RIGOROUS BOUNDS ON THE GROUND-STATE ENERGY FOR MATTER AND ITS STABILITY

Siri Sirininlakul

A Thesis Submitted in Partial Fulfillment of the Requirements

for the Degree of Doctor of Philosophy in Physics

Suranaree University of Technology

Academic Year 2005

ISBN 974-533-526-6

ขอบเขตที่ชัดเจนของพลังงานสถานะพื้นและเสถียรภาพของสสาร

นายสิริ สิรินิลกุล

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรดุษฎีบัณฑิต

สาขาวิชาฟิสิกส์

มหาวิทยาลัยเทคโนโลยีสุรนารี

ปีการศึกษา 2548

ISBN 974-533-526-6

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Suranaree University of Technology has approved this thesis submitted in partial fulfillment of the requirements for the Degree of Doctor of Philosophy.

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สิริ สิรินิลกุล : ขอบเขตที่ชัดเจนของพลังงานสถานะพื้นและเสถียรภาพของสสาร (RIGOROUS BOUNDS ON THE GROUND-STATE ENERGY FORATTER AND ITS STABILITY) อาจารย์ที่ปรึกษา : ศาสตราจารย์. ดร.เอ็ดเวิร์ด มานูเกียน, 395 หน้า. ISBN 974-533-526-6

การวิเคราะห์เชิงคณิตศาสตร์ที่ชัดเจนโดยใช้หลักการขั้นพื้นฐานของการกีดกันของเพาลีได้พบเงื่อนไขของความมีเสถียรภาพในก้อนสสารที่มีอยู่ช้านานในโลกของเรา โดยได้คำนวณหาขอบเขตล่างและขอบเขตบนสำหรับพลังงานสถานะพื้นอย่างแม่นตรงด้วยวิธีกาหายวิธี ผลลัพธ์ที่ได้ถูกแสดงในรูปฟังก์ชันของจำนวนอิเล็กตรอนและจำนวนนิวเคลียส หนึ่งในจำนวนขอบเขตล่างที่ได้มา มีการคำนวณหาค่าตามขั้นตอนต่อไปนี้ ขอบเขตล่างของค่าคาดหมายของพลังงานจลน์ของอิเล็กตรอนอยู่ในรูปของ $\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})$, (กฎ $\rho^2(\mathbf{x})$) เมื่อ $\rho(\mathbf{x})$ คือความหนาแน่นของอิเล็กตรอน: $\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x}) = N$ ในขณะที่ขอบเขตล่างที่คำนวณได้โดยวิธีของลีปและแทริ่ง อยู่ในรูปกฎ $\rho^{5/3}(\mathbf{x})$ ขอบเขตล่างของพลังงานศักย์ผลักระหว่างอิเล็กตรอน-อิเล็กตรอนได้มาโดยการประมาณค่าจากทฤษฎีไม่ยึดเหนี่ยว การคำนวณหาค่าขอบเขตบนทำโดยการทดลองเลือกฟังก์ชันคลื่นของอิเล็กตรอนซึ่งวิธีแรกโดยการจำกัดอิเล็กตรอนอยู่ภายในกล่องที่ไม่ซ้อนทับกันจำนวน N กล่องและมี k นิวคลีไออยู่ที่ตำแหน่งกึ่งกลางของกล่องจำนวน k กล่อง ในขณะที่วิธีที่สองโดยการพิจารณากลุ่มที่ประกอบด้วย ไฮโดรเจนิกอะตอมจำนวน k อะตอม ที่มีประจุนิวเคลียส $Z_1|e|, \ldots, Z_k|e|$ ซึ่งแต่ละนิวเคลียสมีอิเล็กตรอนหนึ่งตัวอยู่ในสถานะพื้น และจำนวน อิเล็กตรอนอิสระจำนวน $(N-k)$ อิเล็กตรอนที่ไม่มีพลังงานจลน์ แต่ละกลุ่มแยกห่างกันเป็นระยะอนันต์ พบว่า ในขณะที่แต่ละกลุ่มแยกจากกัน ถ้าสสารจำนวนมากถูกนำมารวมกัน จำนวนอิเล็กตรอนและนิวคลีไอจำเป็นต้องเพิ่มขึ้นและประจุสูงสุดของแต่ละนิวเคลียสมีค่าในขอบเขตที่ขอบเขตนั่นคือ ถ้า N มีค่าเข้าสู่อนันต์หมายความว่า k มีค่าเข้าสู่อนันต์ด้วยและจะไม่มีนิวเคลียสใดอยู่ในสสารได้โดยมีประจุบวกที่ไม่จำกัด เราได้พิสูจน์การพองตัวของสสารเนื่องจากการเพิ่มของจำนวนอิเล็กตรอนและความน่าจะเป็นที่ไม่เป็นศูนย์ที่จะพบอิเล็กตรอนในทรงกลมรัศมี R ค่าความน่าจะเป็นจะต้องเพิ่มขึ้นไม่ช้ากว่า $N^{1/3}$ โดย N มีค่ามาก จึงไม่ต้องสงสัยว่าทำไมสสารจึงมีปริมาตรที่ใหญ่ และเรายังได้เสนอการตั้งค่าขอบเขตล่างที่ไม่เป็นศูนย์เพื่อที่จะวัดการขยายตัวของสสาร เรายังได้พิสูจน์ความมีเสถียรภาพและการพองตัวของสสารในสองมิติ การวิเคราะห์ทั้งหมด

นี้นำไปสู่การประมาณค่าใหม่กับสสารที่เป็นไปตามหลักการกีดกันโดยให้ผลตรงข้ามกับสสารที่เรียกว่า‘‘สสารประเภทโบซอน” ซึ่งถ้าสสารประเภทโบซอนมีการหดตัว ค่า R ไม่สามารถลดลงเร็วกว่า $N^{-1/3}$ เมื่อ N มีค่ามาก แม้มีความยุ่งยากทางคณิตศาสตร์แต่ผลสุดท้ายได้ถูกแสดงในรูปสมการที่ง่ายและพร้อมที่จะถูกตีความหมายทางฟิสิกส์

สาขาวิชาฟิสิกส์ ลายมือชื่อนักศึกษา ____________

ปีการศึกษา 2548 ลายมือชื่ออาจารย์ที่ปรึกษา ____________

SIRI SIRININLAKUL : RIGOROUS BOUNDS ON THE GROUND-STATE ENERGY FOR MATTER AND ITS STABILITY. THESIS ADVISOR : PROF. EDOUARD B. MANOUKIAN, Ph.D. 395 PP. ISBN 974-533-526-6

STABILITY OF MATTER/ THE SPIN AND STATISTICS CONNECTION/ INFLATION OF MATTER/ CLUSTER PHYSICS AND QUANTUM THEORY OF VERY LARGE SYSTEMS/ MATTER IN BULK.

A mathematically rigorous analysis is carried out of the stability of matter in bulk by invoking, in the process, the fundamental Pauli exclusion principle which has far reaching consequences in nature relevant to our world. To do this, we derive several lower *and* upper bounds for the exact ground-state energy as functions of the number N of electrons and of the nuclear charges. One of the lower bounds obtained is based on positivity properties followed by deriving a lower bound for the expectation value of the exact kinetic energy of the electrons, involving some power of the integral $\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})$ (a $\rho^2(\mathbf{x})-$law), where $\rho(\mathbf{x})$ is the electron density : $\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x}) = N$, while another traces the classics Lieb-Thirring approach, which is however much more involved, based on the $\rho^{5/3}(\mathbf{x})-$law, followed by establishing a "No-binding Theorem", leading, in the process, to a lower bound to the repulsive electron-electron potential energy. The upper bounds are based on specific constructions with appropriate choices of trial wavefunctions for the electrons. One upper bound is based on localizing the electrons in N non-overlapping ordered boxes, with the k nuclei centered at the origins of the first k boxes, while another is obtained by introducing N infinitely separated clusters consisting of : k hydrogenic atoms with nuclear charges $Z_1|e|,\ldots,Z_k|e|$ each containing one electron all in their ground states, and $(N-k)$ free electrons with vanishingly small kinetic energies. We learn, in particular, that as more and more matter is put together, thus increasing the number N of electrons, the number k of nuclei, as separate clusters, would necessarily increase and not arbitrarily fuse together, and their individual charges remain bounded, i.e., $N \to \infty$, implies that $k \to \infty$, and no nuclei may be found in matter that would carry arbitrarily large portions of the total positive charge available. We prove the inflation of matter, as N increases, by showing that the infinite electron density limit does not occur, and that for a non-vanishing probability of having the electrons in matter within a sphere of radius R, the latter *necessarily grows* not any slower than $N^{1/3}$ for large N. No wonder why matter occupies so large a volume ! We also establish a non-zero lower bound for a measure of the extension of matter. Due to the overwhelming interest in recent years in physics in two dimensions, we prove rigorously the stability and inflation of matter in two dimensions as well. Our methods of analyses lead to new estimates on matter when the exclusion principle is revoked dealing with so-called "bosonic matter". In particular, we show that if deflation occurs, upon the collapse of such matter, then R necessarily cannot decrease faster than $N^{-1/3}$ for large N. Although the mathematical intricacies and the corresponding intermediate estimates turn out to be quite tedious and involved, generating a forest of formulas, the final results are expressed in terms of simple expressions and are readily physically interpreted.

School of Physics — Student's Signature ______

Academic Year 2005 — Advisor's Signature ______

ACKNOWLEDGEMENTS

I am grateful to Prof. Dr. Edouard B. Manoukian for being my thesis advisor and for his guidance throughout this work. He gave me a very good research experience which led to a successful completion of the project.

I would like to thank my parents and my relatives for their understanding, support and encouragement over the years of my study.

I wish to thank Dr. Chaiyapoj Muthaporn, Dr. Nattapong Yongram, Mr. Suppiya Siranan, Mr. Seckson Sukkhasena and Ms. Kanchana Limboonsong for their cooperation, discussion on this work and for great support.

I wish to thank Srinakharinwirote University, for giving me an UDC scholarship.

I would like to acknowledge with thanks the encouragement and great advice that Asst. Prof. Niramon Pattanasuwan, the Head of the Physics Department of Srinakharinwirote University, gave me while studying for my Ph.D..

I acknowledge with thanks for discussions with Assoc. Prof. Dr. Prapasri Asawakun related to density functionals and for her suggestions.

Finally, I would like also give my special thanks to Prof. Dr. Walter E. Thirring of the Theoretical Physics Institute of the University of Vienna (Institut für Theoretische Physik der Universität Wien) for the interest he has shown in this work throughout its development, for his encouragement, for his comments concerning the stability of matter, in particular, in two dimensions, and for his several written communications with our group involving this line of investigation.

Siri Sirininlakul

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CHAPTER I

INTRODUCTION

Undoubtedly, one of the most important and serious problems that quantum physics has faced over the years, since its birth over a three-quarter of a century ago, is that of the stability of matter. That is of consistently demonstrating as to why matter in our world consisting of a large number of electrons, in spite of their mutual repulsions, but with increasing attractions to its nuclei, as their number increase, and continuously accelerating around them, does not eventually lead to its collapse, as expected on classical grounds, and a perfect balance between these phenomenae occurs and matter remains stable. The so-called Pauli exclusion principle turns out to be not only sufficient for stability but also necessary. That is, if one invokes the exclusion principle then stability may be established. On the other hand, if the exclusion principle is revoked leading with what is called “bosonic matter” then instability, i.e., collapse, of such matter may be established. A very detailed technical treatment of “bosonic matter” has been the subject matter of the recent doctoral thesis of Muthaporn (2005) providing original contributions to the problems involving such matter and contains extensive references. *The burden on a theoretical physicist is to actually spell out, mathematically, the details for establishing the stability of matter and work out its consequences by invoking, in the process, the Pauli exclusion principle* and not just providing qualitative arguments for stability, as is often done by a phenomenologist, and is the subject matter of this thesis.

The Pauli exclusion principle, or more generally the Spin and Statistics Theorem, in its simplest form, states that no two identical particles of half-odd integer spins (fermions) can occupy the same state while any number of identical particles of integer spins (bosons) may do so without limitation. The practical effect of this theorem prevails over the whole of science and provides the basis for explaining the periodic table of elements from which we are made of. Without the Spin and Statistics connection our world will be unstable and ceases to exist. The translator of the classic book by the Nobel Laureate S.–I. Tomonaga (1997), on the “Story of Spin”, T. Oka, a Robert Milikan Distinguished Service Professor at the Enrico Fermi Institute of Chicago, writes the following concerning this theorem : “*The existence of Spin, and the Statistics associated with it, is the most subtle and ingenious design of Nature–without it the whole universe would collapse*”. The legendary Freeman Dyson (1967) in regard to matter, without the Spin and Statistics connection, writes : “*Matter in bulk would collapse into a condensed high–density phase. The assembly of any two macroscopic objects would release energy comparable to that of an atomic bomb*”. E.H. Lieb (1990), regarding “bosonic matter”, i.e., matter for which the Pauli exclusion principle does not apply, as mentioned above, writes : “*Such “matter” would be very unpleasant stuff to have lying around the house*”. The Spin and Statistics Theorem is usually credited to Stoner (1924), Pauli (1925), Pauli and Weisskopf (1934), Pauli (1936), Ivanenko and Sokolov (1937), Fierz(1939), Pauli and Belifante (1940), deWet (1940), Pauli (1950), Wightman (1956), Hall and Wightman (1957), Schwinger (1958a, 1958b), Bourgogne (1958), L*ü*ders and Zumino (1958), Jost (1960), Brown and Schwinger (1961), Schwinger (1988).

Already in 1931, the practical relevance of the Spin and Statistics Theorem was recognized : “*We take a piece of metal or stone when we think about it, we are astonished that this quantity of matter should occupy so large a volume. Admittedly, the molecules are packed tightly together, and likewise the atoms within each molecule. But why are the atoms themselves so big ? Consider for example the Bohr model of an atom of lead. Why do so few of the 82 electrons run in the orbits close to the nucleus ? The attraction of the 82 positive charges in the nucleus is so strong. Many more of the 82 electrons could be concentrated into the inner orbits, before their mutual repulsion would become too large. What prevents the atom from collapsing in this way ? Answer : only the Pauli principle. ‘No two electrons in the same state’. That is why atoms are so unnecessarily big, and why metal or stone are so bulky*”. These words were addressed by Ehrenfest to Pauli (Ehrenfest, 1931, 1959) as quoted by Dyson (1967).

The first systematic analysis as to why matter is stable was carried out by Dyson and Lenard (1967), Lenard and Dyson (1968) in a rather very complex way of the underlying analysis. Since then much improvements were made (Lieb, 1976, 1980, 1983, 1990; Leib and Thirring, 1975, 1976; Manoukian and Sirininlakul, 2005) on the problem of stability. The basic analysis in the modern developments rested on a remarkable result due to Julian Schwinger (1961) which simply gives rise to an upper bound for counting the eigenvalues of a given Hamiltonian. Recently, an *exact* functional expression (Manoukian and Limboonsong, 2006), not just a bound, have been obtained for the number of eigenvalues, within a given range, of a given Hamiltonian. The relevant papers which led to modern developments of the fundamental problem of stability were due to Fermi (1927), Heisenberg (1927), Hartee (1927, 1928), Thomas (1927), Dirac (1930), Fock (1930), Slater (1930), Lenz (1932), Sommerfeld (1932), von Weizsäcker (1935), Sobolev (1938), Gombas (1949), Scott (1952), Sheldon (1955), Kompaneets and Paulovski (1956), Kirzhnitz (1957), Birman (1961), Teller (1962), Fisher (1964), Balázs (1967), Dyson (1968), Kato (1951, 1972), Rosen (1971), Stein (1970), Conlon (1984), Conlon, Lieb and Yau (1988), Helffer and Robert (1990), Hoffmann–Ostenhof (1977), Leib (1976, 1979, 1980, 1983, 1990), Leib and Lebowitz (1972), Leib and Simon (1974, 1977), Leib and Thirring (1976), Wang (1983), Perez, Malta and Coutino (1988), Wiedl (1996), Manoukian and Sirininlakul (2004, 2005, 2006b), covering essentially the history of which is relevant to the problem of the stability of matter. In addition to the earlier investigations of Dyson and Lenard (1967, 1968) mentioned above, the contribution of Leib and Thirring (1975) has embodied the central result of this problem, in which they bound the ground-state energy from below, as Dyson and Lenard, by a single power of N (the number of electrons in a piece of matter) multiplied by a negative constant whose magnitude is much smaller than that found by Dyson and Lenard. It is expected that an ultimate treatment of stability of matter should involve the full machinery of quantum electrodynamics (Schwinger, 1951a, 1951b, 1953, 1954, 1958c; Manoukian, 1985, 1986; Thirring (Lieb Selecta), 1991).

The drastic difference between matter with the exclusion principle and "bosonic matter" with Coulomb interactions, is that the ground-state energy E_N for the former $-E_N \sim N$, with N denoting the number of negative charges (the electrons), while for the latter $-E_N \sim N^\alpha$, with $\alpha > 1$. A power law behaviour with $\alpha > 1$ implies that of instability as the formation of a single system consisting of $(2N + 2N)$ particles is favoured over two separate systems brought together, each consisting of $(N + N)$ particles, and the energy released upon the collapse of the two systems into one, being proportional to $[(2N)^\alpha - 2(N)^\alpha]$, will be overwhelmingly large for realistic large N, e.g., $N \sim 10^{23}$. *Thus the actual demonstration of a single power of N for the ground-state energy of matter is essential*.

The Hamiltonian into consideration in this work is defined by

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + V_1 + V_2 - \sum_{i=1}^{N}\sum_{j=1}^{k} Z_j e^2 |\mathbf{x}_i - \mathbf{R}_j|^{-1} \tag{1.1}$$

where

$$V_1 = \sum_{i<j}^{N} e^2 |\mathbf{x}_i - \mathbf{x}_j|^{-1} \tag{1.2}$$

$$V_2 = \sum_{i<j}^{k} Z_i Z_j e^2 |\mathbf{R}_i - \mathbf{R}_j|^{-1}\ , \quad \sum_{j=1}^{k} Z_j = N, \quad k \geqslant 2 \tag{1.3}$$

with fixed positive charges, $\mathbf{x}_i$, $\mathbf{R}_j$ refer to the positions of the negative and positive charges, respectively, and m denotes the mass of the electron. We note that for $k = 1$, the V_2 term in (1.3) will be absent in the expression for H and one would be dealing with an atom. *Throughout, we are interested in the case for which $k \geqslant 2$ relevant to matter*. We consider neutral matter, i.e., for which $\sum_{j=1}^{k} Z_j = N$ as indicated in (1.3).

The purpose of this thesis is to carry a mathematically rigorous analysis of the problem of stability of matter in bulk by invoking, in the process, the fundamental Pauli exclusion principle which, as mentioned above, has far reaching consequences in nature relevant directly to our world. To do this, we derive several lower *and* upper bounds for the exact ground-state energy of matter, corresponding to the Hamiltonian H in (1.1)–(1.3), as functions of the number N of electrons and of the nuclear charges $Z_1|e|, \ldots, Z_k|e|$. One of the lower bounds (Chapter II) is based on positivity properties followed by deriving a lower bound for the expectation value of the exact kinetic energy of the electrons involving some power of the integral $\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})$, where $\rho(\mathbf{x})$ is the electron density, i.e.,

$$\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x}) = N. \tag{1.4}$$

The other one traces the classic Lieb–Thirring approach and is much more involved and is based on deriving a lower bound for the expectation value of the kinetic energy involving the integral $\int \mathrm{d}^3\mathbf{x}\,\rho^{5/3}(\mathbf{x})$ followed by establishing a "No–binding Theorem" leading to a lower bound to the repulsive electron–electron potential energy V_1 in (1.2). The upper bounds (chapter III) are based on specific constructions with appropriate choices of trial wavefunctions for the electrons. The first upper bound is obtained by localizing the electrons in N non-overlapping ordered boxes, with the k nuclei centered at the origins of the first k boxes. The second upper bound is obtained by introducing N infinitely separated clusters consisting of : k hydrogenic atoms with nuclear charges $Z_1|e|, \ldots, Z_k|e|$ each containing one electron all in their ground states, and $(N-k)$ free electrons with vanishingly small kinetic energies. We learn, in particular, that as more and more matter is put together, thus increasing the number N of electrons, the number k of nuclei, as separate clusters, would necessarily increase and not arbitrarily fuse together (Chapter IV), and their individual charges remain bounded, i.e., $N \to \infty$, implies that $k \to \infty$, and no nuclei may be found in nature that would carry arbitrarily large portions of the total positive charge available. In Chapter IV, we establish the inflation of matter by showing that for a non-vanishing probability of having the electrons in matter within a sphere of radius R, the latter necessarily *grows* not any slower than $N^{1/3}$ for large N. No wonder why matter occupies so large a volume(!) bringing us into contact with the classic debate of Ehrenfest and Pauli mentioned earlier. Our methods of study developed allow us also to obtain new estimates on matter when the exclusion principle is revoked dealing with the so-called "bosonic matter" as elaborated upon earlier. This is carried out in Appendices A and B of this thesis. In particular, we prove that if deflation occurs of such matter, upon collapse, then R necessarily cannot decrease faster than $N^{-1/3}$ for large N. The mathematical analyses methods are based on modern functional analyses techniques (e.g., Yosida, 1980; Mitrinovíc, Pečarić and Fink, 1993) and fitting particles within specific regions (e.g., Casselman, 2004; Pfender and Ziegler, 2004; Croft, Falconer and Guy, 1991). Due to the overwhelming interest in recent years in physics in two dimensions (e.g., Geyer 1995; Badhuri, 1996; Semenoff, 1987; Forte, 1992) and its relevance to our world, we prove rigorously, in Chapter V, the stability and inflation of such matter by invoking the exclusion principle. [Some of the present field theories (e.g., Green and Schwarz, 1988; Schwarz, 1985) speculate that at early stages of our universe the dimensionality of space was not necessarily coinciding with three, and by a process which has been referred to as compactification of space, the present three-dimensional character of space arose upon the evolution and the cooling down of the universe. Due to technical reasons mentioned in the introductory section 5.1, the stability problem is not considered in the present work for dimensions higher than three.] Chapter VI deals with our main conclusions. Although the mathematical details and the corresponding intermediate estimates turn out to be quite tedious and involved, the final results are expressed in terms of simple expressions and are readily interpreted.

CHAPTER II

RIGOROUS LOWER BOUNDS FOR THE GROUND-STATE ENERGY OF MATTER

2.1 Introduction

The purpose of this chapter is to derive rigorous lower bounds for the exact ground-state of matter based on the Hamiltonian (1.1)–(1.3). The first, given in (Sect. 2.3), relies heavily on positivity conditions together with a derivation of a lower bound (Sect. 2.2) for the expectation value of the exact kinetic energy of the electrons involving some power of an integral of $\rho^2(\mathbf{x})$ with $\rho(\mathbf{x})$ being the particle density (see Eq.(2.37)). Another, though technically much more involved, derivation of a lower bound is also given of the exact ground-state energy in Sect. 2.6 based on the following chain of analyses and tracing the Lieb–Thirring approach. First we carry out a fairly detailed analysis of the so-called Thomas–Fermi atom which surprisingly turns out to be relevant to the exact theory for matter based on the Hamiltonian in question through a "No-binding Theorem" studied in Sect. 2.5. The later theorem then leads to a lower bound for the exact electron-electron interaction potential energy. These results are then combined in Sect. 2.6 to derive the second lower bound for the ground-state energy which follows the celebrated Lieb–Thirring approach to study the stability of matter. The second lower bound for the expectation value of the kinetic energy involves an integral of $\rho^{5/3}(\mathbf{x})$ rather than of $\rho^2(\mathbf{x})$. The method of deriving the first lower bound for the ground-state energy mentioned above turns out to be quite useful when extended to bosonic systems which is studied in detail in Appendices A and B of the thesis.

2.2 Lower Bound for the Expectation Value of the Exact Kinetic Energy of Matter

To obtain a lower bound for the ground-state energy of matter, first we have to find a lower bound for the expectation value kinetic energy T which is the first term on the right-hand side of (1.1). We first consider the Hamiltonian of a single particle

$$H = H_0 + V \tag{2.1}$$

where H_0 is the free Hamiltonian $\mathbf{p}^2/2m$.

By introducing a variable coupling parameter $g \geqslant 0$, with $g = 1$ corresponding to above the Hamiltonian, we rewrite (2.1) in the form

$$H(g) = H_0 + gV(\mathbf{x}). \tag{2.2}$$

We rewrite the potential, by using in the process the step function

$$\begin{aligned} V(\mathbf{x}) =& V(\mathbf{x})(1) \\ =& V(\mathbf{x})\left[\Theta(V(\mathbf{x})) + \Theta(-V(\mathbf{x}))\right] \\ =& V(\mathbf{x})\Theta(V(\mathbf{x})) + V(\mathbf{x})\Theta(-V(\mathbf{x})) \\ \geqslant& V(\mathbf{x})\Theta(-V(\mathbf{x})). \end{aligned} \tag{2.3}$$

Since $V(\mathbf{x})\Theta(V(\mathbf{x})) \geqslant 0$, where $\Theta(V(\mathbf{x})) + \Theta(-V(\mathbf{x})) = 1$.

Let $-v = V(\mathbf{x})\Theta(-V(\mathbf{x}))$ where $v(\mathbf{x}) \geqslant 0$, from (2.3) we then obtain

$$V(\mathbf{x}) \geqslant -\, v(\mathbf{x}). \tag{2.4}$$

Substitute this into (2.2), to obtain

$$H(g) = H_0 + gv(\mathbf{x})$$

$$H(g) \geqslant H_0 - gv(\mathbf{x}). \tag{2.5}$$

Let $N_{-\xi}(H(g))$ denote the number of eigenvalues of $H_g \leqslant -\xi$, with $\xi > 0$. For future developments, we establish an order relationship between the eigenvalues of two self-adjacent operators $H(g)$ and $H_0 - gv(\mathbf{x})$, whose spectra are bounded from below, such that for all vectors $|\Psi\rangle$ in their domains, we obtain

$$\langle\Psi|H(g)|\Psi\rangle \geqslant \langle\Psi|H_0 - gv(\mathbf{x})|\Psi\rangle \geqslant -\xi. \tag{2.6}$$

Also the number of bound-state of $H_0 - gv(\mathbf{x})$ cannot be less than those of $H(g)$,

$$N_{-\xi}\left(H_0 - gv(\mathbf{x})\right) \geqslant N_{-\xi}\left(H_0 + gv(\mathbf{x})\right). \tag{2.7}$$

Similarly $0 < g' < g$,

$$H_0 - g'v(\mathbf{x}) \geqslant H_0 - gv(\mathbf{x}) \tag{2.8}$$

and

$$N_{-\xi}\left(H_0 - gv(\mathbf{x})\right) \geqslant N_{-\xi}\left(H_0 - g'v(\mathbf{x})\right). \tag{2.9}$$

From (2.3)–(2.9), we have the important relation :

$$N_{-\xi}\left(H_0 - v(\mathbf{x})\right) = [\text{Number of } g'\text{'s in } 0 < g' \leqslant g \text{ for which}$$

$$H_0 - g'v(\mathbf{x}) \text{ has the eigenvalue} = -\xi] \tag{2.10}$$

so that $H_0 - g'v(\mathbf{x})$ has energy $\equiv -\xi$.

From (2.10), we introduce the new eigenvalue equation :

$$
\begin{aligned}
(H_0 - g'v(\mathbf{x}))\,|\Psi\rangle &= -\,\xi\,|\Psi\rangle\,, \qquad \langle\Psi|\;\Psi\rangle = 1 \\
\left(\frac{\mathbf{p}^2}{2m} - g'v(\mathbf{x})\right)\bigg|\;\Psi\bigg\rangle &= -\,\xi\,|\Psi\rangle \\
\left(\frac{\mathbf{p}^2}{2m} + \xi\right)\bigg|\;\Psi\bigg\rangle &= g'v(\mathbf{x})|\Psi\rangle \\
&= g'\sqrt{v(\mathbf{x})}\sqrt{v(\mathbf{x})}\;|\Psi\rangle \\
&= g'\sqrt{v(\mathbf{x})}\;|\phi\rangle
\end{aligned}
\tag{2.11}
$$

where $|\phi\rangle = \sqrt{v(\mathbf{x})}\;|\Psi\rangle$.

Multiply (2.11) by $\sqrt{v(\mathbf{x})}$, to obtain

$$
\begin{aligned}
\sqrt{v(\mathbf{x})}\;\left(\frac{\mathbf{p}^2}{2m} + \xi\right)\bigg|\;\Psi\bigg\rangle &= g'\sqrt{v(\mathbf{x})}\;\sqrt{v(\mathbf{x})}|\phi\rangle \\
\sqrt{v(\mathbf{x})}\,|\Psi\rangle &= g'\sqrt{v(\mathbf{x})}\;\frac{1}{\left(\frac{\mathbf{p}^2}{2m} + \xi\right)}\sqrt{v(\mathbf{x})}|\phi\rangle \\
|\phi\rangle &= g'A|\phi\rangle \\
A|\phi\rangle &= \frac{1}{g'}|\phi\rangle
\end{aligned}
\tag{2.12}
$$

where A is the positive operator

$$
A = \sqrt{v(\mathbf{x})}\;\frac{1}{\left(\frac{\mathbf{p}^2}{2m} + \xi\right)}\sqrt{v(\mathbf{x})}
\tag{2.13}
$$

The eigenvalue of the operator A is $1/g'$ and $0 < g' < g$. Also

$$A^\rho = \sum_{j=1}^{\infty} \frac{1}{g_j'^\rho} \, |g_j'\rangle\langle g_j'|. \tag{2.14}$$

From (2.13), for $\rho \geqslant 0$, in particular

$$\int \mathrm{d}^\nu \mathbf{x} \, \langle \mathbf{x}| \, A^\rho \, |\mathbf{x}\rangle \geqslant \frac{1}{g^\rho} \times [\text{Number of all } g'\text{'s as eigenvalues of } A$$
$$\text{in } 0 < g' \leqslant g \text{ for which } H_0 - g'v(\mathbf{x})$$
$$\text{has the eigenvalue } = -\xi] \, . \tag{2.15}$$

From (2.10) and (2.15), we obtain

$$N_{-\xi}\left(H_0 - gv(\mathbf{x})\right) \leqslant g^\rho \int \mathrm{d}^\nu \mathbf{x} \, \langle \mathbf{x}| \, A^\rho \, |\mathbf{x}\rangle \tag{2.16}$$

giving from (2.16), the so-called Schwinger inequality.

In three dimensions $(\nu = 3)$, we choose $\rho = 2$ on the right-hand side of (2.15). Thus with the definition of A in (2.13), we obtain for the right-hand side of (2.15) with $g(\mathbf{x}) = 1$

$$\begin{aligned}\int \mathrm{d}^3\mathbf{x} \, \langle \mathbf{x}| \, A^2 \, |\mathbf{x}\rangle &= \int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^3\mathbf{x}' \, \langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle \, \langle \mathbf{x}'| \, A \, |\mathbf{x}\rangle \\ &= \int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^3\mathbf{x}' \, \langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle \, \langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle^* \\ &= \int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^3\mathbf{x}' \, |\langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle|^2 \\ &= \int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^3\mathbf{x}' \, v(\mathbf{x}) \, v(\mathbf{x}') \left| \left\langle \mathbf{x} \left| \frac{1}{\left[\frac{\mathbf{p}^2}{2m} + \xi\right]} \right| \mathbf{x}' \right\rangle \right|^2 . \end{aligned} \tag{2.17}$$

For $\left\langle \mathbf{x} \left| \left[\frac{\mathbf{p}^2}{2m}+\xi\right]^{-1} \right| \mathbf{x}' \right\rangle$, let $\hat{A}(\mathbf{p}) = \left[\frac{\mathbf{p}^2}{2m}+\xi\right]^{-1}$, we obtain the following chain of the equalities :

$$
\begin{aligned}
&\left\langle \mathbf{x} \left| \frac{1}{\left[\frac{\mathbf{p}^2}{2m}+\xi\right]} \right| \mathbf{x}' \right\rangle \\
&= \left\langle \mathbf{x} \left| \hat{A}(\mathbf{p}) \right| \mathbf{x}' \right\rangle \\
&= \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \int \frac{\mathrm{d}^3\mathbf{p'}}{(2\pi\hbar)^3} \langle \mathbf{x} \mid \mathbf{p} \rangle \left\langle \mathbf{p} \left| \hat{A}(\mathbf{p}) \right| \mathbf{p'} \right\rangle \langle \mathbf{p'} \mid \mathbf{x}' \rangle \\
&= \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \int \frac{\mathrm{d}^3\mathbf{p'}}{(2\pi\hbar)^3} \mathrm{e}^{\mathrm{i}\frac{\mathbf{p}}{\hbar}\cdot\mathbf{x}} \left\langle \mathbf{p} \left| \hat{A}(\mathbf{p}) \right| \mathbf{p'} \right\rangle \mathrm{e}^{-\mathrm{i}\frac{\mathbf{p'}}{\hbar}\cdot\mathbf{x}'} \\
&= \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \int \frac{\mathrm{d}^3\mathbf{p'}}{(2\pi\hbar)^3} \mathrm{e}^{\mathrm{i}(\mathbf{p}\cdot\mathbf{x}-\mathbf{p'}\cdot\mathbf{x}')/\hbar} \left\langle \mathbf{p} \left| \hat{A}(\mathbf{p}) \right| \mathbf{p'} \right\rangle \\
&= \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \int \frac{\mathrm{d}^3\mathbf{p'}}{(2\pi\hbar)^3} \mathrm{e}^{\mathrm{i}(\mathbf{p}\cdot\mathbf{x}-\mathbf{p'}\cdot\mathbf{x}')/\hbar} \hat{A}(\mathbf{p}) \, (2\pi\hbar)^3 \, \delta^3 \left(\mathbf{p}-\mathbf{p'}\right) \\
&= \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \hat{A}(\mathbf{p}) \, (2\pi\hbar)^3 \int \frac{\mathrm{d}^3\mathbf{p'}}{(2\pi\hbar)^3} \mathrm{e}^{\mathrm{i}(\mathbf{p}\cdot\mathbf{x}-\mathbf{p'}\cdot\mathbf{x}')/\hbar} \delta^3 \left(\mathbf{p}-\mathbf{p'}\right) \\
&= \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \hat{A}(\mathbf{p}) \, \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot(\mathbf{x}-\mathbf{x'})/\hbar} \\
&= \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \frac{\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot(\mathbf{x}-\mathbf{x'})/\hbar}}{\left[\frac{\mathbf{p}^2}{2m}+\xi\right]} \\
&= \frac{2\pi}{(2\pi\hbar)^3} \int_0^\infty \frac{p^2 \, \mathrm{d}p}{\left(\frac{p^2}{2m}+\xi\right)} \int_{-1}^{1} \mathrm{d}(\cos\theta) \, \mathrm{e}^{\mathrm{i}\eta p \; \cos\theta/\hbar}, \quad \boldsymbol{\eta} = |\mathbf{x}-\mathbf{x}'| \\
&= \frac{2\pi}{(2\pi\hbar)^3} \frac{\hbar}{i\eta} \int_0^\infty p \, \mathrm{d}p \, \frac{\mathrm{e}^{\mathrm{i}\eta p/\hbar} - \mathrm{e}^{-\mathrm{i}\eta p/\hbar}}{\left(\frac{p^2}{2m}+\xi\right)} \\
&= \frac{2\pi\hbar}{(2\pi\hbar)^3} \frac{1}{i\eta} \int_{-\infty}^{\infty} \frac{p}{\left(\frac{p^2}{2m}+\xi\right)} \, \mathrm{d}p \, \mathrm{e}^{\mathrm{i}\eta p/\hbar}
\end{aligned}
$$

$$= \frac{1}{(2\pi\hbar)^2}\frac{2m}{i\eta}\int_{-\infty}^{\infty}\frac{p}{(p^2+2m\xi)}\,\mathrm{d}p\;\mathrm{e}^{\mathrm{i}\eta p/\hbar}$$

$$= \frac{1}{(2\pi\hbar)^2}\frac{2m}{i\eta}\frac{i\sqrt{2m\xi}}{2i\sqrt{2m\xi}}\,(2\pi i)\;\mathrm{e}^{-\eta\sqrt{2m\xi}/\hbar}$$

$$= \frac{m}{(2\pi\hbar^2)}\frac{1}{\eta}\;\exp\left(-\frac{\eta}{\hbar}\sqrt{2m\xi}\right)$$

$$= \frac{m}{2\pi\hbar^2}\frac{1}{|\mathbf{x}-\mathbf{x}'|}\exp\left(-\frac{|\mathbf{x}-\mathbf{x}'|}{\hbar}\sqrt{2m\xi}\right). \tag{2.18}$$

Substitution (2.18) into (2.17), to obtain

$$\int \mathrm{d}^3\mathbf{x}\,\langle\mathbf{x}|\,A^2\,|\mathbf{x}\rangle = \left(\frac{m}{2\pi\hbar^2}\right)^2\int \mathrm{d}^3\mathbf{x}\int \mathrm{d}^3\mathbf{x}'\;v(\mathbf{x})\;v(\mathbf{x}')\frac{\mathrm{e}^{-2|\mathbf{x}-\mathbf{x}'|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}-\mathbf{x}'|^2}. \tag{2.19}$$

Finally substitution (2.19) into (2.16), to obtain the so-called Schwinger inequality :

$$N_{-\xi}\left(H_0 - v(\mathbf{x})\right) \leqslant \left(\frac{m}{2\pi\hbar^2}\right)^2\int \mathrm{d}^3\mathbf{x}\int \mathrm{d}^3\mathbf{x}'\;v(\mathbf{x})\;v(\mathbf{x}')\frac{\mathrm{e}^{-2|\mathbf{x}-\mathbf{x}'|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}-\mathbf{x}'|^2}. \tag{2.20}$$

Recently an equality, that is, an exact functional expression for $N_{-\xi}(H_0-v(\mathbf{x}))$ has been derived (Manoukian and Limboonsong, 2006) not just an upper bound as in (2.20).

We note that the integrand in (2.20) is positive, and the exponential factor is bounded above by one. We first use Young's inequality

$$\left|\int \mathrm{d}^3\mathbf{x}\int \mathrm{d}^3\mathbf{x}' f(\mathbf{x})g(\mathbf{x}-\mathbf{x}')h(\mathbf{x}')\right| \leqslant \left\{\int \mathrm{d}^3\mathbf{x}\;|f(\mathbf{x})|^p\right\}^{1/p}\left\{\int \mathrm{d}^3\mathbf{x}\;|g(\mathbf{x})|^q\right\}^{1/q}$$
$$\times\left\{\int \mathrm{d}^3\mathbf{x}|h(\mathbf{x})|^s\right\}^{1/s}. \tag{2.21}$$

Let $p=2,\ s=2,\ q=1$ and

$$f(\mathbf{x}) = v(\mathbf{x}), \tag{2.22a}$$

$$g(\mathbf{x}-\mathbf{x}') = \frac{\mathrm{e}^{-2|\mathbf{x}-\mathbf{x}'|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}-\mathbf{x}'|^2}, \tag{2.22b}$$

$$h(\mathbf{x}') = v(\mathbf{x}') \tag{2.22c}$$

substitute the values for $p,\ s,\ q$, in (2.21), to obtain

$$\begin{aligned}
&\left| \int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^3\mathbf{x'}\ \ v(\mathbf{x})\ \frac{\mathrm{e}^{-2|\mathbf{x}-\mathbf{x}'|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}-\mathbf{x}'|^2}\ v(\mathbf{x}') \right| \\
&\leqslant \left(\int \mathrm{d}^3\mathbf{x}\, |v(\mathbf{x})|^2 \right)^{1/2} \left(\int \mathrm{d}^3\mathbf{x}\ \left| \frac{\mathrm{e}^{-2|\mathbf{x}|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}|^2} \right| \right) \\
&\quad \times \left(\int \mathrm{d}^3\mathbf{x}\, |v(\mathbf{x})|^2 \right)^{1/2} \\
&= \left(\int \mathrm{d}^3\mathbf{x}\, [v(\mathbf{x})]^2 \right)^{1/2} \left(\int \mathrm{d}^3\mathbf{x}\, [v(\mathbf{x})]^2 \right)^{1/2} \\
&\quad \times \left(\int \mathrm{d}^3\mathbf{x}\ \left| \frac{\mathrm{e}^{-2|\mathbf{x}|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}|^2} \right| \right) \\
&\leqslant \left(\int \mathrm{d}^3\mathbf{x}\, [v(\mathbf{x})]^2 \right) \left(\int \mathrm{d}^3\mathbf{x}\ \frac{\mathrm{e}^{-2|\mathbf{x}|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}|^2} \right).
\end{aligned} \tag{2.23}$$

For the second term on the right-hand side of (2.23) we have

$$\begin{aligned}
\int \mathrm{d}^3\mathbf{x}\ \frac{\mathrm{e}^{-2|\mathbf{x}|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}|^2} &= \int \mathrm{d}^3\mathbf{x}\ \frac{\mathrm{e}^{-2x\sqrt{2m\xi}/\hbar}}{x^2} \\
&= \int_0^\infty x^2 \mathrm{d}x \int_0^\pi \sin\theta\ \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi\ \frac{\mathrm{e}^{-2x\sqrt{2m\xi}/\hbar}}{x^2} \\
&= 4\pi \int_0^\infty \mathrm{d}x\ \mathrm{e}^{-2x\sqrt{2m\xi}/\hbar} \\
&= \frac{4\pi\hbar}{\sqrt{8m\xi}}
\end{aligned} \tag{2.24}$$

which upon substituting (2.24) into (2.23), to obtain

$$\int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^3\mathbf{x}'\, v(\mathbf{x}) \frac{\mathrm{e}^{-2|\mathbf{x}-\mathbf{x}'|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}-\mathbf{x}'|^2}\, v(\mathbf{x}') \leqslant \left(\frac{4\pi\hbar}{\sqrt{8m\xi}}\right)\left(\int \mathrm{d}^3\mathbf{x}\, [v(\mathbf{x})]^2\right) \tag{2.25}$$

and substituting (2.25) into (2.20), gives

$$\begin{aligned} N_{-\xi}\left(H_0 - v(\mathbf{x})\right) &\leqslant \left(\frac{m}{2\pi\hbar^2}\right)^2 \left(\frac{4\pi\hbar}{\sqrt{8m\xi}}\right)\left(\int \mathrm{d}^3\mathbf{x}\, [v(\mathbf{x})]^2\right) \\ &= \left(\frac{m}{2\hbar^2}\right)^{3/2} \frac{1}{\pi\sqrt{\xi}} \int \mathrm{d}^3\mathbf{x}\, \left(v(\mathbf{x})\right)^2 \end{aligned}$$

$$\therefore \quad N_{-\xi}\left(H_0 - v(\mathbf{x})\right) \leqslant \left(\frac{m}{2\hbar^2}\right)^{3/2} \frac{1}{\pi\sqrt{\xi}} \int \mathrm{d}^3\mathbf{x}\, \left(v(\mathbf{x})\right)^2 \tag{2.26}$$

where $v(\mathbf{x}) \geqslant 0$.

For ξ such that

$$1 = \left(\frac{m}{2\hbar^2}\right)^{3/2} \frac{1}{\pi\sqrt{\xi}} \int \mathrm{d}^3\mathbf{x}\, \left(v(\mathbf{x})\right)^2$$

$$\xi = \left(\frac{m}{2\hbar^2}\right)^{3} \frac{1}{\pi^2} \left(\int \mathrm{d}^3\mathbf{x}\, \left(v(\mathbf{x})\right)^2\right)^2. \tag{2.27}$$

To obtain $N_{-\xi}\left(H_0 - v(\mathbf{x})\right) < 1$ we choose ξ such that

$$\xi = \left(\frac{m}{2\hbar^2}\right)^{3} \frac{1+\delta}{\pi^2} \left(\int \mathrm{d}^3\mathbf{x}\, \left(v(\mathbf{x})\right)^2\right)^2 \tag{2.28}$$

for any $\delta > 0$, however small, or

$$-\xi = -\left(\frac{m}{2\hbar^2}\right)^{3} \frac{(1+\delta)}{\pi^2} \left(\int \mathrm{d}^3\mathbf{x}\, [v(\mathbf{x})]^2\right)^2 \tag{2.29}$$

so that $N_{-\xi}(\mathbf{p}^2/2m - v(\mathbf{x})) < 1$, which implies that $N_{-\xi}(\mathbf{p}^2/2m - v(\mathbf{x})) = 0$, and the right-hand side of (2.29) provides a lower bound to the spectrum of $[\mathbf{p}^2/2m - v(\mathbf{x})]$ since its spectrum would then be empty for energies less or equal to $-\xi$. That is, (2.29) gives the following lower bound for the ground-state energy of the Hamiltonian,

$$-\left(\frac{m}{2\hbar^2}\right)^3 \frac{(1+\delta)}{\pi^2}\left(\int \mathrm{d}^3\mathbf{x}\,[v(\mathbf{x})]^2\right)^2 . \tag{2.30}$$

For a one particle system, we may then obtain a lower bound for kinetic energy T, as follows. First we consider the one particle state which $\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x}) = 1$, where $\rho(\mathbf{x}) = |\Psi(\mathbf{x})|^2$ and $\Psi(\mathbf{x})$ is the wavefunction, and define the positive function

$$v(\mathbf{x}) = \gamma \frac{\rho^{\alpha}(\mathbf{x})}{\int \mathrm{d}^3\mathbf{x}\,\rho^{\alpha+1}(\mathbf{x})} T \tag{2.31}$$

where α, γ are to be determined and $v(\mathbf{x})$ is not the potential energy for any Hamiltonian. It is just introduced in order to be able to obtain a lower bound for T. Substituting (2.31) into $\langle \Psi \,| H_0 - v(\mathbf{x}) |\, \Psi \rangle$, to obtain

$$\left\langle \Psi \left| \frac{\mathbf{p}^2}{2m} - v(\mathbf{x}) \right| \Psi \right\rangle = -(\gamma - 1)\, T \tag{2.32}$$

and in reference to the bound in (2.30), we obtain

$$\left\langle \Psi \left| \frac{\mathbf{p}^2}{2m} - v(\mathbf{x}) \right| \Psi \right\rangle \geqslant -\left(\frac{m}{2\hbar^2}\right)^3 \frac{(1+\delta)}{\pi^2}\left(\int \mathrm{d}^3\mathbf{x}\,[v(\mathbf{x})]^2\right)^2 . \tag{2.33}$$

From (2.32) and (2.33), we obtain

$$\begin{aligned}
-(\gamma-1)\, T &\geqslant -\left(\frac{m}{2\hbar^2}\right)^3 \frac{(1+\delta)}{\pi^2}\left(\int \mathrm{d}^3\mathbf{x}\,[v(\mathbf{x})]^2\right)^2 \\
&= -\left(\frac{m}{2\hbar^2}\right)^3 \frac{(1+\delta)}{\pi^2}\left(\int \mathrm{d}^3\mathbf{x}\,\left(\gamma \frac{\rho^{\alpha}(\mathbf{x})}{\int \mathrm{d}^3\mathbf{x}\,\rho^{\alpha+1}(\mathbf{x})} T\right)^2\right)^2 \\
&= -\left(\frac{m}{2\hbar^2}\right)^3 \frac{(1+\delta)}{\pi^2}\gamma^4 T^4 \frac{\int \mathrm{d}^3\mathbf{x}\,\rho^{2\alpha}(\mathbf{x})}{\left(\int \mathrm{d}^3\mathbf{x}\,\rho^{\alpha+1}(\mathbf{x})\right)^4}
\end{aligned}$$

$$\therefore \quad (\gamma-1)\, T \leqslant \left(\frac{m}{2\hbar^2}\right)^3 \frac{(1+\delta)}{\pi^2}\gamma^4 T^4 \frac{\left(\int \mathrm{d}^3\mathbf{x}\,\rho^{2\alpha}(\mathbf{x})\right)^2}{\left(\int \mathrm{d}^3\mathbf{x}\,\rho^{\alpha+1}(\mathbf{x})\right)^4} . \tag{2.34}$$

To determine α, we consider the right-hand side of inequality (2.34). This suggests to choose $2\alpha = \alpha + 1$, giving $\alpha = 1$. So the inequality (2.34) will become

$$(\gamma - 1)\, T \leqslant \left(\frac{m}{2\hbar^2}\right)^3 \frac{(1+\delta)}{\pi^2}\gamma^4 T^4 \frac{1}{\left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^2}$$

$$T^3 \geqslant \frac{(\gamma - 1)}{\gamma^4} \left(\frac{2\hbar^2}{m}\right)^3 \frac{\pi^2}{(1+\delta)} \left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^2$$

$$T \geqslant \left(\frac{\gamma - 1}{\gamma^4}\right)^{1/3} \frac{4\pi^{2/3}}{(1+\delta)^{1/3}} \left(\frac{\hbar^2}{2m}\right) \left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^{2/3}. \tag{2.35}$$

Optimizing (2.35) over γ, to obtain

$$\frac{\mathrm{d}}{\mathrm{d}\gamma}\frac{\gamma - 1}{\gamma^4} = 0$$

$$\frac{-3}{\gamma^4} + \frac{4}{\gamma^5} = 0$$

$$\gamma = \frac{4}{3}. \tag{2.36}$$

Substitute γ from (2.37) into (2.35), to obtain for the expectation value of the kinetic energy T for one particle system

$$T \geqslant \left(\frac{\frac{4}{3} - 1}{\left(\frac{4}{3}\right)^4}\right)^{1/3} \frac{4\pi^{2/3}}{(1+\delta)^{1/3}} \left(\frac{\hbar^2}{2m}\right) \left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^{2/3}$$

$$= \frac{3}{4^{4/3}} \frac{4\pi^{2/3}}{(1+\delta)^{1/3}} \left(\frac{\hbar^2}{2m}\right) \left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^{2/3}$$

$$= \frac{3}{(1+\delta)^{1/3}} \left(\frac{\pi}{2}\right)^{2/3} \left(\frac{\hbar^2}{2m}\right) \left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^{2/3}$$

$$\therefore \quad T \geqslant \frac{3}{(1+\delta)^{1/3}} \left(\frac{\pi}{2}\right)^{2/3} \left(\frac{\hbar^2}{2m}\right) \left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^{2/3}. \tag{2.37}$$

From (2.37), we rewrite the expectation value of the kinetic energy T (for one particle systems), whose the particle number density is denote by $\rho(\mathbf{x})$, in compact form

$$T \geqslant B \left(\frac{\hbar^2}{2m}\right) \left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^{2/3} \tag{2.38}$$

where

$$B = \frac{3}{(1+\delta)^{1/3}} \left(\frac{\pi}{2}\right)^{2/3}. \tag{2.39}$$

For multi-particle systems, we consider N identical fermions, each of mass m and introduce the particle number density in three dimensions :

$$\rho(\mathbf{x}) = N \sum_{\sigma_1,\ldots,\sigma_N} \int \mathrm{d}^3\mathbf{x}_2 \ldots \mathrm{d}^3\mathbf{x}_N \left|\Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, \ldots, \mathbf{x}_N\sigma_N)\right|^2 \tag{2.40}$$

where $\sigma_1, \ldots, \sigma_N$ specify spin projection values each $\underline{q} = (2s+1)$ values for a particle of spin s.

The total number of particle N is obtained from the normalization condition

$$\int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) = N \tag{2.41}$$

and the wavefunctions $\Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, \ldots, \mathbf{x}_N\sigma_N)$ are assumed to satisfy the appropriate statistics which in this case are anti-symmetric in the exchange of any two particles which amounts into the interchange of the position-spin labeling : $(\mathbf{x}_i\sigma_i) \Leftrightarrow (\mathbf{x}_j\sigma_j)$.

In reference to (2.31), with $\gamma = 4/3,\ \alpha = 1$, and the positive function $v(\mathbf{x})$

$$v(\mathbf{x}) = \frac{4}{3} \frac{\rho(\mathbf{x})}{\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})}\, T \tag{2.42}$$

where

$$T = \left\langle \Psi \left| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \right| \Psi \right\rangle. \tag{2.43}$$

It is easily verified that

$$\left\langle \Psi \left| \sum_{i=1}^{N} v(\mathbf{x}_i) \right| \Psi \right\rangle = \frac{4}{3} T \tag{2.44}$$

where $\sum_{i=1}^{N} v(\mathbf{x}_i) = v(\mathbf{x})$ and $v(\mathbf{x})$ is not the potential energy for any Hamiltonian. It is just introduced in order to be able to obtain the expectation value of the kinetic energy T (for N identical fermions) in three dimensions.

We consider the operator

$$\sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i) \right] \tag{2.45}$$

defining a hypothetical Hamiltonian of N non-interacting fermions which, however, interact with the external "potential" $v(\mathbf{x})$.

From (2.43) and (2.44), we have

$$\left\langle \Psi \left| \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i) \right] \right| \Psi \right\rangle = -\frac{1}{3} T. \tag{2.46}$$

To derive a lower bound to the lower end of the spectrum of the "Hamiltonian" (operator) in (2.45), we note that, allowing for multiplicity and spin degeneracy, we can put the N fermions in the lowest energy of levels of the "Hamiltonian"in conformity with Pauli's exclusion principle, if N number of such levels. If N is larger than this number of levels, the remaining free fermions may be chosen to have arbitrary small $(\to 0)$ kinetic energies, and be infinitely separated, to define the lowest energy of the Hamiltonian in (2.45). That is, in all cases, the Hamiltonian (2.45) is bounded below by the spin multiplicity $(2s+1) = \underline{q}$ times the ground-state energy in (2.30). From (2.33), (for N identical fermions) we obtain

$$\left\langle \Psi \left| \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i) \right] \right| \Psi \right\rangle \geqslant -\underline{q} \left(\frac{m}{2\hbar^2} \right)^3 \frac{(1+\delta)}{\pi^2} \left(\int \mathrm{d}^3\mathbf{x} \, [v(\mathbf{x})]^2 \right)^2. \tag{2.47}$$

Substitute (2.42), (2.46) into (2.47) and using the normalization condition $\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x}) = N$, to obtain the expectation value of the kinetic energy T (for N identical fermions)

$$
\begin{aligned}
-\frac{1}{3}T \geqslant& -\underline{q}\left(\frac{m}{2\hbar^2}\right)^3 \frac{(1+\delta)}{\pi^2}\left(\int \mathrm{d}^3\mathbf{x}\,[v(\mathbf{x})]^2\right)^2 \\
=& -\underline{q}\left(\frac{m}{2\hbar^2}\right)^3 \frac{(1+\delta)}{\pi^2}\left(\frac{4}{3}\right)^4 T^4 \frac{1}{\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^2} \\
T \geqslant& \frac{1}{\underline{q}^{1/3}}\frac{3}{4^{4/3}}\frac{4\pi^{2/3}}{(1+\delta)^{1/3}}\left(\frac{\hbar^2}{2m}\right)\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3} \\
=& \frac{1}{\underline{q}^{1/3}}\frac{3}{(1+\delta)^{1/3}}\left(\frac{\pi}{2}\right)^{2/3}\left(\frac{\hbar^2}{2m}\right)\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3} \\
=& B_F\left(\frac{\hbar^2}{2m}\right)\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3} \\
\therefore \quad T \geqslant& B_F\left(\frac{\hbar^2}{2m}\right)\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3} \qquad (2.48)
\end{aligned}
$$

where

$$
B_F = \frac{1}{\underline{q}^{1/3}}\frac{3}{(1+\delta)^{1/3}}\left(\frac{\pi}{2}\right)^{2/3} \qquad (2.49)
$$

as a modification of the "Lieb-Thirring inequality for the kinetic energy (for N identical fermions)".

2.3 Lower Bound for the Exact Ground-State Energy of Matter I

Consider a real function $v(\mathbf{x})$, where $\mathbf{x}$ is a vector in 3-dimensions, we have

$$
v(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\widetilde{v}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \qquad (2.50)
$$

and

$$\widetilde{v}(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}\; v(\mathbf{x})\; \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{2.51}$$

and we *choose* $v(\mathbf{x}) \geqslant 0$ such that $v(0) < \infty$, and that its Fourier transform is real and $\widetilde{v}(\mathbf{k}) \geqslant 0$ as well. Let $\phi(\mathbf{x})$ be a real function, we have

$$\phi(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi\hbar)^3}\; \widetilde{\phi}(\mathbf{k})\; \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$$

$$\phi(\mathbf{x}_j) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\; \widetilde{\phi}(\mathbf{k})\; \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \tag{2.52}$$

and the Fourier transform of $\phi(\mathbf{x})$ is given by

$$\widetilde{\phi}(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}\; \phi(\mathbf{x})\; \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{2.53}$$

Let $A_1, \ldots, A_k$ $(k \geqslant 2)$ be real and positive numbers. We have

$$\begin{aligned}
A_1\phi(\mathbf{x}_1) &= A_1 \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\; \widetilde{\phi}(\mathbf{k})\; \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_1} \\
A_2\phi(\mathbf{x}_2) &= A_2 \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\; \widetilde{\phi}(\mathbf{k})\; \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_2} \\
&\vdots \\
A_k\phi(\mathbf{x}_k) &= A_k \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\; \widetilde{\phi}(\mathbf{k})\; \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_k}
\end{aligned} \tag{2.54}$$

and

$$A_1\phi(\mathbf{x}_1) + A_2\phi(\mathbf{x}_2) + \ldots + A_k\phi(\mathbf{x}_k) = \sum_{j=1}^{k} A_j \phi(\mathbf{x}_j) \tag{2.55}$$

Substitute $\phi(\mathbf{x}_j) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\widetilde{\phi}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j}$ into $\sum_{j=1}^{k} A_j \phi(\mathbf{x}_j)$, to obtain

$$\sum_{j=1}^{k} A_j \phi(\mathbf{x}_j) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\widetilde{\phi}(\mathbf{k}) \left(\sum_{j=1}^{k} A_j\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \right). \tag{2.56}$$

Insert $\frac{\sqrt{\widetilde{v}(\mathbf{k})}}{\sqrt{\widetilde{v}(\mathbf{k})}}$ into the right-hand side (2.56). Then we may write

$$\sum_{j=1}^{k} A_j \phi(\mathbf{x}_j) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\frac{\widetilde{\phi}(\mathbf{k})}{\sqrt{\widetilde{v}(\mathbf{k})}} \left(\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \right). \tag{2.57}$$

Now we recall the Cauchy-Schwartz inequality

$$\left(\sum_{j=1}^{n} a_j b_j \right)^2 \leqslant \sum_{j=1}^{n} |a_j|^2 \sum_{j=1}^{n} |b_j|^2 \tag{2.58}$$

We square (2.57) and using the Cauchy-Schwartz inequality, gives

$$\begin{aligned} \left(\sum_{j=1}^{k} A_j \phi(\mathbf{x}_j) \right)^2 &= \left(\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\frac{\widetilde{\phi}(\mathbf{k})}{\sqrt{\widetilde{v}(\mathbf{k})}} \left(\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \right) \right)^2 \\ &\leqslant \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left| \frac{\widetilde{\phi}(\mathbf{k})}{\sqrt{\widetilde{v}(\mathbf{k})}} \right|^2 \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left| \sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \right|^2. \end{aligned} \tag{2.59}$$

Consider $\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left| \sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \right|^2$ on left-hand side of (2.59), to obtain

$$\begin{aligned} &\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left| \sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \right|^2 \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left(\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \right) \cdot \left(\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \right)^* \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left(\sum_{i=1}^{k} A_i \sqrt{\widetilde{v}(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_i} \right) \cdot \left(\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \right) \end{aligned}$$

$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \sum_{i=1}^{k} A_i \sum_{j=1}^{k} A_j \, \widetilde{v}(\mathbf{k}) \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)}$$

$$= \sum_{i,j=1}^{k} A_i A_j \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \, \widetilde{v}(\mathbf{k}) \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)}$$

$$= \sum_{i,j=1}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) \tag{2.60}$$

where $A_1, \ldots, A_k \ (k \geqslant 2)$ be real and positive number, $\widetilde{v}(\mathbf{k}) \geqslant 0$ and

$$v(\mathbf{x}_i - \mathbf{x}_j) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \, \widetilde{v}(\mathbf{k}) \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}_i - \mathbf{x}_j)} \tag{2.61}$$

Substitute (2.61) to the right-hand side of (2.59), to obtain

$$\left(\sum_{j=1}^{k} A_j \phi\left(\mathbf{x}_j\right) \right)^2 \leqslant \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left| \widetilde{\phi}(\mathbf{k}) \right|^2}{\widetilde{v}(\mathbf{k})} \sum_{i,j=1}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) \tag{2.62}$$

We can rewrite (2.62) as

$$\frac{\left(\sum_{j=1}^{k} A_j \phi\left(\mathbf{x}_j\right) \right)^2}{\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left| \widetilde{\phi}(\mathbf{k}) \right|^2}{\widetilde{v}(\mathbf{k})}} \leqslant \sum_{i,j=1}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j). \tag{2.63}$$

For any real number a, b such that $b > 0$, we have

$$\begin{aligned} (a-b)^2 &\geqslant 0 \\ a^2 - 2ab + b^2 &\geqslant 0 \\ a^2 &\geqslant 2ab - b^2 \\ \frac{a^2}{2b} &\geqslant \frac{2ab}{2b} - \frac{b^2}{2b} \end{aligned}$$

$$\frac{a^2}{2b} \geqslant a - \frac{b}{2}. \tag{2.64}$$

Define

$$a = \sum_{j=1}^{k} A_j \phi\left(\mathbf{x}_j\right) \tag{2.65}$$

$$b = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} \tag{2.66}$$

as to be used on the left-hand side of the inequality in (2.64), the latter leads to

$$\frac{1}{2} \frac{\left(\sum\limits_{j=1}^{k} A_j\, \phi\left(\mathbf{x}_j\right)\right)^2}{\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}} \geqslant \sum_{j=1}^{k} A_j\, \phi\left(\mathbf{x}_j\right) - \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}$$

$$\frac{1}{2} \sum_{i,j=1}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) \geqslant \sum_{j=1}^{k} A_j\, \phi\left(\mathbf{x}_j\right) - \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}. \tag{2.67}$$

Consider the left-hand side of the inequality in (2.67),

$$\frac{1}{2} \sum_{i,j=1}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) = \sum_{i<j}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) + \frac{1}{2} \sum_{i=j}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j)$$

$$= \sum_{i<j}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) + \frac{1}{2} v(0) \sum_{j=1}^{k} A_j^2$$

$$\sum_{i<j}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) = \frac{1}{2} \sum_{i,j=1}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) - \frac{1}{2} v(0) \sum_{j=1}^{k} A_j^2. \tag{2.68}$$

Substitute (2.67) into (2.68), giving

$$\sum_{i<j}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) \geqslant \sum_{j=1}^{k} A_j \phi\left(\mathbf{x}_j\right) - \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} - \frac{1}{2} v(0) \sum_{j=1}^{k} A_j^2. \tag{2.69}$$

Let $V(\mathbf{x})$ be real such that $V(\mathbf{x}) \geqslant v(\mathbf{x})$, and $\rho(\mathbf{x})$ real, and so far arbitrary,

$$\phi(\mathbf{x}) = \int \mathrm{d}^3\mathbf{x}'\rho(\mathbf{x}')\,V(\mathbf{x}'-\mathbf{x}). \tag{2.70}$$

We may also write

$$\phi(\mathbf{x}_j) = \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}_j). \tag{2.71}$$

Substituting (2.71) into (2.68), we have

$$\sum_{i<j}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) \geqslant \sum_{j=1}^{k} A_j \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}_j) - \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}$$
$$- \frac{1}{2}v(0)\sum_{j=1}^{k} A_j^2. \tag{2.72}$$

We note that with

$$\phi(\mathbf{x}') = \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}') \tag{2.73}$$

and with $\widetilde{\phi}(\mathbf{k})$ is the Fourier transform of $\phi(\mathbf{x}')$

$$\widetilde{\phi}(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}'\phi(\mathbf{x}')\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \tag{2.74}$$

we may write

$$\widetilde{\phi}(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}')\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \tag{2.75}$$

and

$$\widetilde{\phi}^*(\mathbf{k}) = \int \mathrm{d}^3\mathbf{y}' \int \mathrm{d}^3\mathbf{y}\,\rho^*(\mathbf{y})\,V^*(\mathbf{y}-\mathbf{y}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}'}. \tag{2.76}$$

Since $\rho(\mathbf{x})$ and $V(\mathbf{x}-\mathbf{x}')$ are real functions, that is $\rho(\mathbf{x}) = \rho^*(\mathbf{x})$ and $V(\mathbf{x}-\mathbf{x}') = V^*(\mathbf{x}-\mathbf{x}')$, from (2.75), we obtain

$$\begin{aligned}\widetilde{\phi}(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \\ &= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V^*(\mathbf{x}-\mathbf{x}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'}. \end{aligned} \tag{2.77}$$

Using the inverse Fourier transforms of $\widetilde{\rho}(\mathbf{k})$, $\widetilde{\rho}^*(\mathbf{k})$, $\widetilde{V}(\mathbf{k})$ and $\widetilde{V}^*(\mathbf{k})$, we obtain

$$\rho(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{2.78}$$

$$\rho^*(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{2.79}$$

$$V(\mathbf{x}-\mathbf{x}') = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{V}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \tag{2.80}$$

$$V^*(\mathbf{x}-\mathbf{x}') = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{V}^*(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \tag{2.81}$$

which upon substituting (2.81) into (2.77) gives

$$\begin{aligned}\widetilde{\phi}(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\, \widetilde{V}^*(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot(\mathbf{x}-\mathbf{x}')}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \\ &= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\, \widetilde{V}^*(\mathbf{k}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{x}}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}'} \\ &= \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) \int \mathrm{d}^3\mathbf{k}'\, \widetilde{V}^*(\mathbf{k}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{x}} \int \frac{\mathrm{d}^3\mathbf{x}'}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}'}. \end{aligned} \tag{2.82}$$

For further analysis we use the integral representation of the delta function in 3-dimensions :

$$\delta^3(\mathbf{k}-\mathbf{k'}) = \frac{1}{(2\pi)^3} \int \mathrm{d}^3\mathbf{x}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \tag{2.83}$$

$$\delta^3(\mathbf{x}-\mathbf{x}') = \frac{1}{(2\pi)^3}\int \mathrm{d}^3\mathbf{k}\, \mathrm{e}^{\mathrm{i}(\mathbf{x}-\mathbf{x}')\cdot\mathbf{k}} \tag{2.84}$$

$$F(\mathbf{x}') = \int \mathrm{d}^3\mathbf{x}\, F(\mathbf{x})\, \delta^3(\mathbf{x}-\mathbf{x}'). \tag{2.85}$$

Applying the integral representation of the delta function in 3-dimensions into (2.79), gives

$$\begin{aligned}\widetilde{\phi}(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) \int \mathrm{d}^3\mathbf{k}'\, \widetilde{V}^*(\mathbf{k}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{x}}\, \delta^3(\mathbf{k}'-\mathbf{k}) \\ &= \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, \widetilde{V}^*(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \end{aligned} \tag{2.86}$$

Substitute (2.78) and apply the integral representation of the delta function in 3-dimensions into (2.86), to obtain

$$\begin{aligned}\widetilde{\phi}(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, \widetilde{V}^*(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\ &= \int \mathrm{d}^3\mathbf{x} \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\, \widetilde{\rho}(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{x}}\, \widetilde{V}^*(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\ &= \int \mathrm{d}^3\mathbf{k}'\, \widetilde{\rho}(\mathbf{k}')\, \widetilde{V}^*(\mathbf{k}) \int \frac{\mathrm{d}^3\mathbf{x}}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}} \\ &= \int \mathrm{d}^3\mathbf{k}'\, \widetilde{\rho}(\mathbf{k}')\, \widetilde{V}^*(\mathbf{k})\, \delta^3(\mathbf{k}'-\mathbf{k}) \\ &= \widetilde{\rho}(\mathbf{k})\, \widetilde{V}^*(\mathbf{k}) \\ \therefore \quad \widetilde{\phi}(\mathbf{k}) &= \widetilde{\rho}(\mathbf{k})\, \widetilde{V}^*(\mathbf{k}). \end{aligned} \tag{2.87}$$

Similarly we have

$$\widetilde{\phi}^*(\mathbf{k}) = \int \mathrm{d}^3\mathbf{y}' \int \mathrm{d}^3\mathbf{y}\, \rho^*(\mathbf{y})\, V^*(\mathbf{y}-\mathbf{y}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}'}$$

$$
\begin{aligned}
&= \int \mathrm{d}^3\mathbf{y}' \int \mathrm{d}^3\mathbf{y}\, \rho^*(\mathbf{y})\, V(\mathbf{y}-\mathbf{y}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}'} \\
&= \int \mathrm{d}^3\mathbf{y}' \int \mathrm{d}^3\mathbf{y} \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k}'')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}''\cdot\mathbf{y}} \\
&\quad \times \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\, \widetilde{V}(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot(\mathbf{y}-\mathbf{y}')}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}'} \\
&= \int \mathrm{d}^3\mathbf{y} \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k}'')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}''\cdot\mathbf{y}} \int \mathrm{d}^3\mathbf{k}'\, \widetilde{V}(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{y}} \\
&\quad \times \int \frac{\mathrm{d}\mathbf{y}'}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{y}'} \\
&= \int \mathrm{d}^3\mathbf{y} \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k}'')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}''\cdot\mathbf{y}} \int \mathrm{d}^3\mathbf{k}'\, \widetilde{V}(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{y}} \delta^3(\mathbf{k}'-\mathbf{k}) \\
&= \int \mathrm{d}^3\mathbf{y} \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k}'')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}''\cdot\mathbf{y}}\, \widetilde{V}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}} \\
&= \int \mathrm{d}^3\mathbf{k}''\, \widetilde{\rho}^*(\mathbf{k}'') \int \frac{\mathrm{d}^3\mathbf{y}}{(2\pi)^3}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}''\cdot\mathbf{y}}\, \widetilde{V}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}} \\
&= \int \mathrm{d}^3\mathbf{k}''\, \widetilde{\rho}^*(\mathbf{k}'') \int \frac{\mathrm{d}^3\mathbf{y}}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}'')\cdot\mathbf{y}}\, \widetilde{V}(\mathbf{k}) \\
&= \int \mathrm{d}^3\mathbf{k}''\, \widetilde{\rho}^*(\mathbf{k}'')\, \delta^3(\mathbf{k}-\mathbf{k}'')\, \widetilde{V}(\mathbf{k}) \\
&= \widetilde{\rho}^*(\mathbf{k})\, \widetilde{V}(\mathbf{k})
\end{aligned}
$$

$$
\therefore \quad \widetilde{\phi}^*(\mathbf{k}) = \widetilde{\rho}^*(\mathbf{k})\, \widetilde{V}(\mathbf{k}). \tag{2.88}
$$

Since $\left|\widetilde{\phi}(\mathbf{k})\right|^2 = \widetilde{\phi}^*(\mathbf{k}) \cdot \widetilde{\phi}(\mathbf{k})$, from (2.87) and (2.88), we have

$$
\begin{aligned}
\left|\widetilde{\phi}(\mathbf{k})\right|^2 &= \widetilde{\phi}^*(\mathbf{k})\widetilde{\phi}(\mathbf{k}) \\
&= \widetilde{\rho}(\mathbf{k})\, \widetilde{V}^*(\mathbf{k}) \cdot \widetilde{\rho}^*(\mathbf{k})\, \widetilde{V}(\mathbf{k})
\end{aligned}
$$

$$
\begin{aligned}
&= \widetilde{\rho}^*(\mathbf{k})\,\widetilde{\rho}(\mathbf{k})\cdot\widetilde{V}^*(\mathbf{k})\,\widetilde{V}(\mathbf{k}) \\
&= |\widetilde{\rho}(\mathbf{k})|^2\left|\widetilde{V}(\mathbf{k})\right|^2
\end{aligned}
\tag{2.89}
$$

and hence

$$
\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,|\widetilde{\rho}(\mathbf{k})|^2\,\frac{\left|\widetilde{V}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}. \tag{2.90}
$$

Since $V(\mathbf{y}) \geqslant v(\mathbf{y})$, so $V(\mathbf{y}-\mathbf{y'}) \geqslant v(\mathbf{y}-\mathbf{y'})$, we have

$$
\begin{aligned}
\widetilde{\varphi}^*(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{y}' \int \mathrm{d}^3\mathbf{y}\,\rho^*(\mathbf{y})\,v^*(\mathbf{y}-\mathbf{y}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}'} \\
&= \int \mathrm{d}^3\mathbf{y}' \int \mathrm{d}^3\mathbf{y}\,\rho(\mathbf{y})\,v(\mathbf{y}-\mathbf{y}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}'} \\
&= \int \mathrm{d}^3\mathbf{y}' \int \mathrm{d}^3\mathbf{y}\,\rho(\mathbf{y}) \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\,\widetilde{v}(\mathbf{k}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot(\mathbf{y}-\mathbf{y}')}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}'} \\
&= \int \mathrm{d}^3\mathbf{y}\,\rho(\mathbf{y}) \int \mathrm{d}^3\mathbf{k}'\,\widetilde{v}(\mathbf{k}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{y}} \int \frac{\mathrm{d}\mathbf{y}'}{(2\pi)^3}\;\mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{y}'} \\
&= \int \mathrm{d}^3\mathbf{y}\,\rho(\mathbf{y}) \int \mathrm{d}^3\mathbf{k}'\,\widetilde{v}(\mathbf{k}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{y}}\,\delta^3(\mathbf{k}-\mathbf{k}') \\
&= \int \mathrm{d}^3\mathbf{y}\,\rho(\mathbf{y})\,\widetilde{v}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}}.
\end{aligned}
\tag{2.91}
$$

Divide (2.91) by $\widetilde{v}(\mathbf{k})$, to obtain

$$
\begin{aligned}
\frac{\widetilde{\varphi}^*(\mathbf{k})}{\widetilde{v}(\mathbf{k})} &= \int \mathrm{d}^3\mathbf{y}\,\rho(\mathbf{y})\,\frac{\widetilde{v}(\mathbf{k})}{\widetilde{v}(\mathbf{k})}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}} \\
&= \int \mathrm{d}^3\mathbf{y}\,\rho(\mathbf{y})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}}
\end{aligned}
\tag{2.92}
$$

which upon multiplying by $\widetilde{\varphi}(\mathbf{k})$, gives

$$\frac{\widetilde{\phi}(\mathbf{k})\widetilde{\varphi}^*(\mathbf{k})}{\widetilde{v}(\mathbf{k})} = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}')\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \int \mathrm{d}^3\mathbf{y}\,\rho(\mathbf{y})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}} \tag{2.93}$$

and hence

$$\begin{aligned}
&\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{\widetilde{\phi}(\mathbf{k})\widetilde{\varphi}^*(\mathbf{k})}{\widetilde{v}(\mathbf{k})} \\
&\quad = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}')\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \int \mathrm{d}^3\mathbf{y}\,\rho(\mathbf{y})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}} \\
&\quad = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}') \int \mathrm{d}^3\mathbf{y}\,\rho(\mathbf{y}) \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{y}-\mathbf{x}')} \\
&\quad = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}') \int \mathrm{d}^3\mathbf{y}\,\rho(\mathbf{y})\,\delta^3(\mathbf{y}-\mathbf{x}') \\
&\quad = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}')\,\rho(\mathbf{x}').
\end{aligned} \tag{2.94}$$

We now rewrite

$$\begin{aligned}
&\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{\widetilde{\phi}(\mathbf{k})\widetilde{\varphi}^*(\mathbf{k})}{\widetilde{v}(\mathbf{k})} \\
&\quad = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\rho^*(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}')\,\rho(\mathbf{x}') \\
&\quad = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\rho^*(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}') \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\,\widetilde{\rho}(\mathbf{k}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{x}'} \\
&\quad = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\rho^*(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\,\widetilde{V}(\mathbf{k}'')\,\mathrm{e}^{\mathrm{i}\mathbf{k}''\cdot(\mathbf{x}-\mathbf{x}')} \\
&\qquad \times \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\,\widetilde{\rho}(\mathbf{k}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{x}'} \\
&\quad = \int \mathrm{d}^3\mathbf{x}\,\rho^*(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\,\widetilde{V}(\mathbf{k}'')\,\mathrm{e}^{\mathrm{i}\mathbf{k}''\cdot\mathbf{x}} \int \mathrm{d}^3\mathbf{k}'\,\widetilde{\rho}(\mathbf{k}')
\end{aligned}$$

$$
\begin{aligned}
&\times \int \frac{\mathrm{d}^3\mathbf{x}'}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{x}'} \\
&= \int \mathrm{d}^3\mathbf{x}\, \rho^*(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{V}(\mathbf{k}'')\, \mathrm{e}^{\mathrm{i}\mathbf{k}''\cdot\mathbf{x}} \\
&\quad \times \int \mathrm{d}^3\mathbf{k}'\, \widetilde{\rho}(\mathbf{k}')\, \delta^3(\mathbf{k}'-\mathbf{k}'') \\
&= \int \mathrm{d}^3\mathbf{x}\, \rho^*(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{V}(\mathbf{k}'')\, \mathrm{e}^{\mathrm{i}\mathbf{k}''\cdot\mathbf{x}}\, \widetilde{\rho}(\mathbf{k}'') \\
&= \int \mathrm{d}^3\mathbf{x} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{V}(\mathbf{k}'')\, \mathrm{e}^{\mathrm{i}\mathbf{k}''\cdot\mathbf{x}}\, \widetilde{\rho}(\mathbf{k}'') \\
&= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k}) \int \mathrm{d}^3\mathbf{k}''\, \widetilde{V}(\mathbf{k}'')\, \widetilde{\rho}(\mathbf{k}'') \int \frac{\mathrm{d}^3\mathbf{x}}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}''-\mathbf{k})\cdot\mathbf{x}} \\
&= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k}) \int \mathrm{d}^3\mathbf{k}''\, \widetilde{V}(\mathbf{k}'')\, \widetilde{\rho}(\mathbf{k}'')\, \delta^3(\mathbf{k}''-\mathbf{k}) \\
&= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k})\, \widetilde{V}(\mathbf{k})\, \widetilde{\rho}(\mathbf{k}) \\
&= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2\, \widetilde{V}(\mathbf{k}). \qquad (2.95)
\end{aligned}
$$

From (2.94) and (2.95), we have

$$
\int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}')\, \rho(\mathbf{x}') = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2\, \widetilde{V}(\mathbf{k}) \qquad (2.96)
$$

which upon substituting (2.90) and (2.96) into (2.72), gives

$$
\begin{aligned}
\sum_{i<j}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) \geqslant{}& \sum_{j=1}^{k} A_j \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}_j) - \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2\, \frac{\left|\widetilde{V}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} \\
&+ \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2\, \widetilde{V}(\mathbf{k}) \\
&- \frac{1}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}')\, \rho(\mathbf{x}')
\end{aligned}
$$

$$-\frac{1}{2}v(0)\sum_{j=1}^{k}A_j^2. \tag{2.97}$$

Since $V(\mathbf{x}) \geqslant v(\mathbf{x}) \geqslant 0$, we obtain $\sum_{i<j}^{k} A_iA_jV(\mathbf{x}_i - \mathbf{x}_j) \geqslant \sum_{i<j}^{k} A_iA_jv(\mathbf{x}_i - \mathbf{x}_j)$, so that (2.97) will become

$$\begin{aligned}
\sum_{i<j}^{k} A_iA_jV(\mathbf{x}_i - \mathbf{x}_j) \geqslant & \sum_{j=1}^{k} A_j \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}_j) - \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\;|\widetilde{\rho}(\mathbf{k})|^2\;\frac{\left|\widetilde{V}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} \\
& + \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,|\widetilde{\rho}(\mathbf{k})|^2\,\widetilde{V}(\mathbf{k}) \\
& - \frac{1}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}')\,\rho(\mathbf{x}') \\
& - \frac{1}{2}v(0)\sum_{j=1}^{k}A_j^2 \\
= & \sum_{j=1}^{k} A_j \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}_j) \\
& - \frac{1}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}')\,\rho(\mathbf{x}') \\
& - \frac{1}{2}v(0)\sum_{j=1}^{k}A_j^2 - \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\;|\widetilde{\rho}(\mathbf{k})|^2\;\frac{\left|\widetilde{V}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} \\
& + \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,|\widetilde{\rho}(\mathbf{k})|^2\,\widetilde{V}(\mathbf{k})
\end{aligned}$$

$$\begin{aligned}
\sum_{i<j}^{k} A_iA_jV(\mathbf{x}_i - \mathbf{x}_j) \geqslant & \sum_{j=1}^{k} A_j \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}_j) \\
& - \frac{1}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,V(\mathbf{x}-\mathbf{x}')\,\rho(\mathbf{x}') \\
& - \frac{1}{2}v(0)\sum_{j=1}^{k}A_j^2
\end{aligned}$$

$$-\frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ |\widetilde{\rho}(\mathbf{k})|^2\left[\frac{\left|\widetilde{V}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}-\widetilde{V}(\mathbf{k})\right] \tag{2.98}$$

where, needless to say, $\int \mathrm{d}^3\mathbf{k}\ |\ \widetilde{\rho}(\mathbf{k})|^2\ \widetilde{V}(\mathbf{k})$ is real. Let $v(\mathbf{x}) = e^2(1-\mathrm{e}^{-\lambda|\mathbf{x}|})/|\mathbf{x}|$, $\lambda > 0$, then the Fourier transform of $v(\mathbf{x})$ is

$$\begin{aligned}
\widetilde{v}(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}\, v(\mathbf{x})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&= \int \mathrm{d}^3\mathbf{x}\, \frac{e^2(1-\mathrm{e}^{-\lambda|\mathbf{x}|})}{|\mathbf{x}|}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&= \int \mathrm{d}^3\mathbf{x}\, \frac{e^2(1-\mathrm{e}^{-\lambda x})}{x}\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|\cos\theta} \\
&= \int_0^\infty x^2 \mathrm{d}x \int_0^\pi \sin\theta\,\mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi\, \frac{e^2(1-\mathrm{e}^{-\lambda x})}{x}\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|\cos\theta} \\
\widetilde{v}(\mathbf{k}) &= \int_0^\infty \mathrm{d}x\, x^2\, \frac{e^2(1-\mathrm{e}^{-\lambda x})}{x} \int_0^\pi \mathrm{d}\theta\, \sin\theta\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|\cos\theta} \int_0^{2\pi} \mathrm{d}\varphi.
\end{aligned} \tag{2.99}$$

The φ integration is

$$\int_0^{2\pi} \mathrm{d}\varphi = 2\pi \tag{2.100}$$

The θ integration is

$$\begin{aligned}
\int_0^\pi \sin\theta\,\mathrm{d}\theta\,\mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|\cos\theta} &= -\int_1^{-1} \mathrm{d}u\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}|xu} \qquad , u=\cos\theta \\
&= \int_{-1} \mathrm{d}u\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}|xu} \\
&= \frac{1}{i|\mathbf{k}||\mathbf{x}|}\left(\mathrm{e}^{\mathrm{i}|\mathbf{k}||\mathbf{x}|}-\mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|}\right).
\end{aligned} \tag{2.101}$$

Substitute (2.100) and (2.101) into (2.99), gives

$$\widetilde{v}(\mathbf{k}) = 2\pi e^2 \int_0^\infty \mathrm{d}x\; x^2\; \frac{(1-\mathrm{e}^{-\lambda x})}{x}\frac{1}{i|\mathbf{k}||\mathbf{x}|}\left(\mathrm{e}^{\mathrm{i}|\mathbf{k}||\mathbf{x}|}-\mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|}\right)$$

$$= 2\pi e^2 \int_0^\infty \mathrm{d}x\; x^2\; \frac{(1-\mathrm{e}^{-\lambda x})}{x}\frac{1}{i|\mathbf{k}|x}\left(\mathrm{e}^{\mathrm{i}|\mathbf{k}|x}-\mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}\right)$$

$$= \frac{2\pi e^2}{i|\mathbf{k}|}\int_0^\infty \mathrm{d}x\;(1-\mathrm{e}^{-\lambda x})\left(\mathrm{e}^{\mathrm{i}|\mathbf{k}|x}-\mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}\right)$$

$$= \frac{2\pi e^2}{i|\mathbf{k}|}\left[\int_0^\infty \mathrm{d}x\;\left(\mathrm{e}^{\mathrm{i}|\mathbf{k}|x}-\mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}-\mathrm{e}^{(i|\mathbf{k}|-\lambda)x}+\mathrm{e}^{-(i|\mathbf{k}|+\lambda)x}\right)\right]$$

$$= \frac{2\pi e^2}{i|\mathbf{k}|}\left[\int_0^\infty \mathrm{d}x\;\mathrm{e}^{\mathrm{i}|\mathbf{k}|x}-\int_0^\infty \mathrm{d}x\;\mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}-\int_0^\infty \mathrm{d}x\;\mathrm{e}^{(i|\mathbf{k}|-\lambda)x}\right.$$

$$\left.+\int_0^\infty \mathrm{d}x\;\mathrm{e}^{-(i|\mathbf{k}|+\lambda)x}\right]$$

$$= \frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{\mathrm{e}^{\mathrm{i}|\mathbf{k}|x}}{i|\mathbf{k}|}\Bigg|_0^\infty+\frac{\mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}}{i|\mathbf{k}|}\Bigg|_0^\infty-\frac{\mathrm{e}^{(i|\mathbf{k}|-\lambda)x}}{i|\mathbf{k}|-\lambda}\Bigg|_0^\infty-\frac{\mathrm{e}^{-(i|\mathbf{k}|+\lambda)x}}{i|\mathbf{k}|+\lambda}\Bigg|_0^\infty\right]$$

$$= \frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{\mathrm{e}^\infty}{i|\mathbf{k}|}-\frac{1}{i|\mathbf{k}|}-\frac{1}{i|\mathbf{k}|}-\left(\frac{\mathrm{e}^\infty}{i|\mathbf{k}|-\lambda}-\frac{1}{i|\mathbf{k}|-\lambda}\right)+\left(\frac{1}{i|\mathbf{k}|+\lambda}\right)\right]$$

$$= \frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{\mathrm{e}^\infty}{i|\mathbf{k}|}-\frac{1}{i|\mathbf{k}|}-\frac{1}{i|\mathbf{k}|}-\frac{\mathrm{e}^\infty}{i|\mathbf{k}|+\lambda}+\frac{1}{i|\mathbf{k}|-\lambda}+\frac{1}{i|\mathbf{k}|+\lambda}\right]$$

$$= \frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{1}{i|\mathbf{k}|-\lambda}+\frac{1}{i|\mathbf{k}|+\lambda}-\frac{2}{i|\mathbf{k}|}\right]$$

$$= \frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{(i|\mathbf{k}|+\lambda)(i|\mathbf{k}|)+(i|\mathbf{k}|-\lambda)(i|\mathbf{k}|)-2(i|\mathbf{k}|+\lambda)(i|\mathbf{k}|-\lambda)}{(i|\mathbf{k}|-\lambda)(i|\mathbf{k}|+\lambda)(i|\mathbf{k}|)}\right]$$

$$= \frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{2\lambda^2}{(i|\mathbf{k}|^3-i|\mathbf{k}|\lambda^2)}\right]$$

$$= \frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{2\lambda^2}{(i|\mathbf{k}|^3-i|\mathbf{k}|\lambda^2)}\right]$$

$$\widetilde{v}(\mathbf{k}) = \frac{4\pi\lambda^2 e^2}{|\mathbf{k}|^2(|\mathbf{k}|^2+\lambda^2)}. \tag{2.102}$$

To evaluate the Fourier transform of the Coulomb potential, $V(\mathbf{x}) = e^2/|\mathbf{x}|$, the Fourier transform of $V(\mathbf{x})$ is not defined at $\mathbf{k} = 0$. However, if we work with the Yukawa potential,

$$V_\lambda(\mathbf{x}) = \frac{e^2 \mathrm{e}^{-\lambda|\mathbf{x}|}}{|\mathbf{x}|} \ , \lambda > 0 \tag{2.103}$$

the Fourier transform will be defined and we take the limit $\lambda \to 0$ to recover the Coulomb potential. So that, to obtain the Fourier transform of the Coulomb potential, we have to seek the Fourier transform of $V_\lambda(\mathbf{x})$. To obtain, let $\widetilde{v}_\lambda(\mathbf{k})$ is the Fourier transform of Yukawa potential ,$V_\lambda(\mathbf{x})$, we obtain

$$\begin{aligned}
\widetilde{v}_\lambda(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}\, v(\mathbf{x})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&= \int \mathrm{d}^3\mathbf{x}\, \frac{e^2 \mathrm{e}^{-\lambda|\mathbf{x}|}}{|\mathbf{x}|}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&= e^2 \int_0^\infty x^2 \mathrm{d}x \int_0^\pi \sin\theta\, \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi\, \frac{\mathrm{e}^{-\lambda x}}{x}\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}|x\cos\theta} \\
\widetilde{v}(\mathbf{k}) &= e^2 \int_0^\infty \mathrm{d}x\, x^2\, \frac{\mathrm{e}^{-\lambda x}}{x} \int_0^\pi \mathrm{d}\theta\, \sin\theta\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}|x\cos\theta} \int_0^{2\pi} \mathrm{d}\varphi.
\end{aligned} \tag{2.104}$$

Reference (2.100)–(2.101), applying to (2.104), we obtain

$$\begin{aligned}
\widetilde{v}_\lambda(\mathbf{k}) &= 2\pi e^2 \int_0^\infty \mathrm{d}x\, x^2\, \frac{\mathrm{e}^{-\lambda x}}{x} \frac{1}{i|\mathbf{k}|x} \left(\mathrm{e}^{\mathrm{i}|\mathbf{k}|x} - \mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}\right) \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \int_0^\infty \mathrm{d}x\, \mathrm{e}^{-\lambda x} \left(\mathrm{e}^{\mathrm{i}|\mathbf{k}|x} - \mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}\right) \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \int_0^\infty \mathrm{d}x\, \left(\mathrm{e}^{(-\lambda+\mathrm{i}|\mathbf{k}|)x} - \mathrm{e}^{-(\lambda+\mathrm{i}|\mathbf{k}|)x}\right) \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \lim_{a\to\infty} \left[\int_0^a \mathrm{d}x\, \left(\mathrm{e}^{(-\lambda+\mathrm{i}|\mathbf{k}|)x} - \mathrm{e}^{-(\lambda+\mathrm{i}|\mathbf{k}|)x}\right)\right]
\end{aligned}$$

$$
\begin{aligned}
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \lim_{a\to\infty} \left[\left. \frac{\mathrm{e}^{(-\lambda+\mathrm{i}|\mathbf{k}|)x}}{-\lambda+\mathrm{i}|\mathbf{k}|} \right|_0^a + \left. \frac{\mathrm{e}^{-(\lambda+\mathrm{i}|\mathbf{k}|)x}}{\lambda+\mathrm{i}|\mathbf{k}|} \right|_0^a \right] \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \lim_{a\to\infty} \left[\left. \frac{\mathrm{e}^{(-\lambda+\mathrm{i}|\mathbf{k}|)x}}{-\lambda+\mathrm{i}|\mathbf{k}|} \right|_0^a + \left. \frac{\mathrm{e}^{-(\lambda+\mathrm{i}|\mathbf{k}|)x}}{\lambda+\mathrm{i}|\mathbf{k}|} \right|_0^a \right] \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \lim_{a\to\infty} \left[\frac{\mathrm{e}^{(-\lambda+\mathrm{i}|\mathbf{k}|)a} - 1}{-\lambda+\mathrm{i}|\mathbf{k}|} + \frac{\mathrm{e}^{-(\lambda+\mathrm{i}|\mathbf{k}|)a} - 1}{\lambda+\mathrm{i}|\mathbf{k}|} \right] \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \lim_{a\to\infty} \left[\frac{\mathrm{e}^{-\lambda a}\left(\mathrm{e}^{\mathrm{i}|\mathbf{k}|a}(\lambda+\mathrm{i}|\mathbf{k}|) - \mathrm{e}^{-\mathrm{i}|\mathbf{k}|a}(-\lambda+\mathrm{i}|\mathbf{k}|)\right)}{-|\mathbf{k}|^2-\lambda^2} \right. \\
&\qquad \left. \frac{-(\lambda+\mathrm{i}|\mathbf{k}|) - (-\lambda+\mathrm{i}|\mathbf{k}|)}{-|\mathbf{k}|^2-\lambda^2} \right] \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \left[\frac{-2\mathrm{i}|\mathbf{k}|}{-|\mathbf{k}|^2-\lambda^2} \right] \\
&= \frac{4\pi e^2}{(|\mathbf{k}|^2+\lambda^2)}
\end{aligned}
$$

$$
\therefore \quad \widetilde{v}(\mathbf{k}) = \frac{4\pi e^2}{(|\mathbf{k}|^2+\lambda^2)} \tag{2.105}
$$

and is well defined for $\mathbf{k} = 0$, i.e., for $|\mathbf{k}|^2 = 0$. In fact, it was in response to the short range of nuclear forces that Yukawa introduced λ. For electromagnetism, where the range is infinite, λ becomes zero and $V_\lambda(\mathbf{x}) = \frac{\mathrm{e}^{-\lambda|\mathbf{x}|}}{|\mathbf{x}|}$ reduces to $V_{\lambda\to 0}(\mathbf{x}) \to \frac{1}{|\mathbf{x}|}$ the Coulomb potential. Thus, referring to (2.102), the Fourier transform of the Coulomb potential in 3-dimensions is

$$
\begin{aligned}
\widetilde{V}_{\lambda\to 0}(\mathbf{k}) &= \lim_{\lambda\to 0} \frac{4\pi e^2}{(|\mathbf{k}|^2+\lambda^2)} \\
&= \frac{4\pi e^2}{|\mathbf{k}|^2}.
\end{aligned} \tag{2.106}
$$

From the Coulomb potential, $V(\mathbf{x}) = e^2/|\mathbf{x}|$, we obtain

$$
V(\mathbf{x}_i - \mathbf{x}_j) = \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \tag{2.107}
$$

$$V(\mathbf{x}-\mathbf{x}_j) = \frac{e^2}{|\mathbf{x}-\mathbf{x}_j|} \tag{2.108}$$

$$V(\mathbf{x}-\mathbf{x}') = \frac{e^2}{|\mathbf{x}-\mathbf{x}'|}. \tag{2.109}$$

Consider $v(0)$ when now we choose $v(\mathbf{x}) = e^2(1-\mathrm{e}^{-\lambda|\mathbf{x}|})/|\mathbf{x}|$, then

$$\begin{aligned} v(0) =& \lim_{|\mathbf{x}|\to 0} \frac{e^2(1-\mathrm{e}^{-\lambda|\mathbf{x}|})}{|\mathbf{x}|} \\ =& e^2 \lim_{|\mathbf{x}|\to 0} \left[\sum_{n=1}^{\infty} -\frac{(-\lambda|\mathbf{x}|)^n}{|\mathbf{x}|\, n!}\right] \\ =& e^2 \lim_{|\mathbf{x}|\to 0} \left[\lambda - \frac{1}{2!}\lambda^2|\mathbf{x}| + \frac{1}{3!}\lambda^3|\mathbf{x}|^2 - \frac{1}{4!}\lambda^4|\mathbf{x}|^3 + \cdots - \cdots\right] \\ v(0) =& e^2\lambda. \end{aligned} \tag{2.110}$$

Substitute (2.102), (2.106), (2.107), (2.108), (2.109) and (2.110) into (2.98), to obtain the bound $(k \geqslant 2)$

$$\begin{aligned} \sum_{i<j}^{k} \frac{e^2 A_i A_j}{|\mathbf{x}_i - \mathbf{x}_j|} \geqslant& \sum_{j=1}^{k} e^2 A_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} - \frac{1}{2}\int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \\ & - \frac{e^2\lambda}{2}\sum_{j=1}^{k} A_j^2 - \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ |\widetilde{\rho}(\mathbf{k})|^2 \left[\frac{\left|\frac{4\pi e^2}{p^2}\right|^2}{\frac{4\pi\lambda^2 e^2}{p^2(p^2+\lambda^2)}} - \frac{4\pi e^2}{p^2}\right] \\ =& \sum_{j=1}^{k} e^2 A_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} - \frac{1}{2}\int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \\ & - \frac{e^2\lambda}{2}\sum_{j=1}^{k} A_j^2 - R(\mathbf{k}) \end{aligned} \tag{2.111}$$

where

$$
\begin{aligned}
R(\mathbf{k}) =& \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \, |\widetilde{\rho}(\mathbf{k})|^2 \left[\frac{\left| \frac{4\pi e^2}{|\mathbf{k}|^2} \right|^2}{\frac{4\pi\lambda^2 e^2}{|\mathbf{k}|^2(|\mathbf{k}|^2+\lambda^2)}} - \frac{4\pi e^2}{|\mathbf{k}|^2} \right] \\
=& \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \, |\widetilde{\rho}(\mathbf{k})|^2 \left[\left| \frac{4\pi e^2}{|\mathbf{k}|^2} \right|^2 \frac{|\mathbf{k}|^2(|\mathbf{k}|^2+\lambda^2)}{4\pi\lambda^2 e^2} - \frac{4\pi e^2}{|\mathbf{k}|^2} \right] \\
=& \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \, |\widetilde{\rho}(\mathbf{k})|^2 \left[\left(\frac{4\pi e^2(|\mathbf{k}|^2+\lambda^2)}{|\mathbf{k}|^2\lambda^2} \right) - \frac{4\pi e^2}{|\mathbf{k}|^2} \right] \\
=& \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \, |\widetilde{\rho}(\mathbf{k})|^2 \left[\left(\frac{4\pi e^2(|\mathbf{k}|^2+\lambda^2)}{|\mathbf{k}|^2\lambda^2} \right) - \frac{4\pi e^2}{|\mathbf{k}|^2} \right] \\
=& \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \, |\widetilde{\rho}(\mathbf{k})|^2 \, \frac{4\pi e^2}{\lambda^2} \\
=& \frac{2\pi e^2}{\lambda^2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \, |\widetilde{\rho}(\mathbf{k})|^2 \\
=& \frac{2\pi e^2}{\lambda^2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \, \widetilde{\rho}(\mathbf{k}) \cdot \widetilde{\rho}^*(\mathbf{k}) \\
=& \frac{2\pi e^2}{\lambda^2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{x} \, \rho(\mathbf{x}) \, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \cdot \int \mathrm{d}^3\mathbf{x}' \, \rho(\mathbf{x}') \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \\
=& \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x} \, \rho(\mathbf{x}) \int \mathrm{d}^3\mathbf{x}' \, \rho(\mathbf{x}') \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}'-\mathbf{x})} \\
=& \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x} \, \rho(\mathbf{x}) \int \mathrm{d}^3\mathbf{x}' \rho(\mathbf{x}') \, \delta^3(\mathbf{x}'-\mathbf{x}) \\
R(\mathbf{k}) =& \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x} \, \rho^2(\mathbf{x}). \qquad (2.112)
\end{aligned}
$$

Substituting (2.112) into (2.111), we obtain the bound $(k \geqslant 2)$

$$
\sum_{i<j}^{k} \frac{e^2 A_i A_j}{|\mathbf{x}_i - \mathbf{x}_j|} \geqslant \sum_{j=1}^{k} e^2 A_j \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} - \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x}) \, \rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}
$$

$$- \frac{e^2\lambda}{2}\sum_{j=1}^{k} A_j^2 - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}) \tag{2.113}$$

Eq.(2.113) is the general result of Coulomb potential.

For the Hamiltonian in (1.1), it is then straightforward to use (2.113) twice, once for the repulsive potentials in (1.2), with $A_i, A_j = 1$ and $k \longrightarrow N$, giving

$$\sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \geqslant \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} - \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

$$- \frac{e^2\lambda}{2}\sum_{j=1}^{N}(1) - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}) \tag{2.114}$$

and then again for the repulsive potentials in (1.3), with $A_i = Z_i, A_j = Z_j$ and $\mathbf{x}_j \longrightarrow \mathbf{R}_j$ for $k \geqslant 2$, giving

$$\sum_{i<j}^{k} \frac{e^2 Z_i Z_j}{|\mathbf{R}_i - \mathbf{R}_j|} \geqslant \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|} - \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

$$- \frac{e^2\lambda}{2}\sum_{j=1}^{k} Z_j^2 - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}). \tag{2.115}$$

Upon substituting (2.114) and (2.115) into (1.1), we obtain for the Hamiltonian in (1.1) the bound :

$$H \geqslant \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} - \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

$$- \frac{e^2\lambda}{2}\sum_{j=1}^{N}(1) - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}) + \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|}$$

$$- \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} - \frac{e^2\lambda}{2}\sum_{j=1}^{k} Z_j^2 - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})$$

$$-\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_j e^2}{|\mathbf{x}_i-\mathbf{R}_j|}. \tag{2.116}$$

With $\sum\limits_{i=1}^{k} Z_i = N,\ k \geqslant 2$ and $\sum\limits_{i=1}^{N}(1) = N$, (2.116) can be rewritten as

$$\begin{aligned}
H \geqslant &\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}+\sum_{j=1}^{N}e^2\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|}-\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\\
&-\frac{e^2\lambda N}{2}-\frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})+\sum_{j=1}^{k}e^2 Z_j\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|}\\
&-\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}-\frac{e^2\lambda}{2}\sum_{i=1}^{k}Z_i^2-\frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\\
&-\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_j e^2}{|\mathbf{x}_i-\mathbf{R}_j|}\\
=&\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}-\frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})-\frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})-\frac{e^2\lambda N}{2}\\
&-\frac{e^2\lambda}{2}\sum_{i=1}^{k}Z_i^2+\sum_{j=1}^{N}e^2\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|}+\sum_{j=1}^{k}e^2 Z_j\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|}\\
&-e^2\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}-\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_j e^2}{|\mathbf{x}_i-\mathbf{R}_j|}\\
=&\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}-\frac{4\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})-\frac{e^2\lambda}{2}\left(N+\sum_{i=1}^{k}Z_i^2\right)\\
&+\sum_{j=1}^{N}e^2\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|}+\sum_{j=1}^{k}e^2 Z_j\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|}\\
&-e^2\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}-\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_j e^2}{|\mathbf{x}_i-\mathbf{R}_j|}
\end{aligned}$$

$$\therefore \quad H \geqslant \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} - \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{e^2\lambda}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right)$$

$$+ \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} + \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|}$$

$$- e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\; \frac{\rho(\mathbf{x})\, \rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} - \sum_{i=1}^{N} \sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|}. \tag{2.117}$$

This gives the following bound for $\langle \Psi | \, H \, | \Psi \rangle$ with $k \geqslant 2$

$$\langle \Psi | \, H \, | \Psi \rangle \geqslant T - \langle \Psi | \, \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) \, | \Psi \rangle - \langle \Psi | \, \frac{e^2\lambda}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right) | \Psi \rangle$$

$$- \langle \Psi | \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} \, | \Psi \rangle + \langle \Psi | \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|} \, | \Psi \rangle$$

$$- \langle \Psi | \, e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\; \frac{\rho(\mathbf{x})\, \rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \, | \Psi \rangle$$

$$- \langle \Psi | \sum_{i=1}^{N} \sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \, | \Psi \rangle \tag{2.118}$$

where

$$T = \langle \Psi | \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \, | \Psi \rangle \,. \tag{2.119}$$

For the fermionic case, we consider N identical fermions, each of mass m and introduce the particle number density in three dimensions in (2.40) with total number of particle N self consistently obtained from the normalization condition in (2.41). The wavefunctions $\Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N)$ are assumed to satisfy the appropriate statistics which in this case are anti-symmetric in the exchange of any two particles which amounts into the interchange of the position-spin labeling : $(\mathbf{x}_i\sigma_i) \Leftrightarrow (\mathbf{x}_j\sigma_j)$ with the normalization condition

$$\langle\Psi|\Psi\rangle = \int \mathrm{d}^3\mathbf{x}, \mathrm{d}^3\mathbf{x}_2...\mathrm{d}^3\mathbf{x}_N \; \Psi^*(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N)\; \Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N)$$

$$= \sum_{\sigma_1,...,\sigma_N}^{n} \int \mathrm{d}^3\mathbf{x}, \mathrm{d}^3\mathbf{x}_2...\mathrm{d}^3\mathbf{x}_N \, |\Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N)|^2$$

$$=1. \tag{2.120}$$

To investigate the nature of the second term on the right-hand side of (2.118), substitute (2.40) into (2.118), to obtain

$$\langle\Psi|\, \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\, |\Psi\rangle$$

$$= \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}_2...\mathrm{d}^3\mathbf{x}_N \; \Psi^*(\mathbf{x}'\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N)$$

$$\times \left(\int \mathrm{d}^3\mathbf{x}\; \rho^2(\mathbf{x})\right) \Psi(\mathbf{x}'\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N)$$

$$= \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\, \langle\Psi|\Psi\rangle$$

$$= \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}). \tag{2.121}$$

For the third term on the right-hand side of (2.118), substitute (2.40) into (2.118), to obtain

$$\langle\Psi|\, \frac{e^2\lambda}{2} \left(N + \sum_{i=1}^{k} Z_i^2\right) |\Psi\rangle = \left(N + \sum_{i=1}^{k} Z_i^2\right) \langle\Psi|\Psi\rangle$$

$$= \left(N + \sum_{i=1}^{k} Z_i^2\right)$$

$$\therefore \quad \langle\Psi|\, \frac{e^2\lambda}{2} \left(N + \sum_{i=1}^{k} Z_i^2\right) |\Psi\rangle = \left(N + \sum_{i=1}^{k} Z_i^2\right). \tag{2.122}$$

For the fourth term on the right-hand side of (2.118), substitute (2.40) into (2.118), to obtain

$$\langle\Psi|\sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|}\,|\Psi\rangle$$

$$= \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}', \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N\ \Psi^*(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|}\right)\ \Psi(\mathbf{x}', \mathbf{x}_2, \ldots \mathbf{x}_N)$$

$$= \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|}$$

$$\times \sum_{\sigma_1,\ldots,\sigma_N} \int \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N\ |\Psi(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2$$

$$= \frac{e^2}{N} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

$$+ \frac{e^2}{N} \int \mathrm{d}^3\mathbf{x}_2 \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}_2)}{|\mathbf{x}-\mathbf{x}_2|}$$

$$+ \ldots + \frac{e^2}{N} \int \mathrm{d}^3\mathbf{x}_N \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}_N)}{|\mathbf{x}-\mathbf{x}_N|}$$

$$= e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

$$= e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}. \tag{2.123}$$

For the fifth term on the right-hand side of (2.118), substitute (2.40) into (2.118), to obtain

$$\langle\Psi|\sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|}\,|\Psi\rangle$$

$$= \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}', \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \; \Psi^*(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|} \right) \Psi(\mathbf{x}', \mathbf{x}_2, \ldots \mathbf{x}_N)$$

$$= \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|} \langle \Psi | \Psi \rangle$$

$$= \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|}. \tag{2.124}$$

For the sixth term on the right-hand side of (2.118), substitute (2.40) into (2.118), to obtain

$$\langle \Psi | \, e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \; \frac{\rho(\mathbf{x}) \, \rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \, | \Psi \rangle$$

$$= \int \mathrm{d}^3\mathbf{x}'', \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \; \Psi^*(\mathbf{x}'', \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \right) \Psi(\mathbf{x}'', \mathbf{x}_2, \ldots \mathbf{x}_N)$$

$$= e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x}) \, \rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \langle \Psi | \Psi \rangle$$

$$= e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \; \frac{\rho(\mathbf{x}) \, \rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}. \tag{2.125}$$

For the seventh term on the right-hand side of (2.118), substitute (2.40) into (2.118), to obtain

$$\langle \Psi | \sum_{i=1}^{N} \sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \, | \Psi \rangle$$

$$= \int \mathrm{d}^3\mathbf{x}, \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \; \Psi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\sum_{i=1}^{N} \sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \right) \Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$= \sum_{j=1}^{k} \sum_{i=1}^{N} \int \mathrm{d}^3\mathbf{x}, \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \, \Psi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \right) \Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$= \sum_{j=1}^{k} \sum_{j=1}^{N} \int \mathrm{d}^3\mathbf{x} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|}$$

$$\times \sum_{\sigma_1, \ldots, \sigma_N} \int \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \, |\Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2$$

$$= \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x} \frac{Z_j e^2}{|\mathbf{x} - \mathbf{R}_j|} \, \frac{\rho(\mathbf{x})}{N} + \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x}_2 \frac{Z_j e^2}{|\mathbf{x}_2 - \mathbf{R}_j|} \, \frac{\rho(\mathbf{x}_2)}{N}$$

$$+ \ldots + \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x}_N \frac{Z_j e^2}{|\mathbf{x}_N - \mathbf{R}_j|} \, \frac{\rho(\mathbf{x}_N)}{N}$$

$$= \sum_{j=1}^{k} Z_j e^2 \int \mathrm{d}^3\mathbf{x} \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|}. \tag{2.126}$$

In reference to (2.123)–(2.126), we obtain

$$\langle\Psi| \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} \, |\Psi\rangle = \langle\Psi| \, e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x}) \, \rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \, |\Psi\rangle \tag{2.127}$$

$$\langle\Psi| \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|} \, |\Psi\rangle = \langle\Psi| \sum_{i=1}^{N} \sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \, |\Psi\rangle \, . \tag{2.128}$$

In reference to (2.122)–(2.126), substitute them into (2.118), to obtain the bound (for $k \geqslant 2$)

$$\langle\Psi| \, H \, |\Psi\rangle \geqslant T - \langle\Psi| \, \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x} \, \rho^2(\mathbf{x}) \, |\Psi\rangle - \langle\Psi| \, \frac{e^2 \lambda}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right) |\Psi\rangle \, . \tag{2.129}$$

Optimizing (2.129) over λ , we obtain

$$
\begin{aligned}
0 =& \frac{\mathrm{d}}{\mathrm{d}\lambda} \langle \Psi | H | \Psi \rangle \\
=& \frac{\mathrm{d}}{\mathrm{d}\lambda} T - \frac{\mathrm{d}}{\mathrm{d}\lambda} \left(\frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) \right) - \frac{\mathrm{d}}{\mathrm{d}\lambda} \left(\frac{\lambda e^2}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right) \right) \\
=& 0 + \frac{8\pi e^2}{\lambda^3} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{e^2}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right) \\
\lambda^3 =& \frac{16\pi \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})}{\left(N + \sum_{i=1}^{k} Z_i^2 \right)} \\
\lambda =& \left(\frac{16\pi \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})}{\left(N + \sum_{i=1}^{k} Z_i^2 \right)} \right)^{1/3}
\end{aligned} \tag{2.130}
$$

which upon substituting (2.130) into (2.129), gives the remarkably simple bound $(k \geqslant 2)$

$$
\begin{aligned}
\langle \Psi | H | \Psi \rangle \geqslant& T - \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{\lambda e^2}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right) \\
=& T - 4\pi e^2 \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) \left(\frac{\left(N + \sum_{i=1}^{k} Z_i^2 \right)}{16\pi \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})} \right)^{2/3} \\
&- \frac{e^2}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right) \left(\frac{16\pi \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})}{\left(N + \sum_{i=1}^{k} Z_i^2 \right)} \right)^{1/3} \\
=& T - \left(\frac{\pi^{1/3} e^2}{2^{2/3}} + 2^{1/3}\pi^{1/3} e^2 \right) \left(N + \sum_{i=1}^{k} Z_i^2 \right)^{2/3} \left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) \right)^{1/3}
\end{aligned}
$$

$$=T - \frac{3e^2}{2^{2/3}}\,\pi^{1/3}\left(N + \sum_{i=1}^{k} Z_i^2\right)^{2/3}\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{1/3}$$

$$\therefore \quad \langle\Psi|H|\Psi\rangle \geqslant T - \frac{3e^2}{2^{2/3}}\,\pi^{1/3}\left(N + \sum_{i=1}^{k} Z_i^2\right)^{2/3}\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{1/3}. \tag{2.131}$$

For $k = 1$, the V_2 term, $V_2 = \sum_{i<j}^{k} Z_i Z_j\, e^2 |\mathbf{R}_i - \mathbf{R}_j|^{-1}$, will be absent ($V_2 = 0$) in the expression for H in (1.1) and we can rewrite the Coulomb potential between electron and proton interaction $(k = 1)$, $\sum_{i=1}^{N}\sum_{j=1}^{1} Z_1 e^2 |\mathbf{x}_i - \mathbf{R}_1|^{-1}$, as

$$\sum_{i=1}^{N}\sum_{j=1}^{1}\frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_1|} = \sum_{j=1}^{N}\frac{N e^2}{|\mathbf{x}_j - \mathbf{R}|}. \tag{2.132}$$

Substitute (2.132) into (2.117), and let $\sum_{i<j}^{k} Z_i Z_j\, e^2 |\mathbf{R}_i - \mathbf{R}_j|^{-1} = 0$, to obtain for the Hamiltonian for $k = 1$ as

$$\begin{aligned}
H \geqslant & \sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m} + \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} - \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \\
& - \frac{e^2\lambda N}{2} - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}) - \sum_{j=1}^{N}\frac{N e^2}{|\mathbf{x}_j - \mathbf{R}|} \\
= & \sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m} + \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} - e^2\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \\
& + \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} - \frac{e^2\lambda N}{2} \\
& - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}) - \sum_{j=1}^{N}\frac{N e^2}{|\mathbf{x}_j - \mathbf{R}|} \\
= & \sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m} - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}) - \frac{e^2\lambda N}{2} - \sum_{j=1}^{N}\frac{N e^2}{|\mathbf{x}_j - \mathbf{R}|}
\end{aligned}$$

$$+ e^2 \left(\sum_{j=1}^{N} \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} - \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \right)$$

$$+ \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

$$\therefore \quad H \geqslant \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} - \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{e^2\lambda N}{2} - \sum_{j=1}^{N} \frac{Ne^2}{|\mathbf{x}_j - \mathbf{R}|}$$

$$+ e^2 \left(\sum_{j=1}^{N} \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} - \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \right)$$

$$+ \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}. \tag{2.133}$$

To obtain the bound, $\langle\Psi|\, H \,|\Psi\rangle$ for $k = 1$, we get

$$\langle\Psi|\, H \,|\Psi\rangle \geqslant T - \langle\Psi|\, \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\, |\Psi\rangle - \langle\Psi|\, \frac{e^2\lambda N}{2}\, |\Psi\rangle$$

$$- \langle\Psi| \sum_{j=1}^{N} \frac{Ne^2}{|\mathbf{x}_j - \mathbf{R}|}\, |\Psi\rangle + \langle\Psi|\, \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\, |\Psi\rangle$$

$$+ \langle\Psi|\, e^2 \left(\sum_{j=1}^{N} \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} - \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \right) |\Psi\rangle \tag{2.134}$$

where

$$T = \langle\Psi| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m}\, |\Psi\rangle\,. \tag{2.135}$$

For the second term on the right-hand side of (2.134), we obtain (from (2.121))

$$\langle\Psi|\, \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\, |\Psi\rangle = \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}). \tag{2.136}$$

For the third term on the right-hand side of (2.134), we obtain

$$\langle\Psi|\,\frac{e^2\lambda N}{2}\,|\Psi\rangle = \frac{e^2\lambda N}{2}. \tag{2.137}$$

For the fourth term on the right-hand side of (2.134), we obtain

$$\begin{aligned}
\langle\Psi|\sum_{j=1}^{N}\frac{Ne^2}{|\mathbf{x}_j-\mathbf{R}|}\,|\Psi\rangle = &\sum_{j=1}^{N} Ne^2 \int \mathrm{d}^3\mathbf{x}, \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \\
&\times \Psi^*(\mathbf{x},\mathbf{x}_2,\ldots\mathbf{x}_N)\frac{1}{|\mathbf{x}_j-\mathbf{R}|}\Psi(\mathbf{x},\mathbf{x}_2,\ldots\mathbf{x}_N) \\
=&Ne^2\int \mathrm{d}^3\mathbf{x}\frac{1}{|\mathbf{x}-\mathbf{R}|}\,\frac{\rho(\mathbf{x})}{N} \\
&+ Ne^2\int \mathrm{d}^3\mathbf{x}_2\frac{1}{|\mathbf{x}_2-\mathbf{R}|}\,\frac{\rho(\mathbf{x}_2)}{N} \\
&+\ldots + Ne^2\int \mathrm{d}^3\mathbf{x}_N\frac{1}{|\mathbf{x}_N-\mathbf{R}|}\,\frac{\rho(\mathbf{x}_N)}{N} \\
=&Ne^2\int \mathrm{d}^3\mathbf{x}\frac{1}{|\mathbf{x}-\mathbf{R}|}\,\rho(\mathbf{x})
\end{aligned}$$

$$\therefore\quad \langle\Psi|\sum_{j=1}^{N}\frac{Ne^2}{|\mathbf{x}_j-\mathbf{R}|}\,|\Psi\rangle = Ne^2\int \mathrm{d}^3\mathbf{x}\frac{1}{|\mathbf{x}-\mathbf{R}|}\,\rho(\mathbf{x}). \tag{2.138}$$

For the fifth term on the right-hand side of (2.134), we obtain (from (2.125))

$$\langle\Psi|\,\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\,|\Psi\rangle = \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}. \tag{2.139}$$

For the sixth term on the right-hand side of (2.134), we obtain (from (2.127))

$$\langle\Psi|\,e^2\left(\sum_{j=1}^{N}\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} - \int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\right)|\Psi\rangle = 0 \tag{2.140}$$

which upon substituting (2.136), (2.137), (2.138), (2.139), and (2.140) into (2.134) we

obtain

$$\langle\Psi|\, H \,|\Psi\rangle \geqslant T - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{e^2\lambda N}{2} - Ne^2\int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}|}$$
$$+ \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}. \tag{2.141}$$

From (2.141), if we bound the positive term $e^2\int \mathrm{d}^3\,\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\rho(\mathbf{x})|\mathbf{x}-\mathbf{x}'|^{-1}\rho(\mathbf{x}')/2$ below by zero, we obtain

$$\langle\Psi|\, H \,|\Psi\rangle \geqslant T - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{e^2\lambda N}{2} - Ne^2\int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}|}. \tag{2.142}$$

Optimizing (2.142) over λ, gives

$$\begin{aligned}
0 =& \frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\Psi|H|\Psi\rangle \\
=& \frac{\mathrm{d}}{\mathrm{d}\lambda}T - \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\right) - \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{e^2 N\lambda}{2}\right) \\
& - \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(Ne^2\int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}|}\right) \\
=& 0 + \frac{4\pi e^2}{\lambda^3}\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{e^2 N}{2} \\
\lambda^3 =& \frac{8\pi\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})}{N} \\
\lambda =& \left(\frac{8\pi\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})}{N}\right)^{1/3}.
\end{aligned} \tag{2.143}$$

Substitute (2.143) into (2.142), to obtain the remarkably simple bound $(k = 1)$

$$\langle\Psi|\, H \,|\Psi\rangle \geqslant T - 2\pi e^2\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\left(\frac{N}{8\pi\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})}\right)^{2/3}$$
$$- \frac{e^2 N}{2}\left(\frac{8\pi\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})}{N}\right)^{1/3} - Ne^2\int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}|}$$

$$=T - \frac{3e^2}{2}\pi^{1/3}N^{2/3}\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{1/3} - Ne^2\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}|}$$

$$\therefore\quad \langle\Psi|\,H\,|\Psi\rangle \geqslant T - \frac{3e^2}{2}\pi^{1/3}N^{2/3}\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{1/3} - Ne^2\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}|}. \tag{2.144}$$

[From (2.131), it is of utmost importance that $k \geqslant 2$, otherwise, from (2.144), the V_2 term will be absent in the expression for H in (1.1), and there will be an additional term $-e^2N\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})/|\mathbf{x}-\mathbf{R}|$ on the right-hand side of the inequality in (2.131), after having omitted the positive term $e^2\int \mathrm{d}^3\,\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\rho(\mathbf{x})|\mathbf{x}-\mathbf{x}'|^{-1}\rho(\mathbf{x}')/2$. The numerical factor 3 would be also replaced by 3/2.] This suggests to use a lower bound to T which is some power of the integral of ρ^2.

For $k \geqslant 2$, to obtain the lower bound for the ground-state energy of N identical fermions, we use the inequality (2.48). Substitute (2.48) into (2.131), to obtain

$$\langle\Psi|H|\Psi\rangle \geqslant \frac{1}{\underline{q}^{1/3}}\frac{3}{(1+\delta)^{1/3}}\left(\frac{\pi}{2}\right)^{2/3}\left(\frac{\hbar^2}{2m}\right)\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3} - \frac{3e^2}{2^{2/3}}\pi^{1/3}\left(N+\sum_{i=1}^{k}Z_i^2\right)^{2/3}\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{1/3}. \tag{2.145}$$

In the above expression, let

$$A = \left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{1/3} \tag{2.146}$$

$$B = \frac{3}{(1+\varepsilon)}\left(\frac{\pi}{2}\right)^{2/3} \tag{2.147}$$

$$C = \left(N+\sum_{i=1}^{k}Z_i^2\right)^{2/3} \tag{2.148}$$

and we set $(1+\delta)^{1/3} \equiv 1+\varepsilon$, for any $\varepsilon > 0$.

Substitute A and B into (2.145), to obtain lower bound for the ground-state energy of N identical fermions ($k \geqslant 2$)

$$\begin{aligned}
\langle\Psi|H|\Psi\rangle \geqslant & \frac{B}{\underline{q}^{1/3}}\left(\frac{\hbar^2}{2m}\right)A^2 - \frac{3e^2}{2^{2/3}}\,\pi^{1/3}CA \\
= & \frac{B}{\underline{q}^{1/3}}\left(\frac{\hbar^2}{2m}\right)\left(A^2 - \frac{\underline{q}^{1/3}}{B}\left(\frac{2m}{\hbar^2}\right)\frac{3e^2}{2^{2/3}}\,\pi^{1/3}CA\right) \\
= & \frac{B}{\underline{q}^{1/3}}\left(\frac{\hbar^2}{2m}\right)\left(A^2 - \frac{2\underline{q}^{1/3}}{B}\left(\frac{m}{\hbar^2}\right)\frac{3e^2}{2^{2/3}}\,\pi^{1/3}CA\right) \\
= & \frac{B}{\underline{q}^{1/3}}\left(\frac{\hbar^2}{2m}\right)\left(A - \frac{\underline{q}^{1/3}}{B}\left(\frac{m}{\hbar^2}\right)\frac{3e^2}{2^{2/3}}\,\pi^{1/3}C\right)^2 \\
& - \frac{B}{\underline{q}^{1/3}}\left(\frac{\hbar^2}{2m}\right)\left(\frac{\underline{q}^{1/3}}{B}\left(\frac{m}{\hbar^2}\right)\frac{3e^2}{2^{2/3}}\,\pi^{1/3}C\right)^2 \\
> & - \frac{B}{\underline{q}^{1/3}}\left(\frac{\hbar^2}{2m}\right)\left(\frac{\underline{q}^{1/3}}{B}\left(\frac{m}{\hbar^2}\right)\frac{3e^2}{2^{2/3}}\,\pi^{1/3}C\right)^2 \\
= & - \frac{9}{2^{4/3}}\frac{\underline{q}^{1/3}}{B}\pi^{2/3}\left(\frac{me^4}{2\hbar^2}\right)C^2 \\
= & - \frac{9\underline{q}^{1/3}}{2^{4/3}}\frac{(1+\varepsilon)}{3}\left(\frac{2}{\pi}\right)^{2/3}\pi^{2/3}\left(\frac{me^4}{2\hbar^2}\right)\left(N + \sum_{i=1}^{k} Z_i^2\right)^{4/3} \\
= & - \frac{9\underline{q}^{1/3}}{2^{2/3}}\frac{(1+\varepsilon)}{3}\left(\frac{me^4}{2\hbar^2}\right)\left(N + \sum_{i=1}^{k} Z_i^2\right)^{4/3} \\
= & - 1.89\underline{q}^{1/3}(1+\varepsilon)\left(\frac{me^4}{2\hbar^2}\right)\left(N + \sum_{i=1}^{k} Z_i^2\right)^{4/3}
\end{aligned}$$

$$\therefore \quad \langle\Psi|H|\Psi\rangle > - 1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(N + \sum_{i=1}^{k} Z_i^2\right)^{4/3} \tag{2.149}$$

where $\underline{q} = 2s + 1$ is the spin multiplicity, and we have taken ε arbitrarily small.

For $Z_1 = ... = Z_q = 1$, $2 \leqslant q \ll N$, we have

$$\langle\Psi|H|\Psi\rangle > -1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(N + \sum_{i=1}^{q} Z_i^2 + \sum_{i=q+1}^{k} Z_i^2\right)^{4/3},$$

$$= -1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(N + q + \sum_{i=q+1}^{k} Z_i^2\right)^{4/3},$$

$$= -1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(N\left[1 + \frac{q}{N} + \sum_{i=q+1}^{k} \frac{Z_i^2}{N}\right]\right)^{4/3}$$

$$= -1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right) N\left(1 + \sum_{i=q+1}^{k} \frac{Z_i^2}{N}\right) N^{1/3}\left(1 + \sum_{i=q+1}^{k} \frac{Z_i^2}{N}\right)^{1/3}$$

$$= -1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right) N\left(N + \sum_{i=q+1}^{k} Z_i^2\right)\left(N + \sum_{i=q+1}^{k} Z_i^2\right)^{1/3}$$

$$\langle\Psi|H|\Psi\rangle > -1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(N + \sum_{i=q+1}^{k} Z_i^2\right)^{4/3} N. \tag{2.150}$$

For $Z_1 = ... = Z_q = N/q$, $2 \leqslant q \ll N$, we have

$$\langle\Psi|H|\Psi\rangle > -1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(N + \sum_{i=1}^{q} Z_i^2 + \sum_{i=q+1}^{k} Z_i^2\right)^{4/3}$$

$$= -1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(N + \frac{N^2}{q} + \sum_{i=q+1}^{k} Z_i^2\right)^{4/3}$$

$$= -1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left[\frac{N^2}{q}\left(\frac{q}{N} + 1 + \sum_{i=q+1}^{k} \frac{Z_i^2 q}{N^2}\right)\right]^{4/3}$$

$$= -1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left[\frac{N^2}{q}\left(1 + \sum_{i=q+1}^{k} \frac{Z_i^2 q}{N^2}\right)\right]^{4/3}$$

$$= - 1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^2}{q}\right)^{4/3}\left(\frac{N}{q}+\sum_{i=q+1}^{k}Z_i^2\right)^{4/3}$$

$$\therefore \quad \langle\Psi|H|\Psi\rangle > - 1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N}{q}+\sum_{i=q+1}^{k}Z_i^2\right)^{4/3}\left(\frac{N^2}{q}\right)^{4/3}. \tag{2.151}$$

For $Z_1 = \ldots = Z_q = N/q,\ Z_{q+1} = \ldots = Z_k = 0,\ 2 \leqslant q \ll N$,

$$\langle\Psi|H|\Psi\rangle\ > - 1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(N+\sum_{i=1}^{q}Z_i^2+\sum_{i=q+1}^{k}Z_i^2\right)^{4/3}$$

$$= - 1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(N+\sum_{i=1}^{q}Z_i^2+0\right)^{4/3}$$

$$= - 1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(N+\sum_{i=1}^{q}Z_i^2\right)^{4/3},$$

$$= - 1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{8/3}}{q^{4/3}}\left(\frac{q}{N}+1\right)^{4/3}$$

$$= - 1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^2}{q}\right)^{4/3}$$

$$\therefore \quad \langle\Psi|H|\Psi\rangle\ > - 1.89\underline{q}^{1/3}\left(\frac{me^4}{2\hbar^2}\right)N^2\left(\frac{N}{q^2}\right)^{2/3} \tag{2.152}$$

[For $Z_1 = ... = Z_q = N/q$, $2 \leqslant q \ll N$, the N dependence on the right-hand side of (2.150) is $N^{8/3}/q^{4/3}$. One may consider the situation of having q separate ions, each in its ground-state with nuclear charges $|e|Z_1, \ldots, |e|Z_q$ having each only one electron and having separately $(N-q)$ "free" electrons with arbitrarily small kinetic energies with all the N entitities, i.e., the q ions and the $(N-q)$ "free" electrons being infinitely separated from each other. This leads to an upper bound for the ground-state energy of such matter given by the well know expression $-\sum_i Z_i^2 me^4/2\hbar^2$ (which incidently is bounded above by $-Nme^4/2\hbar^2$ for $\sum_i Z_i = N$). From this and (2.149), we conclude that for $Z_1 = \ldots = Z_q = N/q,\ Z_{q+1} = \ldots = Z_k = 0,\ 2 \leqslant q \ll N$, the ground-state energy for fermionic matter will grow not slower than $-N^2$ and is obviously quite relevant physically to the *stability* of matter. It leads to the conclusion that as more and more matter is put together, thus increasing the number N of electrons, the number k of nuclei in such matter, as separate clusters, would necessariliy increase and not arbitrarily fuse together and their individual charges remain *bounded*. That is, as $N \to \infty$, then stability implies that $k \to \infty$ as well, and no nuclei may be found in matter that would carry arbitrarily large portions of the total charge available.

2.4 The Thomas-Fermi Atom in $3D$

The purpose of this section is to determine, as an estimate, an *explicit* expression for the ground-state energy $E(Z)$ for multi-electron neutral atoms as a function of the atomic number Z which will be used in sections 2.5, 2.6 to obtain another lower bound for the exact ground-state energy.

The Hamiltonian of a neutral atom consisting of Z electrons and a nucleus of charge $Z|e|$ is taken to be

$$H = \sum_{i=1}^{Z} \left(\frac{\mathbf{p}_i^2}{2m} - \frac{Ze^2}{r_i} \right) + \sum_{i<j}^{Z} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \tag{2.153}$$

where $r_i = |\mathbf{x}_i|$, and m is the mass of an electron.

In the Thomas-Fermi atom, the interaction that an electron at point $\mathbf{x}$ in an atom experiences is described by an effective spherically symmetric potential $V(\mathbf{x}) = V(r)$, $|\mathbf{x}| = r$ and the density of state is

$$n(\mathbf{x}) = \frac{q}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon}\, G\left(\mathbf{x}\tau; \mathbf{x}0\right) \mathrm{e}^{\mathrm{i}\xi\tau} \tag{2.154}$$

where $\underline{q} = 2s + 1 = 2$ is spin degeneracy or multiplicity and

$$G\left(\mathbf{x}\tau;\mathbf{x}'0\right) = \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3}\ \exp\mathrm{i}\left[\frac{\mathbf{p.(x-x')}}{\hbar} - \frac{\mathbf{p}^2}{2m}\tau - V(\mathbf{x})\tau\right] \qquad (2.155)$$

is the semi-classical expression for the Green function. Now let $\mathbf{x} = \mathbf{x'}$ to obtain

$$G\left(\mathbf{x}\tau;\mathbf{x}0\right) = \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3}\ \exp\mathrm{i}\left[-\frac{\mathbf{p}^2}{2m}\tau - V(\mathbf{x})\tau\right]. \qquad (2.156)$$

Substitute (2.156) into (2.154), to obtain

$$n(\mathbf{x}) = \frac{\underline{q}}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\tau}{\tau-\mathrm{i}\varepsilon}\int\frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3}\ \exp\mathrm{i}\left[\xi\tau - \frac{\mathbf{p}^2}{2m}\tau - V(\mathbf{x})\tau\right] \qquad (2.157)$$

which upon using the integral representation of the step function

$$\Theta(\xi) = \frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\tau}{\tau-\mathrm{i}\varepsilon}\,\mathrm{e}^{\mathrm{i}\xi\tau} \qquad (2.158)$$

gives

$$\Theta\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right) = \frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\tau}{\tau-\mathrm{i}\varepsilon}\ \exp\mathrm{i}\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right) \qquad (2.159)$$

and

$$\Theta\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right) = 1 \qquad (2.160)$$

when $0 < p < \sqrt{2m(\xi - V(\mathbf{x}))}$.

By applying (2.160) on right-hand side of (2.157), we obtain

$$\begin{aligned} n(\mathbf{x}) =& \underline{q}\int\frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3}\,\Theta\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right) \\ =& \frac{\underline{q}}{(2\pi\hbar)^3}\int_0^{\sqrt{2m(\xi-V)}} p^2\,\mathrm{d}p\int\mathrm{d}\Omega \end{aligned}$$

$$=\frac{\underline{q}}{(2\pi\hbar)^3}\int_0^{\sqrt{2m(\xi-V)}} p^2\,\mathrm{d}p\int_0^{\pi}\mathrm{d}\theta\sin\theta\int_0^{2\pi}\mathrm{d}\phi$$

$$=\frac{4\pi\underline{q}}{(2\pi\hbar)^3}\int_0^{\sqrt{2m(\xi-V(\mathbf{x})}} p^2\,\mathrm{d}p$$

$$=\frac{4\pi\underline{q}}{(2\pi\hbar)^3}\frac{\left(\sqrt{2m(\xi-V(\mathbf{x})}\right)^3}{3}$$

$$=\frac{4\underline{q}}{3\pi^2}\left(\frac{2m(\xi-V(\mathbf{x})}{(2\hbar)^2}\right)^{3/2} \tag{2.161}$$

where

$$\int_0^{\pi}\mathrm{d}\theta\sin\theta\int_0^{2\pi}\mathrm{d}\phi=4\pi. \tag{2.162}$$

The parameter ξ determines the boundary of TF atom defined by $\mathbf{x}=\mathbf{x}_B$. Since the electron density $n(\mathbf{x})=0$ for $|\mathbf{x}|\geqslant|\mathbf{x}_B|$. Refer to (2.161), to note that for $V(\mathbf{x}_B)=0$, and $n(\mathbf{x}_B)=0$ at the boundary. We get $\xi=0$. So that the density of electron in TF atom (3-dimensions) is

$$n(\mathbf{x})=\frac{4\underline{q}}{3\pi^2}\left(\frac{-2mV(\mathbf{x})}{(2\hbar)^2}\right)^{3/2} \tag{2.163}$$

where

$$\int \mathrm{d}^3\mathbf{x}\,n(\mathbf{x})=Z. \tag{2.164}$$

For spin $1/2$,

$$n(\mathbf{x})=\frac{1}{3\pi^2}\left(\frac{-2mV(\mathbf{x})}{\hbar^2}\right)^{3/2} \tag{2.165}$$

where the spin degeneracy is

$$\underline{q} =(2s+1) = 2. \tag{2.166}$$

For the sum of the kinetic energies of the electrons in 3-dimensions $(T[n])$, we have

$$\begin{aligned}
T[n] =& \sum_{\sigma} \int \mathrm{d}^3\mathbf{x}\, \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \left[\mathrm{i}\frac{\partial}{\partial\tau} - V(\mathbf{x})\right] G_{\sigma\sigma'}(\mathbf{x}t;\mathbf{x}0) \\
=& \underline{q} \int \mathrm{d}^3\mathbf{x}\, \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \left[\mathrm{i}\frac{\partial}{\partial\tau} - V(\mathbf{x})\right] G_{\sigma\sigma'}(\mathbf{x}t;\mathbf{x}0) \\
=& \underline{q} \int \mathrm{d}^3\mathbf{x}\, \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \left[\mathrm{i}\frac{\partial}{\partial\tau} - V(\mathbf{x})\right] \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \exp\left[-\mathrm{i}\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{x})\right)\tau\right] \\
=& \underline{q} \int \mathrm{d}^3\mathbf{x}\, \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \frac{\mathbf{p}^2}{2m} \exp\left[-\mathrm{i}\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{x})\right)\tau\right]
\end{aligned} \tag{2.167}$$

where

$$\left[\mathrm{i}\frac{\partial}{\partial\tau} - V(\mathbf{x})\right] \exp -\mathrm{i}\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{x})\right)\tau = \frac{\mathbf{p}^2}{2m} \exp -\mathrm{i}\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{x})\right)\tau \tag{2.168}$$

which upon using the integral representation of the step function

$$\Theta(\xi) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon}\, \mathrm{e}^{\mathrm{i}\xi\tau} \tag{2.169}$$

we obtain

$$\Theta\left(-\frac{\mathbf{p^2}}{2m} - V(\mathbf{x})\right) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \exp\left[\mathrm{i}\left(-\frac{\mathbf{p^2}}{2m} - V(\mathbf{x})\right)\tau\right] \tag{2.170}$$

and

$$\Theta\left(-\frac{\mathbf{p^2}}{2m} - V(\mathbf{x})\right) = 1 \tag{2.171}$$

when $0 < p < \sqrt{-2mV(\mathbf{x})}$.

Substitute (2.170) and (2.171) into (2.167), to obtain

$$\begin{aligned}
T[n] =& \underline{q} \int \mathrm{d}^3\mathbf{x} \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \frac{\mathbf{p}^2}{2m} \Theta\left(-\frac{\mathbf{p^2}}{2m} - V(\mathbf{x})\right) \\
=& \frac{\underline{q}}{(2\pi\hbar)^3} \int \mathrm{d}^3\mathbf{x} \int_0^{\sqrt{-2mV(\mathbf{x})}} \mathrm{d}p\, p^2 \frac{p^2}{2m} \int \mathrm{d}\Omega \\
=& \frac{\underline{q}}{(2\pi\hbar)^3} \int \mathrm{d}^3\mathbf{x} \int_0^{\sqrt{-2mV(\mathbf{x})}} \mathrm{d}p\, p^2 \frac{p^2}{2m} \int_0^{\pi} \mathrm{d}\theta \sin\theta \int_0^{2\pi} \mathrm{d}\phi \\
=& \frac{4\pi\underline{q}}{2m(2\pi\hbar)^3} \int \mathrm{d}^3\mathbf{x} \int_0^{\sqrt{-2mV(\mathbf{x})}} \mathrm{d}p\, p^4 \\
=& \frac{4\pi\underline{q}}{2m(2\pi\hbar)^3} \int \mathrm{d}^3\mathbf{x} \left.\frac{p^5}{5}\right|_0^{\sqrt{-2mV(\mathbf{x})}} \\
=& \frac{4\pi\underline{q}}{2m(2\pi\hbar)^3} \int \mathrm{d}^3\mathbf{x} \frac{(-2mV(\mathbf{x}))^{5/2}}{5} \\
=& \frac{4\pi\underline{q}}{10m} \int \mathrm{d}^3\mathbf{x} \frac{(-2mV(\mathbf{x}))^{5/2}}{(2\pi\hbar)^3} \\
=& \frac{4\pi\underline{q}}{10m} \int \mathrm{d}^3\mathbf{x} \,(-2mV(\mathbf{x})) \left(\frac{-2mV(\mathbf{x})}{(2\pi\hbar)^2}\right)^{3/2}.
\end{aligned} \tag{2.172}$$

We rewrite (2.163) as

$$-2mV(\mathbf{x}) = 4\hbar^2 \left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3} [n(\mathbf{x})]^{2/3} \tag{2.173}$$

and

$$\left(\frac{-2mV(\mathbf{x})}{(2\pi\hbar)^2}\right)^{3/2} = \left(\frac{1}{\pi^2}\right)^{3/2} \left(\frac{3\pi^2}{4\underline{q}}\right) [n(\mathbf{x})] \tag{2.174}$$

which upon substituting (2.173) and (2.174) into the right-hand side of (2.172), gives

$$\begin{aligned}
T[n] =& \frac{4\pi \underline{q}}{10m} \int \mathrm{d}^3\mathbf{x}\,(-2mV)\left(\frac{-2mV(\mathbf{x})}{(2\pi\hbar)^2}\right)^{3/2} \\
=& \frac{4\pi \underline{q}}{10m} \int \mathrm{d}^3\mathbf{x}\, 4\hbar^2 \left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3} [n(\mathbf{x})]^{2/3}\, \frac{1}{\pi^3} \left(\frac{3\pi^2}{4\underline{q}}\right) [n(\mathbf{x})] \\
=& \frac{4\pi \underline{q}}{10m} 4\hbar^2 \left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3} \left(\frac{3\pi^2}{4\underline{q}}\right) \frac{1}{\pi^3} \int \mathrm{d}^3\mathbf{x}\ [n(\mathbf{x})]^{2/3} [n(\mathbf{x})] \\
=& \frac{4\pi}{10m}\hbar^2 \left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3} 3\pi^2 \frac{1}{\pi^3} \int \mathrm{d}^3\mathbf{x}\ [n(\mathbf{x})]^{5/3} \\
=& \frac{4\hbar^2}{10\pi^2 m} \frac{(3\pi^2)^{5/3}}{(4\underline{q})^{2/3}} \int \mathrm{d}^3\mathbf{x}\ [n(\mathbf{x})]^{5/3} \\
=& \frac{16\underline{q}\hbar^2}{10\pi^2 m} \left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \int \mathrm{d}^3\mathbf{x}\ [n(\mathbf{x})]^{5/3} \\
\therefore \quad T[n] =& C_1 \int \mathrm{d}^3\mathbf{x}\ [n(\mathbf{x})]^{5/3} \qquad (2.175)
\end{aligned}$$

where

$$C_1 = \frac{16\underline{q}\hbar^2}{10\pi^2 m} \left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}. \qquad (2.176)$$

For spin $1/2$,

$$T[n] = \frac{\hbar^2 (3\pi^2)^{5/3}}{10\pi^2 m} \int \mathrm{d}^3\mathbf{x}\ [n(\mathbf{x})]^{5/3}. \qquad (2.177)$$

To obtain the ground-state energy $E(Z)$, refer (2.153) and from electrostatics, one may define the interaction of the electron-nucleus system in terms of the electron density, and add to it the kinetic energy term. We then obtain the *energy* functional $F[n]$

in 3-dimensions, dependent on the density $n(\mathbf{x})$, defined by

$$F[n] = \frac{16\underline{q}\hbar^2}{10\pi^2 m}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\int \mathrm{d}^3\mathbf{x}\ [n(\mathbf{x})]^{5/3} - Ze^2\int \mathrm{d}^3\mathbf{x}\frac{1}{|\mathbf{x}|}\, n(\mathbf{x})$$
$$+ \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\, n(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\, n(\mathbf{x}'). \tag{2.178}$$

Minimize (2.178), to obtain

$$\begin{aligned}
0 =& \frac{\delta F[n]}{\delta n(\mathbf{x})} \\
=& \frac{16\underline{q}\hbar^2}{10\pi^2 m}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\left(\frac{5}{3}\right)[n(\mathbf{x})]^{2/3} \\
& - \frac{Ze^2}{|\mathbf{x}|} + e^2\int \mathrm{d}^3\mathbf{x}'\frac{1}{|\mathbf{x}-\mathbf{x}'|}\, n(\mathbf{x}') \\
=& \frac{8\underline{q}\hbar^2}{3\pi^2 m}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}[n(\mathbf{x})]^{2/3} \\
& - \frac{Ze^2}{|\mathbf{x}|} + e^2\int \mathrm{d}^3\mathbf{x}'\frac{1}{|\mathbf{x}-\mathbf{x}'|}\, n(\mathbf{x}') \\
=& \frac{8\underline{q}\hbar^2}{3\pi^2 m}\left(\frac{3\pi^2}{4\underline{q}}\right)\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3}[n(\mathbf{x})]^{2/3} \\
& - \frac{Ze^2}{|\mathbf{x}|} + e^2\int \mathrm{d}^3\mathbf{x}'\frac{1}{|\mathbf{x}-\mathbf{x}'|}\, n(\mathbf{x}') \\
=& \frac{2\hbar^2}{m}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3}[n(\mathbf{x})]^{2/3} \\
& - \frac{Ze^2}{|\mathbf{x}|} + e^2\int \mathrm{d}^3\mathbf{x}'\frac{1}{|\mathbf{x}-\mathbf{x}'|}\, n(\mathbf{x}') \\
=& \frac{4\hbar^2}{2m}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3}[n(\mathbf{x})]^{2/3}
\end{aligned}$$

$$- \frac{Ze^2}{|\mathbf{x}|} + e^2 \int \mathrm{d}^3\mathbf{x}' \frac{1}{|\mathbf{x}-\mathbf{x}'|} \, n(\mathbf{x}')$$

$$-\frac{4\hbar^2}{2m} \left(\frac{3\pi^2}{4\underline{q}} \right)^{2/3} [n(\mathbf{x})]^{2/3} = - \frac{Ze^2}{|\mathbf{x}|} + e^2 \int \mathrm{d}^3\mathbf{x}' \frac{1}{|\mathbf{x}-\mathbf{x}'|} \, n(\mathbf{x}'). \tag{2.179}$$

From (2.173), we can rewrite

$$V(\mathbf{x}) = - \frac{4\hbar^2}{2m} \left(\frac{3\pi^2}{4\underline{q}} \right)^{2/3} [n(\mathbf{x})]^{2/3} . \tag{2.180}$$

which upon substituting (2.180) into the left-hand side of (2.179), gives

$$\begin{aligned} V(\mathbf{x}) &= - \frac{Ze^2}{|\mathbf{x}|} + e^2 \int \mathrm{d}^3\mathbf{x}' \frac{1}{|\mathbf{x}-\mathbf{x}'|} \, n(\mathbf{x}') \\ &= - \frac{Ze^2}{|\mathbf{x}|} \left[1 - \frac{|\mathbf{x}|}{Z} \int \mathrm{d}^3\mathbf{x}' \frac{1}{|\mathbf{x}-\mathbf{x}'|} \, n(\mathbf{x}') \right] \\ &= - \frac{Ze^2}{|\mathbf{x}|} \, F(\mathbf{x}) \end{aligned} \tag{2.181}$$

where

$$F(\mathbf{x}) = 1 - \frac{|\mathbf{x}|}{Z} \int \mathrm{d}^3\mathbf{x}' \frac{1}{|\mathbf{x}-\mathbf{x}'|} \, n(\mathbf{x}') \tag{2.182}$$

From (2.163), the density of electron in 3-dimensions

$$n(\mathbf{x}') = \frac{4\underline{q}}{3\pi^2} \left(\frac{-2mV(\mathbf{x}')}{(2\hbar)^2} \right)^{3/2} \tag{2.183}$$

where

$$\int \mathrm{d}^3\mathbf{x}' \, n(\mathbf{x}') = Z \tag{2.184}$$

and

$$\int \mathrm{d}^3\mathbf{x}' = \int_0^\infty dr'\; r'^2 \int_0^\pi \mathrm{d}\theta \sin\vartheta \int_0^{2\pi} \mathrm{d}\phi. \tag{2.185}$$

For the subsequent formulae we use the notation

$$|\mathbf{x}| = r. \tag{2.186}$$

Referring to (2.181), the effective potential in terms of the dimensionless function $f(r)$ is

$$V(r) = -\frac{Ze^2}{r}\, F(r). \tag{2.187}$$

To obtain the electron density in term on $f(r)$, substitute (2.187) into (2.163), to obtain

$$\begin{aligned}
n(r) =& \frac{4\underline{q}}{3\pi^2}\left(\frac{-2mV(r)}{(2\hbar)^2}\right)^{3/2} \\
=& \frac{4\underline{q}}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left[-V(r)\right]^{3/2} \\
=& \frac{4\underline{q}}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left[\frac{Ze^2}{r}\; F(r)\right]^{3/2} \\
=& \frac{4\underline{q}}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left[\frac{Ze^2}{r}\; F(r)\right]^{3/2}
\end{aligned} \tag{2.188}$$

and

$$\begin{aligned}
n(r') =& \frac{4\underline{q}}{3\pi^2}\left(\frac{-2mV(r')}{(2\hbar)^2}\right)^{3/2} \\
=& \frac{4\underline{q}}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left[-V(r')\right]^{3/2}
\end{aligned}$$

$$=\frac{4\underline{q}}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left[\frac{Ze^2}{r'}\,F(r')\right]^{3/2}$$

$$=\frac{4\underline{q}}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left[\frac{Ze^2}{r'}\,F(r')\right]^{3/2}. \tag{2.189}$$

By using (2.185), we rewrite (2.182) as

$$F(r) = 1 - \frac{r}{Z}\int_0^\infty dr'\,r'^2\int_0^\pi \mathrm{d}\vartheta\sin\vartheta\int_0^{2\pi}\mathrm{d}\phi\frac{1}{(r^2+r'^2-2rr'\cos\vartheta)^{1/2}}\,n(r'). \tag{2.190}$$

Substitute (2.189) into the right-hand side of (2.190), to obtain

$$\begin{aligned}F(r) =&1-\frac{r}{Z}\int_0^\infty dr'\,r'^2\left(\frac{4\underline{q}}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left[\frac{Ze^2}{r'}\,F(r')\right]^{3/2}\right)\\ &\times\left(\int_0^\pi \mathrm{d}\vartheta\sin\vartheta\int_0^{2\pi}\mathrm{d}\phi\frac{1}{(r^2+r'^2-2rr'\cos\vartheta)^{1/2}}\right)\\ =&1-\left(\frac{4\underline{q}}{3\pi^2}\right)\frac{r}{Z}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\int_0^\infty dr'\,r'^2\left[\frac{Ze^2}{r'}\,F(r')\right]^{3/2}\\ &\times\left(\int_0^\pi \mathrm{d}\vartheta\sin\vartheta\int_0^{2\pi}\mathrm{d}\phi\frac{1}{(r^2+r'^2-2rr'\cos\vartheta)^{1/2}}\right).\end{aligned} \tag{2.191}$$

Now we use the expansion (Gandshteyn and Ryzhik, 2000, p.980.)

$$\frac{1}{(1+\alpha^2-2t\alpha)^\nu} = \sum_{n=0}^{\infty} C_n^\nu(t)\,\alpha^n \tag{2.192}$$

where the polynomials $C_n^\nu(t)$ are generalizations of the Legendre polynomials.

Accordingly, we may expand $|\mathbf{x}-\mathbf{x}'|^{-\nu}$, as

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|^\nu} =\frac{1}{[r^2+r'^2-2rr'\cos\vartheta]^{\nu/2}}$$

$$
\begin{aligned}
=&\frac{1}{r_>^\nu \left[1+\left(\frac{r_<}{r_>}\right)^2-2\left(\frac{r_<}{r_>}\right)\cos\vartheta\right]^{\nu/2}} \\
=&\frac{1}{r_>^\nu}\frac{1}{\left[1+\left(\frac{r_<}{r_>}\right)^2-2\left(\frac{r_<}{r_>}\right)\cos\vartheta\right]^{\nu/2}} \\
=&\frac{1}{r_>^\nu}\sum_{n=0}^{\infty} C_n^{\nu/2}(t)\ \left(\frac{r_<}{r_>}\right)^n \\
=&\frac{1}{r_>^\nu}\sum_{n=0}^{\infty} C_n^{\nu/2}(\cos\vartheta)\ \left(\frac{r_<}{r_>}\right)^n
\end{aligned} \tag{2.193}
$$

where

$$
t=\cos\vartheta. \tag{2.194}
$$

For $|\mathbf{x}-\mathbf{x}'|^{-1}$, let $\nu=1$, we obtain

$$
\frac{1}{|\mathbf{x}-\mathbf{x}'|}=\frac{1}{r_>}\sum_{n=0}^{\infty} C_n^{1/2}(\cos\vartheta)\ \left(\frac{r_<}{r_>}\right)^n \tag{2.195}
$$

substitute (2.195) into (2.191), to obtain

$$
\begin{aligned}
F(r)=&1-\left(\frac{4\underline{q}}{3\pi^2}\right)\frac{r}{Z}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\int_0^\infty dr'\ r'^2\left[\frac{Ze^2}{r'}\ F(r')\right]^{3/2} \\
&\times\left(\int_0^\pi \mathrm{d}\vartheta\sin\vartheta\int_0^{2\pi}\mathrm{d}\phi\frac{1}{r_>}\sum_{n=0}^{\infty} C_n^{1/2}(\cos\vartheta)\ \left(\frac{r_<}{r_>}\right)^n\right) \\
=&1-\left(\frac{4\underline{q}}{3\pi^2}\right)\frac{r}{Z}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\int_0^\infty dr'\ r'^2\left[\frac{Ze^2}{r'}\ F(r')\right]^{3/2} \\
&\times\left(\int_0^\pi \mathrm{d}\vartheta\sin\vartheta\int_0^{2\pi}\mathrm{d}\phi\frac{1}{r_>}\sum_{n=0}^{\infty} C_n^{1/2}(\cos\vartheta)\ \left(\frac{r_<}{r_>}\right)^n\right)
\end{aligned}
$$

$$=1-\left(\frac{4q}{3\pi^2}\right)\frac{r}{Z}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\int_0^\infty dr'\, r'^2\left[\frac{Ze^2}{r'}\;F(r')\right]^{3/2}\;H(\vartheta) \tag{2.196}$$

where

$$H(\vartheta)=\int_0^\pi \mathrm{d}\vartheta\sin\vartheta\int_0^{2\pi}\mathrm{d}\phi\frac{1}{r_>}\sum_{n=0}^{\infty}C_n^{1/2}(\cos\vartheta)\,\left(\frac{r_<}{r_>}\right)^n. \tag{2.197}$$

The expression for $H(\vartheta)$ now may reduced as follows:

$$\begin{aligned}
H(\vartheta)=&\int\mathrm{d}\Omega\frac{1}{r_>}\sum_{n=0}^{\infty}C_n^{1/2}(\cos\vartheta)\left(\frac{r_<}{r_>}\right)^n\\
=&\int_0^\pi\mathrm{d}\vartheta\;(\sin\vartheta)\int_0^{2\pi}\mathrm{d}\phi\frac{1}{r_>}\sum_{n=0}^{\infty}C_n^{1/2}(\cos\vartheta)\left(\frac{r_<}{r_>}\right)^n\\
=&2\pi\int_0^\pi\mathrm{d}\vartheta\;(\sin\vartheta)\frac{1}{r_>}\sum_{n=0}^{\infty}C_n^{1/2}(\cos\vartheta)\left(\frac{r_<}{r_>}\right)^n\\
=&2\pi\frac{1}{r_>}\left(\frac{r_<}{r_>}\right)^0\int_0^\pi\mathrm{d}\vartheta\;C_0^{1/2}(\cos\vartheta)\,(\sin\vartheta)\\
&+2\pi\sum_{n=1}^{\infty}\frac{1}{r_>}\left(\frac{r_<}{r_>}\right)^n\int_0^\pi\mathrm{d}\vartheta\;C_n^{1/2}(\cos\vartheta)\,(\sin\vartheta)\,.
\end{aligned} \tag{2.198}$$

We now use integrals the combination of Gegenbauer polynomials C_n^ν and some elementary functions (Gandshteyn and Ryzhik, 2000, p.791.)

$$\int_0^\pi C_n^\nu(\cos\vartheta)(\sin\vartheta)^{2\nu}\mathrm{d}\vartheta=\begin{cases}0,\quad(n=1,2,3,\ldots)\\ 2^{-2\nu}\pi\Gamma(2\nu+1)\left[\Gamma(1+\nu)\right]^{-2},\quad(n=0).\end{cases} \tag{2.199}$$

In (2.199), let $\nu=1/2$ to obtain

$$\begin{aligned}
H(\vartheta)=&2\pi\frac{1}{r_>}\left(\frac{r_<}{r_>}\right)^0\int_0^\pi\;C_0^{1/2}(\cos\vartheta)\,(\sin\vartheta)\,\mathrm{d}\vartheta+0\\
=&2\pi\frac{1}{r_>}\;2^{-1}\pi\Gamma(2)\left[\Gamma(3/2)\right]^{-2}
\end{aligned}$$

$$=\frac{\pi^2}{r_>}\ \left[\frac{\pi^{1/2}}{2}\right]^{-2}$$

$$=\frac{4\pi}{r_>} \tag{2.200}$$

where

$$\Gamma(2) =1, \tag{2.201a}$$

$$\Gamma\left(\frac{3}{2}\right) =\frac{\pi^{1/2}}{2}. \tag{2.201b}$$

Substitute (2.200) into (2.196), to obtain

$$F(r) =1-\left(\frac{4\underline{q}}{3\pi^2}\right)\frac{r}{Z}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\int_0^\infty dr'\ r'^2\left[\frac{Ze^2}{r'}\ F(r')\right]^{3/2}\ H(\vartheta)$$

$$=1-\left(\frac{4\underline{q}}{3\pi^2}\right)\frac{r}{Z}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\int_0^\infty dr'\ r'^2\left[\frac{Ze^2F(r')}{r'}\right]^{3/2}\ \frac{4\pi}{r_>}$$

$$=1-4\pi r Z^{1/2}\left[e^2\right]^{3/2}\left(\frac{4\underline{q}}{3\pi^2}\right)\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\int_0^\infty dr'\ \frac{r'^2}{r_>}\left[\frac{F(r')}{r'}\right]^{3/2}. \tag{2.202}$$

We set

$$r =ax, \tag{2.203a}$$

$$r' =ax', \tag{2.203b}$$

$$F(r) =f(x), \tag{2.203c}$$

$$F(r') =f(x'). \tag{2.203d}$$

By applying (2.203) on the both-sides of (2.202), we obtain

$$\begin{aligned}
f(x) =&1-4\pi(ax)Z^{1/2}\left[e^2\right]^{3/2}\left(\frac{4\underline{q}}{3\pi^2}\right)\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\int_0^\infty d(ax')\,\frac{(ax')^2}{ax_>}\left[\frac{f(x')}{(ax)'}\right]^{3/2}\\
=&1-4\pi\frac{a^3}{a^{3/2}}Z^{1/2}\left[e^2\right]^{3/2}\left(\frac{4\underline{q}}{3\pi^2}\right)\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}x\int_0^\infty dx'\,\frac{x'^2}{x_>}\left[\frac{f(x')}{x'}\right]^{3/2}\\
=&1-a^{3/2}Z^{1/2}\left(\frac{2\pi\underline{q}}{3\pi^2}\right)\left(\frac{2me^2}{\hbar^2}\right)^{3/2}x\int_0^\infty dx'\,\frac{x'^2}{x_>}\left[\frac{f(x')}{x'}\right]^{3/2}\\
=&1-x\int_0^\infty dx'\,\frac{x'^2}{x_>}\left[\frac{f(x')}{x'}\right]^{3/2}
\end{aligned}\qquad(2.204)$$

where

$$a^{3/2}=\left(\frac{3\pi}{2\underline{q}}\right)\left(\frac{\hbar^2}{2me^2}\right)^{3/2}\frac{1}{Z^{1/2}}.\qquad(2.205)$$

From (2.205), we have

$$a=\left(\frac{3\pi}{2\underline{q}}\right)^{2/3}\left(\frac{\hbar^2}{2me^2}\right)\frac{1}{Z^{1/3}}\cong 0.8853a_0\frac{1}{Z^{1/3}}.\qquad(2.206)$$

and a_0 is the Bohr radius $\hbar^2/me^2$.

Use (2.203), in (2.187), to write the effective potential in term of the dimensionless function $f(x)$

$$V(x)=-\frac{Ze^2}{a}\frac{f(x)}{x}.\qquad(2.207)$$

Use (2.203), in (2.188) to obtain the electron density in term of $f(x)$

$$\begin{aligned}
n(r)=&\frac{4\underline{q}}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left[\frac{Ze^2}{r}F(r)\right]^{3/2}\\
=&\frac{4\underline{q}}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left(\frac{Ze^2}{a}\frac{f(x)}{x}\right)^{3/2}
\end{aligned}$$

$$=\frac{4q}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left(\frac{Ze^2}{a}\frac{f(x)}{x}\right)^{3/2}$$

$$n(r)\rightarrow n(x)=\frac{q}{6\pi^2}\left(\frac{2me^2}{\hbar^2}\right)^{3/2}\left(\frac{Z}{a}\right)^{3/2}\left(\frac{f(x)}{x}\right)^{3/2} \tag{2.208}$$

and

$$n(r')=\frac{4q}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left[\frac{Ze^2}{r'}\,F(r')\right]^{3/2}$$

$$=\frac{4q}{3\pi^2}\left(\frac{2m}{(2\hbar)^2}\right)^{3/2}\left(\frac{Ze^2}{a}\frac{f(x')}{x'}\right)^{3/2}$$

$$n(r)\rightarrow n(x)=\frac{q}{6\pi^2}\left(\frac{2me^2}{\hbar^2}\right)^{3/2}\left(\frac{Z}{a}\right)^{3/2}\left(\frac{f(x')}{x'}\right)^{3/2}. \tag{2.209}$$

We may also express the kinetic energy of the electrons in term of $f(x)$. Substitute (2.176), (2.185), (2.186) and (2.208) into (2.175), to obtain

$$T[n]=C_1\int \mathrm{d}^3\mathbf{x}\ [n(\mathbf{x})]^{5/3}$$

$$=C_1\int_0^\infty \mathrm{d}r\ r^2\ [n(r)]^{5/3}\int_0^\pi \mathrm{d}\theta\sin\theta\int_0^{2\pi}\mathrm{d}\phi$$

$$=C_1\int_0^\infty \mathrm{d}r\ r^2\ [n(r)]^{5/3}$$

$$=4\pi C_1 a\int_0^\infty \mathrm{d}x\ (ax)^2\ [n(x)]^{5/3}$$

$$=4\pi C_1 a^3\int_0^\infty \mathrm{d}x\ x^2\ [n(x)]^{5/3}$$

$$=4\pi C_1 a^3\int_0^\infty \mathrm{d}x\ x^2\left[\frac{q}{6\pi^2}\left(\frac{2me^2}{\hbar^2}\right)^{3/2}\left(\frac{Z}{a}\right)^{3/2}\left(\frac{f(x)}{x}\right)^{3/2}\right]^{5/3}$$

$$=4\pi C_1\left(\frac{q}{6\pi^2}\left(\frac{2me^2}{\hbar^2}\right)^{3/2}\right)^{5/3}Z^{5/2}a^{1/2}\int_0^\infty \mathrm{d}x\ x^2\left(\frac{f(x)}{x}\right)^{5/2}$$

$$=C_T Z^{5/2} a^{1/2} \int_0^\infty \mathrm{d}x \, \frac{[f(x)]^{5/2}}{x^{1/2}} \tag{2.210}$$

where

$$\begin{aligned}
C_T =& 4\pi \left[\frac{16\underline{q}\hbar^2}{10\pi^2 m} \left(\frac{3\pi^2}{4\underline{q}} \right)^{5/3} \right] \left[\frac{\underline{q}}{6\pi^2} \left(\frac{2me^2}{\hbar^2} \right)^{3/2} \right]^{5/3} \\
=& 4\pi \frac{16\underline{q}\hbar^2}{10\pi^2 m} \left(\frac{3\pi^2}{4\underline{q}} \right)^{5/3} \left(\frac{\underline{q}}{6\pi^2} \right)^{5/3} \left[\left(\frac{2me^2}{\hbar^2} \right)^{3/2} \right]^{5/3} \\
=& \frac{32\underline{q}\hbar^2}{5\pi m} \left(\frac{\pi^2}{4\underline{q}} \right)^{5/3} \left(\frac{\underline{q}}{2\pi^2} \right)^{5/3} \left(\frac{2me^2}{\hbar^2} \right)^{5/2} \\
=& \frac{\underline{q}\hbar^2}{5\pi m} \left(\frac{2me^2}{\hbar^2} \right)^{5/2} \\
=& \frac{2\underline{q}e^2}{5\pi} \left(\frac{2me^2}{\hbar^2} \right)^{3/2}
\end{aligned}$$

$$\therefore \quad C_T = \frac{2\underline{q}e^2}{5\pi} \left(\frac{2me^2}{\hbar^2} \right)^{3/2} . \tag{2.211}$$

From (2.178), we obtain for the electron-nucleus interaction part, the expression

$$\begin{aligned}
-Ze^2 \int \mathrm{d}^3\mathbf{x} \, \frac{1}{|\mathbf{x}|} \, n(\mathbf{x}) =& - Ze^2 \int_0^\infty \mathrm{d}r \, r^2 \, \frac{1}{r} \, n(r) \int_0^\pi \mathrm{d}\theta \sin\theta \int_0^{2\pi} \mathrm{d}\phi \\
=& - 4\pi Z e^2 \frac{a^3}{a} \int_0^\infty \mathrm{d}x \, x^2 \, \frac{1}{x} \, n(x) \\
=& - 4\pi Z e^2 a^2 \int_0^\infty \mathrm{d}x \, x \, n(x)
\end{aligned} \tag{2.212}$$

which upon substituting (2.208) into the right-hand side of (2.212), gives

$$-Ze^2 \int \mathrm{d}^3\mathbf{x} \, \frac{1}{|\mathbf{x}|} \, n(\mathbf{x}) = - 4\pi Z e^2 a^2 \left[\frac{\underline{q}}{6\pi^2} \left(\frac{2me^2}{\hbar^2} \right)^{3/2} \left(\frac{Z}{a} \right)^{3/2} \right]$$

$$
\begin{aligned}
&\times \int_0^\infty \mathrm{d}x\, x \left[\frac{f(x)}{x}\right]^{3/2} \\
&= -\frac{4\pi Z e^2 a^2 \underline{q}}{6\pi^2} \left(\frac{2me^2}{\hbar^2}\right)^{3/2} \left(\frac{Z}{a}\right)^{3/2} \\
&\times \int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{3/2}}{x^{1/2}} \\
&= -\frac{2\underline{q}e^2}{3\pi} \left(\frac{2me^2}{\hbar^2}\right)^{3/2} Z^{5/2} a^{1/2} \int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{3/2}}{x^{1/2}}
\end{aligned}
$$

$$
\therefore -Ze^2 \int \mathrm{d}^3\mathbf{x}\, \frac{1}{|\mathbf{x}|}\, n(\mathbf{x}) = -C_{Ze} Z^{5/2} a^{1/2} \int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{3/2}}{x^{1/2}} \tag{2.213}
$$

where

$$
C_{Ze} = \frac{2\underline{q}e^2}{3\pi} \left(\frac{2me^2}{\hbar^2}\right)^{3/2}. \tag{2.214}
$$

For the electron-electron interaction part, we have from (2.178) and by using, in the process (2.186)

$$
\begin{aligned}
&\frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, n(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, n(\mathbf{x}') \\
&= \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, n(\mathbf{x})\, g(\mathbf{x}') \\
&= \frac{e^2}{2} \int_0^\infty \mathrm{d}r\, r^2\, n(r) \int_0^\pi \mathrm{d}\theta \sin\theta \int_0^{2\pi} \mathrm{d}\phi\, g(\mathbf{x}') \\
&= \frac{e^2}{2} a^3 \int_0^\infty \mathrm{d}x\, x^2\, n(x) \int_0^\pi \mathrm{d}\theta \sin\theta \int_0^{2\pi} \mathrm{d}\phi\, g(\mathbf{x}')
\end{aligned} \tag{2.215}
$$

where

$$
g(\mathbf{x}') = \int \mathrm{d}^3\mathbf{x}' \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, n(\mathbf{x}'). \tag{2.216}
$$

Substitute (2.195) and (2.200) into (2.216), to obtain

$$g(r') = \int_0^\infty \mathrm{d}r'\, r'^2 \int \mathrm{d}\Omega\, \frac{1}{r_>} \sum_{n=0}^{\infty} C_n^{1/2}(\cos\vartheta) \left(\frac{r_<}{r_>}\right)^n n(r')$$

$$= \int_0^\infty \mathrm{d}r'\, r'^2\, n(r') \int \mathrm{d}\Omega\, \frac{1}{r_>} \sum_{n=0}^{\infty} C_n^{1/2}(\cos\vartheta) \left(\frac{r_<}{r_>}\right)^n$$

$$g(x') = \int_0^\infty \mathrm{d}x'\, a\,(ax')^2\, n(x') \int \mathrm{d}\Omega_3 \frac{1}{(ax_>)} \sum_{n=0}^{\infty} C_n^{1/2}(\cos\vartheta) \left(\frac{ax_<}{ax_>}\right)^n$$

$$= \int_0^\infty \mathrm{d}x'\, \frac{a^3}{a}\, x'^2\, n(x') \int \mathrm{d}\Omega \frac{1}{x_>} \sum_{n=0}^{\infty} C_n^{1/2}(\cos\vartheta) \left(\frac{x_<}{x_>}\right)^n$$

$$= a^2 \int_0^\infty \mathrm{d}x'\, x'^2\, n(x')\, H(\vartheta)$$

$$= a^2 \int_0^\infty \mathrm{d}x'\, x'^2\, n(x')\, \frac{4\pi}{x_>}$$

$$= 4\pi a^2 \int_0^\infty \mathrm{d}x'\, \frac{x'^2}{x_>}\, n(x') \tag{2.217}$$

where

$$H(\vartheta) = \int \mathrm{d}\Omega \frac{1}{x_>} \sum_{n=0}^{\infty} C_n^{1/2}(\cos\vartheta) \left(\frac{x_<}{x_>}\right)^n . \tag{2.218}$$

The expansion of $H(\vartheta)$ is

$$H(\vartheta) = \int \mathrm{d}\Omega \frac{1}{x_>} \sum_{n=0}^{\infty} C_n^{1/2}(\cos\vartheta) \left(\frac{x_<}{x_>}\right)^n$$

$$= \int_0^\pi \mathrm{d}\vartheta\, (\sin\vartheta) \int_0^{2\pi} \mathrm{d}\phi \frac{1}{x_>} \sum_{n=0}^{\infty} C_n^{1/2}(\cos\vartheta) \left(\frac{x_<}{x_>}\right)^n$$

$$= 2\pi \int_0^\pi \mathrm{d}\vartheta\, (\sin\vartheta) \frac{1}{x_>} \sum_{n=0}^{\infty} C_n^{1/2}(\cos\vartheta) \left(\frac{x_<}{x_>}\right)^n$$

$$
\begin{aligned}
=&2\pi\frac{1}{x_>}\left(\frac{x_<}{x_>}\right)^0\int_0^\pi \mathrm{d}\vartheta\, C_0^{1/2}(\cos\vartheta)\,(\sin\vartheta) \\
&+2\pi\sum_{n=1}^{\infty}\frac{1}{x_>}\left(\frac{x_<}{x_>}\right)^n\int_0^\pi \mathrm{d}\vartheta\, C_n^{1/2}(\cos\vartheta)\,(\sin\vartheta)\,.
\end{aligned}
\tag{2.219}
$$

To obtain the left-hand side of (2.219), by using (2.199) with $\nu = 1/2$ and applying to the left-hand side of (2.219), we obtain

$$
\begin{aligned}
H(\vartheta) =&2\pi\frac{1}{x_>}\left(\frac{x_<}{x_>}\right)^0\int_0^\pi C_0^{1/2}(\cos\vartheta)\,(\sin\vartheta)\,\mathrm{d}\vartheta + 0 \\
=&2\pi\frac{1}{x_>}\,2^{-1}\pi\Gamma(2)\,[\Gamma(3/2)]^{-2} \\
=&\frac{\pi^2}{x_>}\,\left[\frac{\pi^{1/2}}{2}\right]^{-2} \\
=&\frac{4\pi}{x_>}
\end{aligned}
\tag{2.220}
$$

where

$$
\Gamma(2) =1, \tag{2.221a}
$$

$$
\Gamma(3/2) =\frac{\pi^{1/2}}{2}. \tag{2.221b}
$$

Substitute (2.220) into (2.217), we obtain

$$
\begin{aligned}
g(x') =&a^2\int_0^\infty \mathrm{d}x'\; x'^2\; n(x')\; H(\vartheta) \\
=&a^2\int_0^\infty \mathrm{d}x'\; x'^2\; n(x')\;\frac{4\pi}{x_>} \\
=&4\pi a^2\int_0^\infty \mathrm{d}x'\;\frac{x'^2}{x_>}\; n(x')
\end{aligned}
\tag{2.222}
$$

which upon substituting (2.209) into the right-hand side of (2.217), gives

$$\begin{aligned} g(x') =& 4\pi a^2 \int_0^\infty \mathrm{d}x' \, \frac{x'^2}{x_>} \, n(x') \\ =& 4\pi a^2 \int_0^\infty \mathrm{d}x' \, \frac{x'^2}{x_>} \frac{q}{6\pi^2} \left(\frac{2me^2}{\hbar^2}\right)^{3/2} \left(\frac{Z}{a}\right)^{3/2} \left(\frac{f(x')}{x'}\right)^{3/2} \\ =& 4\pi \frac{q}{6\pi^2} \left(\frac{2me^2}{\hbar^2}\right)^{3/2} Z^{3/2} a^{1/2} \int_0^\infty \mathrm{d}x' \, \frac{x'^2}{x_>} \left(\frac{f(x')}{x'}\right)^{3/2} \\ =& \frac{2q}{3\pi} \left(\frac{2me^2}{\hbar^2}\right)^{3/2} Z^{3/2} a^{1/2} \int_0^\infty \mathrm{d}x' \, \frac{x'^2}{x_>} \left(\frac{f(x')}{x'}\right)^{3/2} . \end{aligned} \tag{2.223}$$

Finally substitute (2.208), (2.209) and (2.223) into (2.215), to obtain

$$\begin{aligned} &\frac{e^2}{2} \int \mathrm{d}^3\mathbf{x} \, \mathrm{d}^3\mathbf{x}' \, n(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \, n(\mathbf{x}') \\ &\quad = \frac{e^2}{2} \, a^3 \int_0^\infty \mathrm{d}x \, x^2 \, n(x) \int_0^\pi \mathrm{d}\theta \sin\theta \int_0^{2\pi} \mathrm{d}\phi \, g(\mathbf{x}') \\ &\quad = \frac{e^2}{2} \, a^3 \, 4\pi \int_0^\infty \mathrm{d}x \, x^2 \, n(x) \, g(\mathbf{x}') \\ &\quad = 2\pi e^2 a^3 \int_0^\infty \mathrm{d}x \, x^2 \, n(x) \, g(\mathbf{x}') \\ &\quad = 2\pi e^2 \frac{2q}{3\pi} \left(\frac{2me^2}{\hbar^2}\right)^{3/2} Z^{3/2} a^3 a^{1/2} \\ &\qquad \times \left(\int_0^\infty \mathrm{d}x \, x^2 \, n(x) \int_0^\infty \mathrm{d}x' \, \frac{x'^2}{x_>} \left(\frac{f(x')}{x'}\right)^{3/2} \right) \\ &\quad = \frac{4qe^2}{3} \left(\frac{2me^2}{\hbar^2}\right)^{3/2} \left(\frac{q}{6\pi^2}\right) \left(\frac{2me^2}{\hbar^2}\right)^{3/2} \left(\frac{Z}{a}\right)^{3/2} Z^{3/2} a^{7/2} \\ &\qquad \times \left(\int_0^\infty \mathrm{d}x \, x^2 \left(\frac{f(x)}{x}\right)^{3/2} \int_0^\infty \mathrm{d}x' \, \frac{x'^2}{x_>} \left(\frac{f(x')}{x'}\right)^{3/2} \right) \end{aligned}$$

$$
\begin{aligned}
&= \left(\frac{2\underline{q}^2 e^2}{9\pi^2}\right)\left(\frac{2me^2}{\hbar^2}\right)^3 Z^3 a^2 \\
&\quad \times \left(\int_0^\infty \mathrm{d}x\, x^2 \left(\frac{f(x)}{x}\right)^{3/2} \int_0^\infty \mathrm{d}x'\, \frac{x'^2}{x_>} \left(\frac{f(x')}{x'}\right)^{3/2}\right) \\
&= C_e Z^3 a^2 \int_0^\infty \mathrm{d}x\, x^2 \left(\frac{f(x)}{x}\right)^{3/2} \int_0^\infty \mathrm{d}x'\, \frac{x'^2}{x_>} \left(\frac{f(x')}{x'}\right)^{3/2}
\end{aligned} \tag{2.224}
$$

where

$$
C_e = \left(\frac{2\underline{q}^2 e^2}{9\pi^2}\right)\left(\frac{2me^2}{\hbar^2}\right)^3 . \tag{2.225}
$$

Adding the contributions, (2.210), (2.213) and (2.224), for the energy functional (2.178), we obtain for the ground-state energy $E(Z)$ the explicit expression :

$$
\begin{aligned}
E(Z) =& \frac{16\underline{q}\hbar^2}{10\pi^2 m}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \int \mathrm{d}^3\mathbf{x}\, [n(\mathbf{x})]^{5/3} - Ze^2 \int \mathrm{d}^3\mathbf{x} \frac{1}{|\mathbf{x}|}\, n(\mathbf{x}) \\
&+ \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, n(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, n(\mathbf{x}') \\
=& C_T Z^{5/2} a^{1/2} \int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{5/2}}{x^{1/2}} - C_{Ze} Z^{5/2} a^{1/2} \int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{3/2}}{x^{1/2}} \\
&+ C_e Z^3 a^2 \int_0^\infty \mathrm{d}x\, x^2 \left[\frac{f(x)}{x}\right]^{3/2} \int_0^\infty \mathrm{d}x'\, \frac{x'^2}{x_>} \left[\frac{f(x')}{x'}\right]^{3/2} .
\end{aligned} \tag{2.226}
$$

To evaluate the above, first we have to find the differential equation satisfied by $f(x)$. From (2.204), we can rewrite as

$$
\begin{aligned}
f(x) =& 1 - x \int_0^\infty dx'\, \frac{x'^2}{x_>} \left[\frac{f(x')}{x'}\right]^{3/2} \\
=& 1 - x \int_0^x dx'\, \frac{x'^2}{x} \left[\frac{f(x')}{x'}\right]^{3/2} - x \int_x^\infty dx'\, \frac{x'^2}{x'} \left[\frac{f(x')}{x'}\right]^{3/2}
\end{aligned}
$$

$$=1-\int_0^x dx'\ [f(x')]^{3/2}\, x'^{1/2}-x\int_x^\infty dx'\frac{[f(x')]^{3/2}}{x'^{1/2}}. \tag{2.227}$$

satisfying the boundary condition (B.C.)

$$f(0)=1. \tag{2.228}$$

By using B.C. in (2.228)and (2.203), Applying to (2.187), we obtain the later boundary condition corresponding to

$$V(r)\sim -\frac{Ze^2}{r} \tag{2.229}$$

for $r\to 0$.

By differentiating with respect to x on the both-sides of (2.227), we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}x}f(x)=&-\frac{\mathrm{d}}{\mathrm{d}x}\left(\int_0^x dx'\ [f(x')]^{3/2}\, x'^{1/2}\right)-\frac{\mathrm{d}}{\mathrm{d}x}\left(x\int_x^\infty dx'\frac{[f(x')]^{3/2}}{x'^{1/2}}\right)\\ =&-\frac{\mathrm{d}}{\mathrm{d}x}\int_0^x dx'\ [f(x')]^{3/2}\, x'^{1/2}-x\frac{\mathrm{d}}{\mathrm{d}x}\int_x^\infty dx'\frac{[f(x')]^{3/2}}{x'^{1/2}}\\ &-\int_x^\infty dx'\frac{[f(x')]^{3/2}}{x'^{1/2}}.\end{aligned} \tag{2.230}$$

Consider the differentiation of definite integral with respect to a parameter

$$\frac{\mathrm{d}}{\mathrm{d}x}\int_b^x \mathrm{d}x'\, g(x') = g(x), \tag{2.231a}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\int_x^b \mathrm{d}x'\, g(x') = -\, g(x). \tag{2.231b}$$

By applying (2.231) to the right-hand side of (2.35), we have

$$\frac{\mathrm{d}}{\mathrm{d}x}f(x)=-\frac{\mathrm{d}}{\mathrm{d}x}\int_0^x dx'\ [f(x')]^{3/2}\, x'^{1/2}-x\frac{\mathrm{d}}{\mathrm{d}x}\int_x^\infty dx'\frac{[f(x')]^{3/2}}{x'^{1/2}}$$

$$
\begin{aligned}
&- \int_x^\infty dx' \frac{[f(x')]^{3/2}}{x'^{1/2}} \\
&= - [f(x)]^{3/2} x^{1/2} + [f(x)]^{3/2} x^{1/2} - \int_x^\infty dx' \frac{[f(x')]^{3/2}}{x'^{1/2}} \\
&= - \int_x^\infty dx' \frac{[f(x')]^{3/2}}{x'^{1/2}} .
\end{aligned}
\tag{2.232}
$$

By differentiating with respect to x again on the both-sides of (2.232), we obtain

$$
\frac{\mathrm{d}^2}{\mathrm{d}x^2} f(x) = - \frac{\mathrm{d}}{\mathrm{d}x} \int_x^\infty dx' \frac{[f(x')]^{3/2}}{x'^{1/2}} .
\tag{2.233}
$$

By applying (2.231) to the right-hand side of (2.233) and from the appropriate B.C., we have

$$
\frac{\mathrm{d}^2}{\mathrm{d}x^2} f(x) = \frac{[f(x)]^{3/2}}{x^{1/2}} \ , \ f(0) = 1.
\tag{2.234}
$$

From the normalization condition (2.164) and (2.208), we have

$$
\begin{aligned}
Z =& \int \mathrm{d}^3\mathbf{x} \, n(\mathbf{x}) \\
=& a^3 \int_0^\infty dx \, x^2 \, n(x) \int_0^\pi \mathrm{d}\theta \sin\theta \int_0^{2\pi} \mathrm{d}\phi \\
=& 4\pi a^3 \int_0^\infty dx \, x^2 \, n(x) \\
=& \frac{4\pi a^3 \underline{q}}{6\pi^2} \left(\frac{2me^2}{\hbar^2} \right)^{3/2} \left(\frac{Z}{a} \right)^{3/2} \int_0^\infty dx \, x^2 \left(\frac{f(x)}{x} \right)^{3/2} \\
=& \frac{2\underline{q}}{3\pi} \left(\frac{2me^2}{\hbar^2} \right)^{3/2} (Za)^{3/2} \int_0^\infty dx \, x \frac{[f(x)]^{3/2}}{x^{1/2}} .
\end{aligned}
\tag{2.235}
$$

which upon substituting (2.206) and (2.234) into the right-hand side of (2.235), we

obtain

$$Z = \frac{2\underline{q}Z^{3/2}}{3\pi}\left(\frac{2me^2}{\hbar^2}\right)^{3/2}\left(\left(\frac{3\pi}{2\underline{q}}\right)^{2/3}\left(\frac{\hbar^2}{2me^2}\right)\frac{1}{Z^{1/3}}\right)^{3/2}\lim_{x_B\to\infty}\int_0^{x_B} dx\, x f''(x)$$

$$= Z\lim_{x_B\to\infty}\int_0^{x_B} dx\, x f''(x). \tag{2.236}$$

From (2.236) and with B.C, we obtain

$$\begin{aligned}
1 &= \lim_{x_B\to\infty}\int_0^{x_B} dx\; x f''(x) \\
&= \lim_{x_B\to\infty}\int_0^{x_B} x\, d(f'(x)) \\
&= \lim_{x_B\to\infty}\left[x f'(x)|_0^{x_B} - \int_0^{x_B} f'(x)\, dx\right] \\
&= \lim_{x_B\to\infty}\left[x f'(x)|_0^{x_B} - f(x)|_0^{x_B}\right] \\
&= \lim_{x_B\to\infty}\left[(x_B f'(x_B) - 0) - (f(x_B) - f(0))\right] \\
&= \lim_{x_B\to\infty}\left[x_B f'(x_B - (f(x_B) + 1)\right] \\
0 &= \lim_{x_B\to\infty}\left[x_B f'(x_B) - f(x_B)\right].
\end{aligned} \tag{2.237}$$

From (2.237) we obtain that

$$\lim_{x_B\to\infty} x_B f'(x_B) = 0, \tag{2.238a}$$

$$\lim_{x_B\to\infty} f(x_B) = 0. \tag{2.238b}$$

To find the asymptotic behavior for $x \to \infty$, we set

$$f(x) = \beta x^{-\alpha} \tag{2.239}$$

and substitute $f(x)$ into left-hand side of (2.234), to obtain

$$\begin{aligned} \frac{\mathrm{d}^2}{\mathrm{d}x^2} f(x) &= -\beta\alpha(-\alpha - 1)x^{-\alpha-2} \\ &= \left(\beta\alpha^2 + \beta\alpha\right)\ x^{-\alpha-2} \end{aligned} \tag{2.240}$$

and then substitute $f(x)$ into right-hand side of (2.234), to obtain

$$\begin{aligned} \frac{[f(x)]^{3/2}}{x^{1/2}} =& \frac{\beta^{3/2}\left[x^{-\alpha}\right]^{3/2}}{x^{1/2}} \\ =& \beta^{3/2} x^{(-3\alpha-1)/2}. \end{aligned} \tag{2.241}$$

Substitute (2.240) and (2.241) into (2.234), to obtain the equation

$$\left(\beta\alpha^2 + \beta\alpha\right)\ x^{-\alpha-2} = \beta^{3/2} x^{(-3\alpha-1)/2}. \tag{2.242}$$

From (2.242), this gives

$$\begin{aligned} -\alpha - 2 =& \frac{-3\alpha - 1}{2} \\ \alpha =& 3 \end{aligned} \tag{2.243}$$

and

$$\begin{aligned} \left(\beta\alpha^2 + \beta\alpha\right) =& \beta^{3/2} \\ \beta^{1/2} =& 12 \end{aligned}$$

$$\beta = 144. \tag{2.244}$$

Substitute α and β into (2.239) to derive

$$f(x) = \frac{144}{x^3} \tag{2.245}$$

for $x \to \infty$.

Eq.(2.238) and (2.245) shows that f(x) vanishes at infinity and that $x_B = \infty$, then also implies that $f'(x) \to 0$ for $x \to \infty$. Accordingly, from (2.234), we can rewrite

$$f'(\infty) - f'(0) = \int_0^\infty \mathrm{d}x \, \frac{[f(x)]^{3/2}}{x^{1/2}}$$

$$f'(0) = -\int_0^\infty \mathrm{d}x \, \frac{[f(x)]^{3/2}}{x^{1/2}} \; < \; 0 \tag{2.246}$$

i.e., it is negative.

Actually the function $f(x)$ vanishes only at infinity. This is easily seen by integrating the differential equation (2.234), over x, between two points $x_1 < x_2$, to obtain

$$f'(x_2) - f'(x_1) = \int_{x_1}^{x_2} \mathrm{d}x \, \frac{\left[f(x)\right]^{3/2}}{x^{1/2}} \tag{2.247}$$

and hence conclude that with $f'(0) < 0$, that

$$f'(0) \leqslant \cdots \leqslant f'(x_1) \leqslant \cdots \leqslant f'(x_2) \leqslant \cdots \leqslant 0 \tag{2.248}$$

for $0 < \cdots < x_1 < \cdots < x_2 < \cdots < \infty$. That is, $f(x)$, starting at $f(0) = 1$, is monotonically non-increasing, approaching zero for $x \to \infty$. The function $f(x)$ cannot vanish for finite x and then increase again as this will be in contradiction with (2.248). Also note that the differential equation (2.234) implies that

$$f''(x) \xrightarrow[x \to \infty]{} 0. \tag{2.249}$$

The function $f(x)$ and its derivative $f'(x)$ may be then determined numerically from the differential equation in (2.234) with the boundary conditions $f(0) = 1$, $f(x) \to 0$ for $x \to \infty$. In particular (Kobayashi, Matsukuma, Nagai and Umeda, 1955), $f'(0) \cong -1.58807$. For the integral in (2.246), we have numerically

$$\int_0^\infty \mathrm{d}x \, \frac{\left[f(x)\right]^{3/2}}{x^{1/2}} = -f'(0) \cong 1.58807. \tag{2.250}$$

By using (2.226), (2.247) and (2.250), we can compute the ground-state energy $E(Z)$.

For the kinetic energy term, the first term on the right-hand side of (2.226), by using (2.206), (2.211) and (2.247), we obtain

$$\begin{aligned} T[n] =& C_T Z^{5/2} a^{1/2} \int_0^\infty \mathrm{d}x \, \frac{[f(x)]^{5/2}}{x^{1/2}} \\ =& C_T Z^{5/2} \left(\left(\frac{3\pi}{2\underline{q}}\right)^{2/3} \left(\frac{\hbar^2}{2me^2}\right) \frac{1}{Z^{1/3}} \right)^{1/2} \int_0^\infty \mathrm{d}x \, \frac{[f(x)]^{5/2}}{x^{1/2}} \\ =& C_T Z^{7/3} \left(\frac{3\pi}{2\underline{q}}\right)^{1/3} \left(\frac{\hbar^2}{2me^2}\right)^{1/2} \int_0^\infty \mathrm{d}x \, \frac{[f(x)]^{5/2}}{x^{1/2}} \\ =& \frac{2\underline{q}e^2}{5\pi} \left(\frac{2me^2}{\hbar^2}\right)^{3/2} Z^{7/3} \left(\frac{3\pi}{2\underline{q}}\right)^{1/3} \left(\frac{\hbar^2}{2me^2}\right)^{1/2} \int_0^\infty \mathrm{d}x \, \frac{[f(x)]^{5/2}}{x^{1/2}} \\ =& \left(\frac{3}{5}\right) \left(\frac{2\underline{q}}{3\pi}\right)^{2/3} \left(\frac{2me^4}{\hbar^2}\right) Z^{7/3} \int_0^\infty \mathrm{d}x \, \frac{[f(x)]^{5/2}}{x^{1/2}}. \end{aligned} \tag{2.251}$$

To obtain above, consider the integral term on the right-hand side of (2.251), and set

$$u = [f(x)]^{5/2}, \tag{2.252a}$$

$$\mathrm{d}v = 2\mathrm{d}\left(x^{1/2}\right) = x^{-1/2}\,\mathrm{d}x, \tag{2.252b}$$

$$v = 2x^{1/2}. \tag{2.252c}$$

By using the appropriate B.C and applying (2.252) to the integral term on the right-hand side of (2.251), we obtain

$$\begin{aligned}\int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{5/2}}{x^{1/2}} =& 2\int_0^\infty \mathrm{d}\left(x^{1/2}\right)\ [f(x)]^{5/2} \\ =& 2\lim_{x_B\to\infty}\left[x^{1/2}\,[f(x)]^{5/2}\Big|_0^{x_B} - \int_0^\infty \mathrm{d}\left([f(x)]^{5/2}\right)x^{1/2}\right] \\ =& 2\lim_{x_B\to\infty}(x_B^{1/2}\,[f(x_B)]^{5/2} - 0) - 2\int_0^\infty \mathrm{d}\left([f(x)]^{5/2}\right)x^{1/2} \\ =& -2\int_0^\infty \mathrm{d}\left([f(x)]^{5/2}\right)x^{1/2} \\ =& -5\int_0^\infty \mathrm{d}x\ [f(x)]^{3/2}\ f'(x)\,x^{1/2} \end{aligned} \tag{2.253}$$

where (from (2.238) and (2.245))

$$2\lim_{x_B\to\infty} x_B^{1/2}\,[f(x_B)]^{5/2} = 0 \tag{2.254}$$

and

$$2\,\mathrm{d}\left([f(x)]^{5/2}\right) = 5\,\mathrm{d}x\ [f(x)]^{3/2}\ f'(x)\,x^{1/2}. \tag{2.255}$$

Accordingly,

$$\begin{aligned}\int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{5/2}}{x^{1/2}} =& -5\int_0^\infty \mathrm{d}x\ [f(x)]^{3/2}\ f'(x)\,\frac{x^{1/2}x^{1/2}}{x^{1/2}} \\ =& -5\int_0^\infty \mathrm{d}x\,\frac{[f(x)]^{3/2}}{x^{1/2}}\,f'(x)\,x \\ =& -5\int_0^\infty \mathrm{d}x\, f''(x)\,f'(x)\,x \\ =& -\frac{5}{2}\int_0^\infty \mathrm{d}\,[f'(x)]^2\ x \end{aligned} \tag{2.256}$$

where

$$\mathrm{d}x\ f''(x)\ f'(x) = \frac{1}{2}\,\mathrm{d}\left[f'(x)\right]^2 \tag{2.257}$$

Now let

$$u = x, \tag{2.258a}$$

$$\mathrm{d}v = \mathrm{d}\left[f'(x)\right]^2, \tag{2.258b}$$

$$v = \left[f'(x)\right]^2 \tag{2.258c}$$

which upon applying to the right-hand side of (2.195), gives

$$\begin{aligned}\int_0^\infty \mathrm{d}x\ \frac{\left[f(x)\right]^{5/2}}{x^{1/2}} &= -\frac{5}{2}\int_0^\infty \mathrm{d}\left[f'(x)\right]^2\ x \\ &= -\frac{5}{2}\left[x\ \left[f'(x)\right]^2\Big|_0^\infty - \int_0^\infty \mathrm{d}x\ \left[f'(x)\right]^2\right] \\ &= -\frac{5}{2}\lim_{x_B\to\infty}\Big(x_B\ \left[f'(x_B)\right]^2 - 0\Big) + \frac{5}{2}\int_0^\infty \mathrm{d}x\ \left[f'(x)\right]^2 \\ &= \frac{5}{2}\int_0^\infty \mathrm{d}x\ \left[f'(x)\right]^2. \end{aligned} \tag{2.259}$$

Again consider the left-hand side of (2.259) and note that

$$\begin{aligned}\int_0^\infty \mathrm{d}x\ \frac{\left[f(x)\right]^{5/2}}{x^{1/2}} &= \int_0^\infty \mathrm{d}x\ \frac{\left[f(x)\right]^{3/2}}{x^{1/2}}\ f(x) \\ &= \int_0^\infty \mathrm{d}x\ f''(x)\ f(x). \end{aligned} \tag{2.260}$$

With the notations

$$u = f(x), \tag{2.261a}$$

$$\mathrm{d}v = \mathrm{d}\left[f'(x)\right], \tag{2.261b}$$

$$v = f'(x) \tag{2.261c}$$

as applied to the right-hand side of (2.260), we obtain

$$\begin{aligned}
\int_0^\infty \mathrm{d}x\ \frac{[f(x)]^{5/2}}{x^{1/2}} &= \int_0^\infty \mathrm{d}x\ f''(x)\ f(x) \\
&= \int_0^\infty \mathrm{d}\left[f'(x)\right]\ f(x) \\
&= \lim_{x_B\to\infty} f(x)\ f'(x)\Big|_0^{x_B} - \int_0^\infty \mathrm{d}\left[f(x)\right]\ f'(x) \\
&= \lim_{x_B\to\infty} \left[f(x_B)\ f'(x_B) - f(0)\ f'(0)\right] - \int_0^\infty \mathrm{d}x\ \left[f(x)\right]^2 \\
&= -\,f'(0) - \int_0^\infty \mathrm{d}x\ \left[f(x)\right]^2 .
\end{aligned} \tag{2.262}$$

From (2.259), we can rewrite as

$$\int_0^\infty \mathrm{d}x\ \left[f'(x)\right]^2 = \frac{2}{5}\int_0^\infty \mathrm{d}x\ \frac{[f(x)]^{5/2}}{x^{1/2}} \tag{2.263}$$

which upon substituting (2.263) into the right-hand side of (2.262), we obtain

$$\begin{aligned}
\int_0^\infty \mathrm{d}x\ \frac{[f(x)]^{5/2}}{x^{1/2}} &= -\,f'(0) - \int_0^\infty \mathrm{d}x\ \left[f(x)\right]^2 \\
&= -\,f'(0) - \frac{2}{5}\int_0^\infty \mathrm{d}x\ \frac{[f(x)]^{5/2}}{x^{1/2}} \\
\int_0^\infty \mathrm{d}x\ \frac{[f(x)]^{5/2}}{x^{1/2}} &= -\,\frac{5}{7}f'(0).
\end{aligned} \tag{2.264}$$

Finally, substitute (2.264) into the right-hand side of (2.251), to obtain for the kinetic energy term

$$T[n] = \left(\frac{3}{5}\right)\left(\frac{2\underline{q}}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right) Z^{7/3}\int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{5/2}}{x^{1/2}}$$

$$= -\left(\frac{3}{7}\right)\left(\frac{2\underline{q}}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right) Z^{7/3}\, f'(0). \tag{2.265}$$

For the electron-nucleus interaction part, the second term on the right-hand side of (2.226) we obtain, by using (2.206), (2.213), (2.214) and (2.247),

$$E_{Ze} = -\, Ze^2 \int \mathrm{d}^3\mathbf{x}\, \frac{1}{|\mathbf{x}|}\, n(\mathbf{x})$$

$$= -\, C_{Ze} Z^{5/2} a^{1/2} \int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{3/2}}{x^{1/2}}$$

$$= C_{Ze} Z^{5/2} a^{1/2} f'(0)$$

$$= C_{Ze} Z^{5/2} \left(\left(\frac{3\pi}{2\underline{q}}\right)^{2/3}\left(\frac{\hbar^2}{2me^2}\right)\frac{1}{Z^{1/3}}\right)^{1/2} f'(0)$$

$$= C_{Ze}\left(\frac{3\pi}{2\underline{q}}\right)^{1/3}\left(\frac{\hbar^2}{2me^2}\right)^{1/2} Z^{7/3} f'(0)$$

$$= \frac{2\underline{q}e^2}{3\pi}\left(\frac{2me^2}{\hbar^2}\right)^{3/2}\left(\frac{3\pi}{2\underline{q}}\right)^{1/3}\left(\frac{\hbar^2}{2me^2}\right)^{1/2} Z^{7/3} f'(0)$$

$$= -\, \frac{2\underline{q}e^2}{3\pi}\left(\frac{2me^2}{\hbar^2}\right)\left(\frac{3\pi}{2\underline{q}}\right)^{1/3} Z^{7/3} f'(0)$$

$$E_{Ze} = \left(\frac{2\underline{q}}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right) Z^{7/3} f'(0). \tag{2.266}$$

Finally, for the electron-electron interaction part, the third term on the right-hand side of (2.226) we obtain, by using (2.206), (2.213), (2.214) and (2.247),

$$
\begin{aligned}
E_{ee}(Z) =& C_e Z^3 a^2 \int_0^\infty \mathrm{d}x\, x^2 \left[\frac{f(x)}{x}\right]^{3/2} \int_0^\infty \mathrm{d}x'\, x'^2 \frac{1}{x_>} \left[\frac{f(x')}{x'}\right]^{3/2} \\
=& C_e Z^3 a^2 \left[\int_0^\infty \mathrm{d}x\, x^2 \frac{1}{x} \left[\frac{f(x)}{x}\right]^{3/2} \int_0^x \mathrm{d}x'\, x'^2 \left[\frac{f(x')}{x'}\right]^{3/2} \right. \\
& \left. + \int_0^\infty \mathrm{d}x\, x^2 \left[\frac{f(x)}{x}\right]^{3/2} \int_x^\infty \mathrm{d}x'\, x'^2 \frac{1}{x'} \left[\frac{f(x')}{x'}\right]^{3/2} \right] \\
=& C_e Z^3 a^2 \left[\int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{3/2}}{x^{1/2}} \int_0^x \mathrm{d}x'\, x'^{1/2} \, [f(x')]^{3/2} \right. \\
& \left. + \int_0^\infty \mathrm{d}x\, x^{1/2} \, [f(x)]^{3/2} \int_x^\infty \mathrm{d}x'\, \frac{[f(x')]^{3/2}}{x'^{1/2}} \right].
\end{aligned}
\tag{2.267}
$$

The obtain an explicit analytical expression for the following integral, consider the first term on the right-hand side of (2.267) :

$$
\begin{aligned}
& \int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{3/2}}{x^{1/2}} \int_0^x \mathrm{d}x'\, x'^{1/2} \, [f(x')]^{3/2} \\
& = \int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{3/2}}{x^{1/2}} \int_0^x \mathrm{d}x'\, x' \frac{[f(x')]^{3/2}}{x'^{1/2}} \\
& = \int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{3/2}}{x^{1/2}} \int_0^x \mathrm{d}x'\, x'\, f''(x) \\
& = \int_0^\infty \mathrm{d}x\, f''(x) \int_0^x \mathrm{d}x'\, x'\, f''(x) \\
& = \int_0^\infty \mathrm{d}x\, f''(x) \int_0^x \mathrm{d}[f'(x')]\, x' \\
& = \int_0^\infty \mathrm{d}x\, f''(x) \left[f'(x')\, x'|_0^x - \int_0^x \mathrm{d}x'\, f'(x') \right] \\
& = \int_0^\infty \mathrm{d}x\, f''(x) \, [f'(x)\, x - f(x) + f(0)]
\end{aligned}
$$

$$= \int_0^\infty \mathrm{d}x\ f''(x)\ f'(x)\ x - \int_0^\infty \mathrm{d}x\ f''(x)\ f(x)$$

$$+ f(0) \int_0^\infty \mathrm{d}x\ f''(x)$$

$$= -\frac{1}{2} \int_0^\infty \mathrm{d}x\ \left[f'(x)\right]^2 - \int_0^\infty \mathrm{d}[f'(x)]\ f(x) + f(0) f'(0)$$

$$= -\frac{1}{2} \int_0^\infty \mathrm{d}x\ \left[f'(x)\right]^2 - \left[f'(x)\ f(x)|_0^\infty - \int_0^\infty \mathrm{d}[f(x)]\ f'(x) \right]$$

$$+ f(0) f'(0)$$

$$= -\frac{1}{2} \int_0^\infty \mathrm{d}x\ \left[f'(x)\right]^2 - f'(0)\ f(0) + \int_0^\infty \mathrm{d}x\ [f'(x)]^2 + f(0) f'(0)$$

$$= \frac{1}{2} \int_0^\infty \mathrm{d}x\ \left[f'(x)\right]^2 . \tag{2.268}$$

Substitute (2.263) and (2.264) into the right-hand side of (2.268), to obtain

$$\int_0^\infty \mathrm{d}x\ \frac{\left[f(x)\right]^{3/2}}{x^{1/2}} \int_0^x \mathrm{d}x'\ x'^{1/2} \left[f(x')\right]^{3/2}$$

$$= \frac{1}{5} \int_0^\infty \mathrm{d}x\ \frac{\left[f(x)\right]^{5/2}}{x^{1/2}}$$

$$= -\frac{1}{5} [\frac{5}{7} f'(0)]$$

$$= -\frac{1}{7} f'(0). \tag{2.269}$$

Consider the second term on the right-hand side of (2.267)

$$\int_0^\infty \mathrm{d}x\ x^{1/2} \left[f(x)\right]^{3/2} \int_x^\infty \mathrm{d}x'\ \frac{\left[f(x')\right]^{3/2}}{x'^{1/2}}$$

$$= \int_0^\infty \mathrm{d}x\ x^{1/2} \left[f(x)\right]^{3/2} \int_x^\infty \mathrm{d}x'\ f''(x')$$

$$= \int_0^\infty \mathrm{d}x\; x^{1/2} \left[f(x)\right]^{3/2} \lim_{x_b \to \infty} f'(x')|_x^{x_B}$$

$$= \int_0^\infty \mathrm{d}x\; x^{1/2} \left[f(x)\right]^{3/2} \lim_{x_b \to \infty} \left(f'(x_B) - f'(x)\right)$$

$$= -\int_0^\infty \mathrm{d}x\; x^{1/2} \left[f(x)\right]^{3/2} f'(x). \tag{2.270}$$

Multiply the right-hand side of (2.270) by $x^{1/2}/x^{1/2}$, to obtain

$$\int_0^\infty \mathrm{d}x\; x^{1/2} \left[f(x)\right]^{3/2} \int_x^\infty \mathrm{d}x' \; \frac{\left[f(x')\right]^{3/2}}{x'^{1/2}}$$

$$= -\int_0^\infty \mathrm{d}x\; x^{1/2} x^{1/2} \frac{\left[f(x)\right]^{3/2}}{x^{1/2}} f'(x)$$

$$= -\int_0^\infty \mathrm{d}x\; x \frac{\left[f(x)\right]^{3/2}}{x^{1/2}} f'(x)$$

$$= -\int_0^\infty \mathrm{d}x\; x\; f''(x)\; f'(x)$$

$$= -\frac{1}{2} \int_0^\infty \mathrm{d}\left[f'(x)\right]^2 \; x$$

$$= -\frac{1}{2}\left[\lim_{x_B \to \infty} x \;\left[f'(x)\right]^2 \Big|_0^{x_B} - \int_0^\infty \mathrm{d}x \;\left[f'(x)\right]^2 \right]$$

$$= -\frac{1}{2}\left[\lim_{x_B \to \infty} \left(x_B \;\left[f'(x_B)\right]^2 - 0\right) - \int_0^\infty \mathrm{d}x \;\left[f'(x)\right]^2 \right]$$

$$= \frac{1}{2} \int_0^\infty \mathrm{d}x \;\left[f'(x)\right]^2$$

$$= \frac{1}{2}\left[\lim_{x_B \to \infty} \left(f'(x_B) - f'(0)\right) - \int_0^\infty \mathrm{d}x \; \frac{\left[f(x)\right]^{5/2}}{x^{1/2}} \right]$$

$$= -\frac{1}{2} f'(0) - \frac{1}{2} \int_0^\infty \mathrm{d}x \; \frac{\left[f(x)\right]^{5/2}}{x^{1/2}}. \tag{2.271}$$

Substitute (2.264) into the second term on the right-hand side of(2.271), to obtain

$$\begin{aligned}\int_0^\infty \mathrm{d}x\, x^{1/2}\,[f(x)]^{3/2} \int_x^\infty \mathrm{d}x'\, \frac{[f(x')]^{3/2}}{x'^{1/2}}\\ &= -\frac{1}{2}f'(0) - \frac{1}{2}\int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{5/2}}{x^{1/2}}\\ &= -\frac{1}{2}f'(0) + \frac{5}{14}f'(0)\\ &= -\frac{1}{7}f'(0).\end{aligned} \tag{2.272}$$

Substitute (2.269) and (2.272) into the right-hand side of (2.267), to obtain

$$\begin{aligned}E_{ee}(Z) =& C_e Z^3 a^2 \left[\int_0^\infty \mathrm{d}x\, \frac{[f(x)]^{3/2}}{x^{1/2}} \int_0^x \mathrm{d}x'\, x'^{1/2}\,[f(x')]^{3/2}\right.\\ &\left. + \int_0^\infty \mathrm{d}x\, x^{1/2}\,[f(x)]^{3/2} \int_x^\infty \mathrm{d}x'\, \frac{[f(x')]^{3/2}}{x'^{1/2}}\right]\\ =& C_e Z^3 a^2 \left[-\frac{1}{7}f'(0) - \frac{1}{7}f'(0)\right]\\ =& -\frac{2}{7}C_e Z^3 a^2 f'(0).\end{aligned} \tag{2.273}$$

Substitute C_e from (2.225) and a from (2.206) into the right-hand side of (2.273), to obtain

$$\begin{aligned}E_{ee}(Z) &= -\frac{2}{7}\left(\frac{2\underline{q}^2 e^2}{9\pi^2}\right)\left(\frac{2me^2}{\hbar^2}\right)^3 Z^3 a^2 f'(0)\\ &= -\frac{2}{7}\left(\frac{2\underline{q}^2 e^2}{9\pi^2}\right)\left(\frac{2me^2}{\hbar^2}\right)^3 Z^3 \left(\left(\frac{3\pi}{2\underline{q}}\right)^{2/3}\left(\frac{\hbar^2}{2me^2}\right)\frac{1}{Z^{1/3}}\right)^2 f'(0)\\ E_{ee}(Z) &= -\frac{1}{7}\left(\frac{2\underline{q}}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right) Z^{7/3} f'(0).\end{aligned} \tag{2.274}$$

From (2.226), we obtain

$$E_{TF}(Z) = T[n] + E_{Ze} + E_{ee} \tag{2.275}$$

Substitute (2.265), (2.266) and (2.274) into (2.275), to obtain

$$\begin{aligned} E_{TF}(Z) =& -\left(\frac{3}{7}\right)\left(\frac{2q}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right)Z^{7/3}\,f'(0) \\ &+\left(\frac{2q}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right)Z^{7/3}f'(0) \\ &-\frac{1}{7}\left(\frac{2q}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right)Z^{7/3}f'(0) \\ =&\frac{3}{7}\left(\frac{2q}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right)Z^{7/3}f'(0). \end{aligned} \tag{2.276}$$

Substitute (2.250) into the right-hand side of (2.276), to obtain for the ground-state energy $E_{TF}(Z)$ of the TF atom the explicit expression :

$$\begin{aligned} E_{TF}(Z) =& -(1.58807)\frac{3}{7}\left(\frac{2q}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right)Z^{7/3} \\ \cong& -0.68060\left(\frac{2q}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right)Z^{7/3}. \end{aligned} \tag{2.277}$$

It remains to show that n_{TF} provides the smallest possible value for $F[n]$ in (2.178), that is

$$F[\sigma] \geqslant F[n_{\text{TF}}]. \tag{2.278}$$

To the above, defined a priori for an arbitrary density $\rho(\mathbf{x}) \geqslant 0$ by

$$\begin{aligned} F[\rho] =& A\int \mathrm{d}^3\mathbf{x}\ [\rho(\mathbf{x})]^{5/3} - Ze^2\int \mathrm{d}^3\mathbf{x}\frac{1}{|\mathbf{x}|}\,\rho(\mathbf{x}) \\ &+\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\,\rho(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\,\rho(\mathbf{x}') \end{aligned} \tag{2.279}$$

where

$$A = \frac{16\underline{q}\hbar^2}{10\pi^2 m}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \tag{2.280}$$

To show that the second term on the right-hand side of (2.279) is negative, we start from the potential solution of Poisson's Equation

$$\boldsymbol{\nabla}^2 \frac{1}{|\mathbf{x}|} = -\,4\pi\delta^2(\mathbf{x}), \tag{2.281a}$$

$$\frac{1}{|\mathbf{x}|} = -\,4\pi\left(\boldsymbol{\nabla}^2\right)^{-1}\delta^3(\mathbf{x}). \tag{2.281b}$$

Substitute into the second term on the right-hand side of (2.279), to obtain

$$\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\,\rho(\mathbf{x}) = -\,4\pi\int \mathrm{d}^3\mathbf{x}\,\left(\boldsymbol{\nabla}^2\right)^{-1}\,\rho(\mathbf{x})\,\delta^3(\mathbf{x}). \tag{2.282}$$

By using the integral representation of the delta function in 3-dimensions :

$$\delta^3(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{2.283}$$

We define the Fourier transform of $\tilde{\rho}^*(\mathbf{k})$ for real function $\rho(\mathbf{x})$

$$\tilde{\rho}^*(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}\,\rho^*(\mathbf{x})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} = \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{2.284}$$

Apply (2.283) and (2.284) into (2.282), to obtain

$$\begin{aligned}\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\,\rho(\mathbf{x}) &= -\,4\pi\int \mathrm{d}^3\mathbf{x}\,\left(\boldsymbol{\nabla}^2\right)^{-1}\,\rho(\mathbf{x})\,\delta^3(\mathbf{x}) \\ &= -\,4\pi\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\left(\boldsymbol{\nabla}^2\right)^{-1}\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\ &= 4\pi\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\frac{1}{\mathbf{k}^2}\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\end{aligned}$$

$$=4\pi \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{1}{\mathbf{k}^2} \tilde{\rho}^*(\mathbf{k}) \tag{2.285}$$

where

$$\nabla^2 \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} = -\,\mathbf{k}^2 \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}, \tag{2.286a}$$

$$\left(\nabla^2\right)^{-1} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} = -\,\frac{1}{\mathbf{k}^2} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{2.286b}$$

So that, from (2.285), we have

$$-Ze^2 \int \mathrm{d}^3\mathbf{x} \frac{1}{|\mathbf{x}|}\, \rho(\mathbf{x}) \;<\; 0. \tag{2.287}$$

To show that the third term on the right-hand side of (2.279) is positive, we start from the potential solution of Poisson's Equation

$$\nabla^2 \frac{1}{|\mathbf{x}-\mathbf{x}'|} = -\,4\pi\delta^3(\mathbf{x}-\mathbf{x}'), \tag{2.288a}$$

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = -\,4\pi \left(\nabla^2\right)^{-1} \delta^3(\mathbf{x}-\mathbf{x}'). \tag{2.288b}$$

Substitute into the third term on the right-hand side of (2.279), to obtain

$$\begin{aligned} &\int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \rho(\mathbf{x})\, \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, \rho(\mathbf{x}') \\ &\qquad = -4\pi \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \rho(\mathbf{x}) \left(\nabla^2\right)^{-1} \delta^3(\mathbf{x}-\mathbf{x}')\, \rho(\mathbf{x}'). \end{aligned} \tag{2.289}$$

By using the integral representation of the delta function in 3-dimensions :

$$\delta^3(\mathbf{x}-\mathbf{x}') = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \tag{2.290}$$

and the Fourier transform of $\tilde{\rho}(\mathbf{k})$ is

$$\rho(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \tilde{\rho}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{2.291}$$

Apply (2.290) and (2.291) into (2.289), we obtain

$$\begin{aligned}
&\int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}' \rho(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, \rho(\mathbf{x}') \\
&= -4\pi \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}' \rho(\mathbf{x})\, \rho(\mathbf{x}')\, \left(\boldsymbol{\nabla}^2\right)^{-1}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \\
&= -4\pi \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}' \rho(\mathbf{x})\, \rho(\mathbf{x}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'}\, \left(\boldsymbol{\nabla}^2\right)^{-1} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}.
\end{aligned} \tag{2.292}$$

The Fourier transform of $\rho(\mathbf{x})$ is

$$\tilde{\rho}(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}'\, \rho(\mathbf{x}')\, \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{x}'}. \tag{2.293}$$

By using (2.286) and (2.293), substitute into the right-hand side of (2.292), to obtain

$$\begin{aligned}
&\int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}' \rho(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, \rho(\mathbf{x}') \\
&= 4\pi \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \rho(\mathbf{x})\, \rho(\mathbf{x}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'}\, \frac{1}{\mathbf{k}^2}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&= 4\pi \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, \tilde{\rho}(\mathbf{k}) \frac{1}{\mathbf{k}^2}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}.
\end{aligned} \tag{2.294}$$

Since $\rho(\mathbf{x})$ is real function, we obtain $\rho(\mathbf{x}) = \rho^*(\mathbf{x})$, by referring (2.291), we obtain

$$\rho(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\, \tilde{\rho}^*(\mathbf{k}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{x}}. \tag{2.295}$$

Now substitute (2.295) into (2.294), giving

$$\begin{aligned}
&\int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}' \rho(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|}\ \rho(\mathbf{x}') \\
&\qquad = 4\pi \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3} \int \mathrm{d}^3\mathbf{x}\ \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{x}}\ \tilde{\rho}^*(\mathbf{k}')\ \tilde{\rho}(\mathbf{k}) \frac{1}{\mathbf{k}^2}\ \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&\qquad = 4\pi \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\ \tilde{\rho}^*(\mathbf{k}')\ \tilde{\rho}(\mathbf{k}) \frac{1}{\mathbf{k}^2} \int \mathrm{d}^3\mathbf{x}\ \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}. \qquad (2.296)
\end{aligned}$$

By using the integral representation of the delta function in 3-dimensions :

$$\delta^3(\mathbf{k}-\mathbf{k}') = \int \frac{\mathrm{d}^3\mathbf{x}}{(2\pi)^3}\ \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}, \qquad (2.297a)$$

$$F(\mathbf{k}) = \int \mathrm{d}^3\mathbf{k}'\ F(\mathbf{k}')\ \delta^3(\mathbf{k}-\mathbf{k}'). \qquad (2.297b)$$

Applying (2.297) on the right-hand side of (2.296), to write

$$\begin{aligned}
&\int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}' \rho(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|}\ \rho(\mathbf{x}') \\
&\qquad = 4\pi \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ \tilde{\rho}(\mathbf{k})\ \frac{1}{\mathbf{k}^2}\ (2\pi)^3 \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\ \tilde{\rho}^*(\mathbf{k}')\ \delta^3(\mathbf{k}-\mathbf{k}') \\
&\qquad = 4\pi \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ \tilde{\rho}(\mathbf{k})\ \frac{1}{\mathbf{k}^2}\ \tilde{\rho}^*(\mathbf{k}) \\
&\qquad = 4\pi \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ |\tilde{\rho}(\mathbf{k})|^2\ \frac{1}{\mathbf{k}^2}. \qquad (2.298)
\end{aligned}$$

We also have

$$e^2 \int \mathrm{d}^3\mathbf{x}\ \mathrm{d}^3\mathbf{x}' \rho(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|}\ \rho(\mathbf{x}') \geqslant 0. \qquad (2.299)$$

Let

$$\rho(\mathbf{x}) = t\rho_1(\mathbf{x}) + \beta\rho_2(\mathbf{x}) \equiv t\rho_1 + \beta\rho_2, \tag{2.300a}$$

$$\rho(\mathbf{x}') = t\rho_1(\mathbf{x}') + \beta\rho_2(\mathbf{x}') \equiv t\rho_1' + \beta\rho_2', \tag{2.300b}$$

$$1 = t + \beta, \tag{2.300c}$$

$$\beta = (1 - t) \tag{2.300d}$$

where $0 \leqslant t \leqslant 1$ and $\rho_1, \rho_2 \geqslant 0$.

For any real and positive ρ_1, ρ_2, we have the elementary inequality

$$\left(t\rho_1 + (1-t)\rho_2\right)^{5/3} \leqslant t\left(\rho_1\right)^{5/3} + (1-t)\left(\rho_2\right)^{5/3}. \tag{2.301}$$

Also

$$\begin{aligned}
\left[t\rho_1 + (1-t)\rho_2\right]\left[t\rho_1' + (1-t)\rho_2'\right] =& t^2\rho_1\rho_1' + (1-t)^2\rho_2\rho_2' + t(1-t)\rho_1\rho_2' \\
& + t(1-t)\rho_1'\rho_2 \\
=& t^2\rho_1\rho_1' + \rho_2\rho_2' - t^2\rho_2\rho_2' + t\rho_1\rho_2' - t\rho_1'\rho_2 \\
& + t\rho_1'\rho_2 - t^2\rho_1'\rho_2 \\
=& t^2\rho_1\rho_1' + \rho_2\rho_2' - t^2\rho_2\rho_2' + t\rho_1\rho_2' - t\rho_1'\rho_2 \\
& + t\rho_1'\rho_2 - t^2\rho_1'\rho_2 + t\rho_1\rho_1' - t\rho_1\rho_1' \\
=& t\rho_1\rho_1' + (1-t)\rho_2\rho_2' \\
& - t(1-t)(\rho_1 - \rho_2)(\rho_1' - \rho_2')
\end{aligned}$$

$$\therefore \quad \big[t\rho_1 + (1-t)\rho_2\big]\big[t\rho_1' + (1-t)\rho_2'\big] = t\rho_1\rho_1' + (1-t)\rho_2\rho_2' - t(1-t)(\rho_1-\rho_2)(\rho_1'-\rho_2'). \quad (2.302)$$

In (2.299), replace $\rho(\mathbf{x})$ with $\big[\rho_1(\mathbf{x}) - \rho_2(\mathbf{x})\big]$ and replace $\rho(\mathbf{x}')$ with $\big[\rho_1(\mathbf{x}') - \rho_2(\mathbf{x}')\big]$, to obtain from (2.298)

$$\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\,\big[\rho_1(\mathbf{x}) - \rho_2(\mathbf{x})\big]\frac{1}{|\mathbf{x}-\mathbf{x}'|}\big[\rho_1(\mathbf{x}') - \rho_2(\mathbf{x}')\big] \geqslant 0. \quad (2.303)$$

In (2.279) and (2.300), replace $\rho(\mathbf{x})$ by $\big[t\rho_1 + (1-t)\rho_2\big]$ and $\rho(\mathbf{x}')$ by $\big[t\rho_1' + (1-t)\rho_2'\big]$, to obtain

$$\begin{aligned} F\big[t\rho_1 + (1-t)\rho_2\big] =& A\int \mathrm{d}^3\mathbf{x}\big[t\rho_1 + (1-t)\rho_2\big]^{5/3} \\ &- Ze^2\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\,\big[t\rho_1 + (1-t)\rho_2\big] \\ &+ \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\big[t\rho_1 + (1-t)\rho_2\big]\frac{1}{|\mathbf{x}-\mathbf{x}'|}\,\big[t\rho_1' + (1-t)\rho_2'\big]. \end{aligned} \quad (2.304)$$

Consider the first term on the right-hand side of (2.304), by using the elementary inequality in (2.301), to obtain

$$\begin{aligned} A\int \mathrm{d}^3\mathbf{x}\big[t\rho_1 + (1-t)\rho_2\big]^{5/3} \leqslant& A\int \mathrm{d}^3\mathbf{x}\,\left(t\,(\rho_1)^{5/3} + (1-t)\,(\rho_2)^{5/3}\right) \\ =& A\int \mathrm{d}^3\mathbf{x}\,t\,(\rho_1)^{5/3} + A\int \mathrm{d}^3\mathbf{x}\,(1-t)\,(\rho_2)^{5/3} \end{aligned}$$

$$\begin{aligned} \therefore\ A\int \mathrm{d}^3\mathbf{x}\big[t\rho_1 + (1-t)\rho_2\big]^{5/3} \leqslant& t\left(A\int \mathrm{d}^3\mathbf{x}\,\,(\rho_1)^{5/3}\right) \\ &+ (1-t)\left(A\int \mathrm{d}^3\mathbf{x}\,\,(\rho_2)^{5/3}\right). \end{aligned} \quad (2.305)$$

Consider the second term on the right-hand side of (2.304) and write it as

$$
\begin{aligned}
-Ze^2 \int \mathrm{d}^3\mathbf{x}\, \frac{1}{|\mathbf{x}|}\, \big[t\rho_1 + (1-t)\rho_2\big] =& - Ze^2 \int \mathrm{d}^3\mathbf{x}\, \frac{1}{|\mathbf{x}|}\, t\rho_1 \\
&- Ze^2 \int \mathrm{d}^3\mathbf{x}\, \frac{1}{|\mathbf{x}|}\, (1-t)\rho_2 \\
=& - t\left(Ze^2 \int \mathrm{d}^3\mathbf{x}\, \frac{1}{|\mathbf{x}|}\, \rho_1 \right) \\
&- (1-t)\left(Ze^2 \int \mathrm{d}^3\mathbf{x}\, \frac{1}{|\mathbf{x}|}\, \rho_2 \right) . \qquad (2.306)
\end{aligned}
$$

Consider the third term on the right-hand side of (2.304), by using (2.302), to obtain

$$
\begin{aligned}
&\frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}' \big[t\rho_1 + (1-t)\rho_2\big] \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, \big[t\rho_1' + (1-t)\rho_2'\big] \\
&= \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, t\rho_1\rho_1' + \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, (1-t)\rho_2\rho_2' \\
&\quad - \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, \big(t(1-t)(\rho_1-\rho_2)(\rho_1'-\rho_2')\big) . \qquad (2.307)
\end{aligned}
$$

From (2.303), the left-hand side of (2.307) is positive, so that (2.307) be rewriten as

$$
\begin{aligned}
&\frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}' \big[t\rho_1 + (1-t)\rho_2\big] \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, \big[t\rho_1' + (1-t)\rho_2'\big] \\
&\leqslant t\left(\frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, \rho_1\rho_1' \right) \\
&\quad + (1-t)\left(\frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, \rho_2\rho_2' \right) . \qquad (2.308)
\end{aligned}
$$

Substitute (2.305), (2.306) and (2.308) into (2.304), to obtain

$$
\begin{aligned}
F\left[t\rho_1+(1-t)\rho_2\right] \leqslant\, & t\left(A\int \mathrm{d}^3\mathbf{x}\ (\rho_1)^{5/3}\right)+(1-t)\left(A\int \mathrm{d}^3\mathbf{x}\ (\rho_2)^{5/3}\right) \\
& -t\left(Ze^2\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\,\rho_1\right)-(1-t)\left(Ze^2\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\,\rho_2\right) \\
& +t\left(\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\,\rho_1\rho_1'\right) \\
& +(1-t)\left(\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\,\rho_2\rho_2'\right) \\
=& t\left(A\int \mathrm{d}^3\mathbf{x}\ (\rho_1)^{5/3}-Ze^2\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\,\rho_1\right. \\
& \left.+\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\,\rho_1\rho_1'\right) \\
& +(1-t)\left(A\int \mathrm{d}^3\mathbf{x}\ (\rho_2)^{5/3}-Ze^2\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\,\rho_2\right. \\
& \left.+\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\,\rho_2\rho_2'\right).
\end{aligned}
\tag{2.309}
$$

Referring to (2.279), we obtain

$$
\begin{aligned}
F[\rho_1] =& A\int \mathrm{d}^3\mathbf{x}\ (\rho_1)^{5/3}-Ze^2\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\,\rho_1 \\
& +\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\,\rho_1\rho_1'
\end{aligned}
\tag{2.310}
$$

and

$$
\begin{aligned}
F[\rho_2] =& A\int \mathrm{d}^3\mathbf{x}\ (\rho_2)^{5/3}-Ze^2\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\,\rho_2 \\
& +\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\,\rho_2\rho_2'
\end{aligned}
\tag{2.311}
$$

Substitute (2.309) and (2.311) into the right-hand side of inequality (2.309), to obtain

$$F\big[t\rho_1 + (1-t)\rho_2\big] \leqslant tF[\rho_1] + (1-t)F[\rho_2]. \tag{2.312}$$

Also, from (2.304), we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}F\big[t\rho_1 + (1-t)\rho_2\big] =& \frac{5}{3}A\int \mathrm{d}^3\mathbf{x}\, \big[t\rho_1 + (1-t)\rho_2\big]^{2/3}(\rho_1-\rho_2) \\ & - Ze^2\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\,(\rho_1-\rho_2) \\ & + e^2\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\,\big[t\rho_1' + (1-t)\rho_2'\big](\rho_1-\rho_2)\end{aligned} \tag{2.313}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t}F\big[t\rho_1 + (1-t)\rho_2\big]\Big|_{t=0} = \int \mathrm{d}^3\mathbf{x}\,(\rho_1-\rho_2)\left[\frac{5}{3}A\rho_2^{2/3} - Ze^2\,\frac{1}{|\mathbf{x}|} - e^2\int \mathrm{d}^3\mathbf{x}'\,\frac{\rho_2'}{|\mathbf{x}-\mathbf{x}'|}\right] \tag{2.314}$$

By choosing $\rho_2 = n_{\mathrm{TF}}$, and $\rho_1 = \sigma \geqslant 0$ arbitrary, we conclude from (2.179) that the expression within the square brackets in (2.314) is zero, thus

$$\frac{\mathrm{d}}{\mathrm{d}t}F\big[t\sigma + (1-t)n_{\mathrm{TF}}\big]\Big|_{t=0} = 0. \tag{2.315}$$

Also (2.312) leads to the bound

$$F\big[\sigma\big] - F\big[n_{\mathrm{TF}}\big] \geqslant \frac{F\big[t\sigma + (1-t)n_{\mathrm{TF}}\big] - F\big[n_{\mathrm{TF}}\big]}{t}. \tag{2.316}$$

Since the left-hand side of (2.316) is independent of t, we may take the limit

$t \to 0$, to obtain

$$F[\sigma] - F[n_{\text{TF}}] \geqslant \lim_{t\to 0}\left(\frac{F[t\sigma + (1-t)n_{\text{TF}}] - F[n_{\text{TF}}]}{t}\right) \tag{2.317}$$

and finally use (2.287) to conclude that

$$F[\sigma] \geqslant F[n_{\text{TF}}] \tag{2.318}$$

with the TF density n_{TF} providing the smallest possible value for the energy functional in (2.279).

2.5 A Thomas-Fermi Energy Functional and a Lower Bound for The Electron-Electron Interaction Potential Energy

The Hamiltonian under consideration for the stability matter is taken to be the N-electron in (1.1),where m denotes the mass of the electron and the $\mathbf{x}_i$, $\mathbf{R}_j$ correspond, respectively, to positions of the electrons and nuclei. Also we consider neutral matter, i.e.,

$$\sum_{i=1}^{k} Z_i = N. \tag{2.319}$$

For anti-symmetric normalized functions $\Psi(\mathbf{x}_1\sigma_1,\dots,\mathbf{x}_N\sigma_N)$ of N electrons, we have for the expectation value of the Hamiltonian H

$$\langle\Psi| H |\Psi\rangle = \sum_{i=1}^{N}\langle\Psi| \frac{\mathbf{p}_i^2}{2m}|\Psi\rangle - \sum_{i=1}^{N}\sum_{j=1}^{k}\langle\Psi| \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|}|\Psi\rangle$$

$$+ \sum_{i<j}^{N}\langle\Psi| \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}|\Psi\rangle + \sum_{i<j}^{k}\langle\Psi| \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|}|\Psi\rangle . \tag{2.320}$$

To derive a lower bound for this expectation value, we recall the definition of electron density

$$\rho(\mathbf{x}) = N \sum_{\sigma_1,\ldots,\sigma_N} \int \mathrm{d}^3\mathbf{x}_2 \ldots \mathrm{d}^3\mathbf{x}_N \, |\Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, \ldots, \mathbf{x}_N\sigma_N)|^2 \tag{2.321}$$

normalized to

$$\int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) = N \tag{2.322}$$

and

$$\begin{aligned}\langle\Psi|\Psi\rangle =& \int \mathrm{d}^3\mathbf{x}, \mathrm{d}^3\mathbf{x}_2 ... \mathrm{d}^3\mathbf{x}_N \; \Psi^*(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N) \; \Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N) \\ =& \sum_{\sigma_1,\ldots,\sigma_N}^{n} \int \mathrm{d}^3\mathbf{x}, \mathrm{d}^3\mathbf{x}_2 ... \mathrm{d}^3\mathbf{x}_N \, |\Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N)|^2 \\ =& 1. \end{aligned} \tag{2.323}$$

From (2.175), we also use the lower bound to the expectation value of the kinetic energy derived there :

$$\begin{aligned} T[\rho] =& \sum_{i=1}^{N} \langle\Psi| \, \frac{\mathbf{p}_i^2}{2m} \, |\Psi\rangle \\ \geqslant& \frac{16\underline{q}\hbar^2}{10\pi^2 m} \left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \int \mathrm{d}^3\mathbf{x} \; [\rho(\mathbf{x})]^{5/3} \end{aligned} \tag{2.324}$$

where $\beta > 0$, by setting $\beta = 1$,we obtain the kinetic energy of TF atom.

In the second term on the right-hand side of (2.320), substitute (2.321) into (2.320), to obtain

$$\sum_{i=1}^{N} \sum_{j=1}^{k} \langle\Psi| \, \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \, |\Psi\rangle = \int \mathrm{d}^3\mathbf{x}, \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \; \Psi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\sum_{i=1}^{N} \sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \right) \Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$= \sum_{j=1}^{k} \sum_{i=1}^{N} \int \mathrm{d}^3\mathbf{x}, \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \; \Psi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \right) \Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$= \sum_{j=1}^{k} \sum_{j=1}^{N} \int \mathrm{d}^3\mathbf{x} \; \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|}$$

$$\times \sum_{\sigma_1, \ldots, \sigma_N} \int \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \, |\Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2$$

$$= \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x} \frac{Z_j e^2}{|\mathbf{x} - \mathbf{R}_j|} \; \frac{\rho(\mathbf{x})}{N}$$

$$+ \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x}_2 \frac{Z_j e^2}{|\mathbf{x}_2 - \mathbf{R}_j|} \; \frac{\rho(\mathbf{x}_2)}{N}$$

$$+ \ldots + \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x}_N \frac{Z_j e^2}{|\mathbf{x}_N - \mathbf{R}_j|} \; \frac{\rho(\mathbf{x}_N)}{N}$$

$$= N \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x} \frac{Z_j e^2}{|\mathbf{x} - \mathbf{R}_j|} \; \frac{\rho(\mathbf{x})}{N}$$

$$\therefore \;\; \sum_{i=1}^{N} \sum_{j=1}^{k} \langle \Psi | \, \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \, | \Psi \rangle = \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x} \; \rho(\mathbf{x}) \; \frac{Z_j e^2}{|\mathbf{x} - \mathbf{R}_j|}. \tag{2.325}$$

In the third term on the right-hand side of (2.320), we first note that

$$\sum_{i<j}^{N} \langle \Psi | \, \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \, | \Psi \rangle = \sum_{i<j}^{N} \int \mathrm{d}^3\mathbf{x}', \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \; \Psi^*(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \right) \; \Psi(\mathbf{x}', \mathbf{x}_2, \ldots \mathbf{x}_N)$$

$$= \frac{e^2}{2} \int d^3\mathbf{x}' \int d^3\mathbf{x}\, \rho(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, \rho(\mathbf{x}')$$

$$\sum_{i<j}^{N} \langle\Psi| \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} |\Psi\rangle = \frac{e^2}{2} \int d^3\mathbf{x}' \int d^3\mathbf{x}\, \rho(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, \rho(\mathbf{x}') \tag{2.326}$$

and for the fourth term on the right-hand side of (2.320) we can write

$$\sum_{i<j}^{k} \langle\Psi| \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|} |\Psi\rangle = \sum_{i<j}^{k} \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \langle\Psi \mid \Psi\rangle$$

$$= \sum_{i<j}^{k} \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|}. \tag{2.327}$$

From (2.324)–(2.327), we obtain the lower bound for (2.320)

$$\langle\Psi| H |\Psi\rangle = \frac{16\underline{q}\hbar^2}{10\pi^2 m} \left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \int d^3\mathbf{x}\, \left[\rho(\mathbf{x})\right]^{5/3} - \sum_{j=1}^{k} \int d^3\mathbf{x}\, \rho(\mathbf{x})\, \frac{Z_j e^2}{|\mathbf{x}-\mathbf{R}_j|}$$

$$+ \frac{e^2}{2} \int d^3\mathbf{x}\, d^3\mathbf{x}'\, \rho(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, \rho(\mathbf{x}') + \sum_{i<j}^{k} \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|}. \tag{2.328}$$

From (2.328), We introduce the functional of a positive function $\rho(\mathbf{x})$ defined by

$$F\left[\rho; Z_1, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\right] = \frac{16\underline{q}\hbar^2}{10\pi^2 m\beta} \left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \int d^3\mathbf{x}\, \left[\rho(\mathbf{x})\right]^{5/3}$$

$$- \sum_{j=1}^{k} Z_j\, e^2 \int d^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|}$$

$$+ \frac{e^2}{2} \int d^3\mathbf{x}\, d^3\mathbf{x}'\, \rho(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \rho(\mathbf{x}')$$

$$+ \sum_{i<j}^{k} \frac{Z_i Z_j\, e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{2.329}$$

depending on positive parameters $Z_1, \ldots, Z_k$ and vectors $\mathbf{R}_1, \ldots, \mathbf{R}_k$. Here $\beta > 0$ is an arbitrary dimensionless parameter. [In particular, for $k = 1$, the last term in (2.329) is absent, and by setting $\mathbf{R}_i = \mathbf{0}$, $\beta = 1$, we obtain the energy functional in (2.178), (2.279).] In this section will be used in the next section to obtain a lower bound for the (repulsive) Coulomb potential for many particles having charges of the same signs.

Minimize (2.329), with respect to $\rho(\mathbf{x})$ we obtain

$$\begin{aligned}
0 =& \frac{\delta F(\rho)}{\delta \rho(\mathbf{x})} \\
=& \frac{16\underline{q}\hbar^2}{10\pi^2 m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\frac{5}{3}\,\rho^{2/3}(\mathbf{x}) - \sum_{i=1}^{k}\frac{Z_i\, e^2}{|\mathbf{x}-\mathbf{R}_i|} + e^2\int \mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\rho(\mathbf{x}') \\
=& \frac{2\hbar^2}{m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3}\rho^{2/3}(\mathbf{x}) - \sum_{i=1}^{k}\frac{Z_i\, e^2}{|\mathbf{x}-\mathbf{R}_i|} + e^2\int \mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\rho(\mathbf{x}'). \qquad (2.330)
\end{aligned}$$

Let $\rho_0(\mathbf{x};k)$ satisfy the Eq.(2.330), we obtain

$$\frac{2\hbar^2}{m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3}\rho_0^{2/3}(\mathbf{x};k) = \sum_{i=1}^{k}\frac{Z_i\, e^2}{|\mathbf{x}-\mathbf{R}_i|} - e^2\int \mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\rho_0(\mathbf{x}';k). \qquad (2.331)$$

Following the proof given in Eq.(2.318), which shows that the TF density actually provides the smallest value, for the energy density functional, we conclude that $\rho_0(\mathbf{x};k)$ satisfying (2.331) provides the smallest value for the functionals $F\big[\rho; Z_1,\dots,Z_k,\mathbf{R}_1,\dots,\mathbf{R}_k\big]$ in (2.329), with the normalization condition

$$\int \mathrm{d}^3\mathbf{x}\,\rho_0(\mathbf{x};k) = \sum_{i=1}^{k} Z_i \qquad (2.332)$$

satisfied. That is

$$F\big[\rho\big] \geqslant F\big[\rho_0\big], \qquad (2.333a)$$

$$F\big[\rho; Z_1,\dots,Z_k,\mathbf{R}_1,\dots,\mathbf{R}_k\big] \geqslant F\big[\rho_0; Z_1,\dots,Z_k,\mathbf{R}_1,\dots,\mathbf{R}_k\big]. \qquad (2.333b)$$

We introduce the functionals

$$F\big[\rho; \lambda Z_1, \dots, \lambda Z_l, Z_{l+1}, \dots, Z_k, \mathbf{R}_1, \dots, \mathbf{R}_k\big] \tag{2.334}$$

and

$$F\big[\rho; \lambda Z_1, \dots, \lambda Z_l, \mathbf{R}_1, \dots, \mathbf{R}_l\big] \tag{2.335}$$

where $l < k$, and $\lambda > 0$ is an arbitrary parameter.

Let $\rho_1(\mathbf{x})$, $\rho_2(\mathbf{x})$ be the corresponding solutions to (2.331) for the functionals in (2.334), (2.335), respectively :

$$\frac{2\hbar^2}{m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3}\rho_1^{2/3}(\mathbf{x}) = \sum_{j=1}^{l}\frac{\lambda Z_j\, e^2}{|\mathbf{x}-\mathbf{R}_j|} + \sum_{j=l+1}^{k}\frac{Z_j\, e^2}{|\mathbf{x}-\mathbf{R}_j|} - e^2\int \mathrm{d}^3\mathbf{x}'\,\frac{\rho_1(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}, \tag{2.336a}$$

$$\frac{2\hbar^2}{m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3}\rho_2^{2/3}(\mathbf{x}) = \sum_{j=1}^{l}\frac{\lambda Z_j\, e^2}{|\mathbf{x}-\mathbf{R}_j|} - e^2\int \mathrm{d}^3\mathbf{x}'\,\frac{\rho_2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}. \tag{2.336b}$$

for simplicity of the notation only, we have suppressed the dependence of ρ_1, ρ_2 on λ, k, l.

We set

$$Q_1(\mathbf{x}) = \frac{2\hbar^2}{m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3}\rho_1^{2/3}(\mathbf{x}), \tag{2.337a}$$

$$Q_2(\mathbf{x}) = \frac{2\hbar^2}{m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3}\rho_2^{2/3}(\mathbf{x}). \tag{2.337b}$$

Upon subtracting, $Q_2(\mathbf{x})$ from $Q_1(\mathbf{x})$ we obtain from (2.336a), (2.336b) :

$$Q_1(\mathbf{x}) - Q_2(\mathbf{x}) = \sum_{j=l+1}^{k}\frac{Z_j\, e^2}{|\mathbf{x}-\mathbf{R}_j|} - e^2\int \mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\big[\rho_1(\mathbf{x}') - \rho_2(\mathbf{x}')\big]$$

$$= \sum_{j=l+1}^{k}\frac{Z_j\, e^2}{|\mathbf{x}-\mathbf{R}_j|}$$

$$-\frac{4\underline{q}}{3\pi^2}\left(\frac{m\beta}{2\hbar^2}\right)^{3/2} e^2 \int \mathrm{d}^3\mathbf{x}' \frac{1}{|\mathbf{x}-\mathbf{x}'|}\Big[Q_1^{3/2}(\mathbf{x}') - Q_2^{3/2}(\mathbf{x}')\Big]. \tag{2.338}$$

Since the sum over j in (2.338) is non-negative, $\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ cannot be strictly negative for all $\mathbf{x}$ otherwise this will be in contradiction with the equation (2.338) itself.

We introduce the set

$$S = \{\mathbf{x}|\, Q_1(\mathbf{x}) - Q_2(\mathbf{x}) < 0\} \tag{2.339}$$

which we will eventually show that it is empty, thus concluding that $Q_1(\mathbf{x}) - Q_2(\mathbf{x}) \geqslant 0$.

We assume that S is non-empty and then run into a contradiction. As we move away from the boundary Ω of S, $\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ changes sign or vanishes, by definition of S, and we then have

$$\hat{\mathbf{n}} \cdot \boldsymbol{\nabla}\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] \geqslant 0 \tag{2.340}$$

where $\hat{\mathbf{n}}$ is a unit vector perpendicular to the boundary at $\mathbf{x}$, otherwise, we would run into a region beyond S where $\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ is still strictly negative. [If S is of infinite extension the non-negativity of $\hat{\mathbf{n}} \cdot \boldsymbol{\nabla}\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ on the boundary still holds.]

The application of the Laplacian to (2.338) gives

$$\nabla^2\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] = -4\pi \sum_{j=l+1}^{k} Z_j\, e^2 \delta^3(\mathbf{x} - \mathbf{R_j}) + 4\pi e^2 \left(\frac{m\beta}{2\hbar^2}\left(\frac{4\underline{q}}{3\pi^2}\right)^{2/3}\right)^{3/2} \Big[Q_1^{3/2}(\mathbf{x}) - Q_2^{3/2}(\mathbf{x})\Big] \tag{2.341}$$

and for $\mathbf{x}$ in the set S, the expression on the right-hand side of this equation is strictly negative since $\left[Q_1^{3/2}(\mathbf{x}) - Q_2^{3/2}(\mathbf{x})\right] < 0$ for such $\mathbf{x}$ by hypothesis.

Accordingly,

$$0 > \int_S \mathrm{d}^3\mathbf{x}\, \nabla^2 \big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] = \int_\Omega \mathrm{d}\Omega\, \hat{\mathbf{n}} \cdot \boldsymbol{\nabla} \big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] \tag{2.342}$$

in contradiction with (2.340), hence S is empty and

$$Q_1(\mathbf{x}) - Q_2(\mathbf{x}) \geqslant 0 \tag{2.343}$$

as a function of $\mathbf{x}$.

In reference to the functional

$$F\big[\rho; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\big] \tag{2.344}$$

let $\rho_3(\mathbf{x})$ satisfy

$$\frac{2\hbar^2}{m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3} \rho_3^{2/3}(\mathbf{x}) = \sum_{j=l+1}^{k} \frac{Z_j\, e^2}{|\mathbf{x} - \mathbf{R}_j|} - e^2 \int \mathrm{d}^3\mathbf{x}' \frac{1}{|\mathbf{x} - \mathbf{x}'|} \rho_3(\mathbf{x}') \tag{2.345}$$

in analogy to (2.336).

We define

$$\begin{aligned} f(\lambda) = {} & F\big[\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big] \\ & - F\big[\rho_2; \lambda Z_1, \ldots, \lambda Z_l, \mathbf{R}_1, \ldots, \mathbf{R}_l\big] \\ & - F\big[\rho_3; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\big] \end{aligned} \tag{2.346}$$

with $l < k$. Since for $\lambda = 0$, ρ_1 and ρ_3 denote the same density, and ρ_2, being just the TF density, is equal to zero for $\lambda = 0$,with mass $m\beta$ and $Z = 1$. When $\rho_2 = 0$, we can rewrite (2.346) as

$$f(0) = F\big[\rho; Z_{l+1}, \dots, Z_k, \mathbf{R}_1, \dots, \mathbf{R}_k\big]$$

$$- F\big[0; \dots \mathbf{R}_1, \dots, \mathbf{R}_l\big]$$

$$- F\big[\rho; Z_{l+1}, \dots, Z_k, \mathbf{R}_{l+1}, \dots, \mathbf{R}_k\big] \tag{2.347}$$

the left-hand side of (2.347) is non-negative while the right-hand side is non-positive, so that we may infer that (for $\lambda = 0$)

$$f(0) = 0. \tag{2.348}$$

For $\lambda = 1$, gives

$$f(1) = F\big[\rho; Z_1, \dots, Z_l, Z_{l+1}, \dots, Z_k, \mathbf{R}_1, \dots, \mathbf{R}_k\big]$$

$$- F\big[\rho_2; Z_1, \dots, Z_l, \mathbf{R}_1, \dots, \mathbf{R}_l\big]$$

$$- F\big[\rho; Z_{l+1}, \dots, Z_k, \mathbf{R}_{l+1}, \dots, \mathbf{R}_k\big]. \tag{2.349}$$

From (2.348), we may write

$$f(1) = \int_0^1 \mathrm{d}\lambda\, f'(\lambda) \tag{2.350}$$

and hence to establish (2.351) it is sufficient to show that $f'(\lambda) \geqslant 0$ for $0 \leqslant \lambda \leqslant 1$. We may infer that

$$f(1) \geqslant 0. \tag{2.351}$$

To the above end, we note from (2.329) with $Z_1 \to \lambda Z_1, \dots, Z_l \to \lambda Z_l$, $\rho \to \rho_1$ that

$$F\big[\rho_1; \lambda Z_1, \dots, \lambda Z_l, Z_{l+1}, \dots, Z_k, \mathbf{R}_1, \dots, \mathbf{R}_k\big]$$

$$
\begin{aligned}
= & \frac{16\underline{q}\hbar^2}{10\pi^2 m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\int \mathrm{d}^3\mathbf{x}\ [\rho_1(\mathbf{x})]^{5/3} \\
& -\lambda\sum_{j=1}^{\ell} Z_j\, e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho_1(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|} \\
& -\sum_{j=\ell+1}^{k} Z_j\, e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho_1(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|} \\
& +\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \rho_1(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\rho_1(\mathbf{x}') \\
& +\lambda^2\sum_{i=1}^{\ell-1}\sum_{j=\ell+1}^{\ell}\frac{Z_i Z_j\, e^2}{|\mathbf{R}_i-\mathbf{R}_j|} \\
& +\sum_{i=1}^{\ell}\lambda Z_i\sum_{j=\ell+1}^{k}\frac{Z_i Z_j\, e^2}{|\mathbf{R}_i-\mathbf{R}_j|}
\end{aligned}
\tag{2.352}
$$

where

$$
\begin{aligned}
\sum_{i<j}^{k} Z_i Z_j e^2\,\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|} = & \lambda^2\sum_{i=1}^{\ell-1}\sum_{j=\ell+1}^{\ell}\frac{Z_i Z_j\, e^2}{|\mathbf{R}_i-\mathbf{R}_j|} \\
& +\sum_{i=1}^{\ell}\lambda Z_i\sum_{j=\ell+1}^{k}\frac{Z_i Z_j\, e^2}{|\mathbf{R}_i-\mathbf{R}_j|}.
\end{aligned}
\tag{2.353}
$$

By setting the functional partial derivative of (2.352), with respect to λ, we obtain

$$
\begin{aligned}
& \frac{\partial}{\partial\lambda}F\big[\rho_1;\lambda Z_1,\ldots,\lambda Z_l, Z_{l+1},\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k\big] \\
& \qquad = \frac{2\hbar^2}{m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3}\int \mathrm{d}^3\mathbf{x}\ \rho_1^{2/3}(\mathbf{x})\ \frac{\partial}{\partial\lambda}\rho_1(\mathbf{x}) \\
& \qquad\quad -\sum_{j=1}^{l}\int \mathrm{d}^3\mathbf{x}\frac{\lambda Z_j\, e^2}{|\mathbf{x}-\mathbf{R}_j|}\frac{\partial}{\partial\lambda}\rho_1(\mathbf{x})
\end{aligned}
$$

$$- \sum_{j=1}^{l} Z_j \, e^2 \int \mathrm{d}^3\mathbf{x} \frac{\rho_1(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|}$$

$$- \sum_{j=\ell+1}^{k} Z_j \, e^2 \int \mathrm{d}^3\mathbf{x} \, \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \, \frac{\partial}{\partial\lambda} \rho_1(\mathbf{x})$$

$$- e^2 \int \mathrm{d}^3\mathbf{x} \, \mathrm{d}^3\mathbf{x}' \frac{1}{|\mathbf{x} - \mathbf{x}'|} \, \rho_1(\mathbf{x}') \, \frac{\partial}{\partial\lambda} \rho_1(\mathbf{x})$$

$$- 2\lambda \sum_{i=1}^{\ell-1} \sum_{j=\ell+1}^{\ell} Z_i Z_j e^2 \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|}$$

$$- \sum_{i=1}^{\ell} Z_i \sum_{j=\ell+1}^{k} Z_j e^2 \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|}. \tag{2.354}$$

Similarly, we can rewrite (2.354) as

$$\frac{\partial}{\partial\lambda} F\big[\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big]$$

$$= \int \mathrm{d}^3\mathbf{x} \left[\frac{2\hbar^2}{m\beta} \left(\frac{3\pi^2}{4\underline{q}} \right)^{2/3} \rho_1^{2/3}(\mathbf{x}) - e^2 \sum_{j=1}^{l} \frac{\lambda Z_j}{|\mathbf{x} - \mathbf{R}_j|} \right.$$

$$\left. - e^2 \sum_{j=l+1}^{k} \frac{Z_j}{|\mathbf{x} - \mathbf{R}_j|} + e^2 \int \mathrm{d}^3\mathbf{x}' \frac{1}{|\mathbf{x} - \mathbf{x}'|} \rho_1(\mathbf{x}') \right] \frac{\partial}{\partial\lambda} \rho_1(\mathbf{x})$$

$$+ e^2 \left(2\lambda \sum_{i=1}^{l-1} \sum_{j=i+1}^{l} \frac{Z_i Z_j}{|\mathbf{R}_i - \mathbf{R}_j|} + \sum_{i=1}^{l} Z_i \sum_{j=l+1}^{k} \frac{Z_j}{|\mathbf{R}_i - \mathbf{R}_j|} \right)$$

$$- \sum_{j=1}^{l} Z_j \, e^2 \int \mathrm{d}^3\mathbf{x} \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \rho_1(\mathbf{x}). \tag{2.355}$$

On account of (2.336), the expression within the square brackets of the $\mathbf{x}$-integral in the first term on the right-hand side of (2.355) is zero. This gives

$$\frac{\partial}{\partial\lambda} F\big[\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big]$$

$$=e^2\left(2\lambda\sum_{i=1}^{l-1}\sum_{j=i+1}^{l}\frac{Z_iZ_j}{|\mathbf{R}_i-\mathbf{R}_j|}+\sum_{i=1}^{l}Z_i\sum_{j=l+1}^{k}\frac{Z_j}{|\mathbf{R}_i-\mathbf{R}_j|}\right)$$

$$-\sum_{j=1}^{l}Z_j\,e^2\int\mathrm{d}^3\mathbf{x}\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\rho_1(\mathbf{x}). \tag{2.356}$$

An expression similar to the one in (2.355) for ρ_2 is

$$\frac{\partial}{\partial\lambda}F\big[\rho_2;\lambda Z_1,\dots,\lambda Z_l,\mathbf{R}_1,\dots,\mathbf{R}_l\big]$$

$$=e^2\left(2\lambda\sum_{i=1}^{l-1}\sum_{j=i+1}^{l}\frac{Z_iZ_j}{|\mathbf{R}_i-\mathbf{R}_j|}+\sum_{i=1}^{l}Z_i\sum_{j=l+1}^{k}\frac{Z_j}{|\mathbf{R}_i-\mathbf{R}_j|}\right)$$

$$-\sum_{j=1}^{l}Z_j\,e^2\int\mathrm{d}^3\mathbf{x}\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\rho_2(\mathbf{x}). \tag{2.357}$$

An expression similar to the one in (2.355) for ρ_3 is

$$\frac{\partial}{\partial\lambda}F\big[\rho_3;Z_l,\dots,Z_k\mathbf{R}_{\ell+1},\dots,\mathbf{R}_k\big]=e^2\sum_{i=1}^{\ell}Z_i\sum_{j=\ell+1}^{k}\frac{Z_j}{|\mathbf{R}_i-\mathbf{R}_j|}. \tag{2.358}$$

Hence from (2.346)

$$\frac{\partial}{\partial\lambda}f(\lambda)=\frac{\partial}{\partial\lambda}F\big[\rho_1;\lambda Z_1,\dots,\lambda Z_l,Z_{l+1},\dots,Z_k,\mathbf{R}_1,\dots,\mathbf{R}_k\big]$$

$$-\frac{\partial}{\partial\lambda}F\big[\rho_2;\lambda Z_1,\dots,\lambda Z_l,\mathbf{R}_1,\dots,\mathbf{R}_l\big]$$

$$-\frac{\partial}{\partial\lambda}F\big[\rho_3;Z_{l+1},\dots,Z_k,\mathbf{R}_{l+1},\dots,\mathbf{R}_k\big]$$

$$=\sum_{i=1}^{l}Z_i\left(\sum_{j=l+1}^{k}\frac{Z_j\,e^2}{|\mathbf{R}_i-\mathbf{R}_j|}-e^2\int\mathrm{d}^3\mathbf{x}\,\frac{\big[\rho_1(\mathbf{x})-\rho_2(\mathbf{x})\big]}{|\mathbf{x}-\mathbf{R}_i|}\right)$$

$$\equiv\sum_{i=1}^{l}Z_i\big[Q_1(\mathbf{R}_i)-Q_2(\mathbf{R}_i)\big]\geqslant 0 \tag{2.359}$$

where we have used (2.343), thus establishing (2.351). Here we note that the summation over j in (2.338) is from $(l+1)$ to k, while the one in (2.359) is over i from 1 to l, and there are no ambiguities in the expression in (2.359).

Accordingly, from (2.346), (2.351) we obtain

$$F\big[\rho_1; Z_1, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big] \geqslant F\big[\rho_2; Z_1, \ldots, Z_l, \mathbf{R}_1, \ldots, \mathbf{R}_l\big] \\ + F\big[\rho_3; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\big]. \qquad (2.360)$$

for any $1 \leqslant l < k$, where ρ_1, ρ_2, ρ_3 are the densities which provide the smallest values for the corresponding functionals, respectively.

Since l, k (with $1 \leqslant l < k$) are arbitrary natural numbers, (2.360) implies that

$$F\big[\rho_0; Z_1, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big] \geqslant \sum_{i=1}^{k} F\big[\rho^i_{\mathrm{TF}}; Z_i, \mathbf{R}_i\big] \qquad (2.361)$$

where each $F\big[\rho^i_{\mathrm{TF}}; Z_i, \mathbf{R}_i\big]$ is the TF functional.

From (2.179) the TF functional

$$-\frac{4\hbar^2}{2m}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3} [n_{TF}(\mathbf{x})]^{2/3} = -\frac{Ze^2}{|\mathbf{x}|} + e^2 \int \mathrm{d}^3\mathbf{x}' \frac{1}{|\mathbf{x}-\mathbf{x}'|}\, n_{TF}(\mathbf{x}') \qquad (2.362)$$

where $n_{\mathrm{TF}}(\mathbf{x})$ is the TF density considered earlier.

From (2.277), the ground-state energy of the TF atom is

$$E_{TF}(Z) = -\,0.68060 \left(\frac{2\underline{q}}{3\pi}\right)^{2/3} \left(\frac{2me^4}{\hbar^2}\right) Z^{7/3}. \qquad (2.363)$$

To evaluated with the TF density ρ^i_{TF} with nuclear charge $Z_i|e|$, situated at $\mathbf{R}_i$, and the mass m of each negatively charged particle simply scaled by β, we replac $\mathbf{x}$ by

$\mathbf{x}+\mathbf{R}_i$ and setting

$$\rho^i_{\mathrm{TF}}(\mathbf{x}+\mathbf{R}_i) = n_{\mathrm{TF}}(\mathbf{x})\Big|_{\substack{m\to m\beta\\ Z\to Z_i}} \tag{2.364}$$

That is,

$$\frac{2\hbar^2}{m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{2/3}\left(\rho^i_{\mathrm{TF}}(\mathbf{x})\right)^{2/3} = \frac{Z_i\, e^2}{|\mathbf{x}-\mathbf{R}_i|} - e^2\int \mathrm{d}^3\mathbf{x}'\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\rho^i_{\mathrm{TF}}(\mathbf{x}'). \tag{2.365}$$

From (2.333), (2.360), (2.363) and (2.365), we obtain

$$F\left[\rho; Z_1,\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k\right] \geqslant \beta E_{\mathrm{TF}}(1)\sum_{i=1}^{k} Z_i^{7/3} \tag{2.366}$$

for arbitrary positive $\rho(\mathbf{x})$, where

$$E_{\mathrm{TF}}(1) = -\,0.68060\left(\frac{2\underline{q}}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right) \tag{2.367}$$

corresponding to particles of masses m.

From (2.360), shows that a system identified by the parameters $[Z_1,\ldots, Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k]$ cannot have an (optimized) energy functional (2.329) less than the sum of the (optimized) energy functional of any two subsystems identified by parameters $\left[Z_1,\ldots,Z_l,\mathbf{R}_1,\ldots,\mathbf{R}_l\right]$, $\left[Z_{l+1},\ldots,Z_k,\mathbf{R}_{l+1},\ldots,\mathbf{R}_k\right]$, $l<k$. Because of this last property, the Theorem embodied in the inequalities (2.360), (2.361) is referred to as a “No Binding Theorem”.

From (2.329) and (2.367) we obtain,

$$\frac{16\underline{q}\hbar^2}{10\pi^2 m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\int \mathrm{d}^3\mathbf{x}\;[\rho(\mathbf{x})]^{5/3} - \sum_{j=1}^{k} Z_j\, e^2\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|}$$

$$+\,\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\,\rho(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\rho(\mathbf{x}') + \sum_{i<j}^{k}\frac{Z_iZ_j\, e^2}{|\mathbf{R}_i-\mathbf{R}_j|}$$

$$\geqslant \beta E_{\mathrm{TF}}(1)\sum_{i=1}^{k} Z_i^{7/3}. \tag{2.368}$$

The energy density functional, expressed in terms of the density $\rho(\mathbf{x})$ on the left-hand side of (2.368) is in the spirit of the TF energy functional considered earlier in (2.178) in the TF theory, with the mass m of the electron replaced by $m\beta$, and with the further generalization of including k nuclei, with the last term, involving '$Z_i Z_j\, e^2$', describing their interactions.

The inequality in (2.368) gives rise to a lower bound to the (repulsive) Coulomb potential energy of k particles of charges $Z_1|e|, \ldots, Z_k|e|$, or charges $-Z_1|e|, \ldots, -Z_k|e|$, i.e., for charges of the same sign as follows :

$$\sum_{i<j}^{k} \frac{Z_i Z_j\, e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \geqslant \sum_{j=1}^{k} Z_j\, e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|} - \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \rho(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \rho(\mathbf{x}') - \frac{16 \underline{q} \hbar^2}{10\pi^2 m\beta} \left(\frac{3\pi^2}{4\underline{q}} \right)^{5/3} \int \mathrm{d}^3\mathbf{x}\, \rho^{5/3}(\mathbf{x}) + \beta E_{\mathrm{TF}}(1) \sum_{i=1}^{k} Z_i^{7/3}. \quad (2.369)$$

In particular for the interaction of N electrons we have, with substitutions $k \to N$, $Z_j \to 1$, $\mathbf{R}_j \to \mathbf{x}_j$ for $j = 1, \ldots, N$:

$$\sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \geqslant \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} - \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \rho(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \rho(\mathbf{x}') - \frac{16 \underline{q} \hbar^2}{10\pi^2 m\beta} \left(\frac{3\pi^2}{4\underline{q}} \right)^{5/3} \int \mathrm{d}^3\mathbf{x}\, \rho^{5/3}(\mathbf{x}) + \beta N E_{\mathrm{TF}}(1). \quad (2.370)$$

Eqs.(2.368), (2.369) and (2.370) will be used in the next section to derive another lower bound for the exact ground-state energy of matter with Coulomb interactions by appropriately choosing $\rho(\mathbf{x})$ in (2.368).

2.6 Lower Bound for the Exact Ground-State Energy of Matter II

For anti-symmetric normalized functions $\Psi(\mathbf{x}_1\sigma_1, \ldots, \mathbf{x}_N\sigma_N)$ of N electrons, we define the expectation value of the Hamiltonian H in (2.320). To derive a lower bound to this expectation value, we recall the definition of electron density

$$\rho(\mathbf{x}) = N \sum_{\sigma_1,\ldots,\sigma_N} \int \mathrm{d}^3\mathbf{x}_2 \ldots \mathrm{d}^3\mathbf{x}_N \, |\Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, \ldots, \mathbf{x}_N\sigma_N)|^2 \tag{2.371}$$

normalized to

$$\int \mathrm{d}^3\mathbf{x} \; \rho(\mathbf{x}) = N. \tag{2.372}$$

Now we use a "Lieb-Thirring inequality (Lieb and Thirring, 1975) for the kinetic energy with spin multiplicity $\underline{q}$":

$$\sum_{i=1}^{N} \langle\Psi| \, \frac{\mathbf{p}_i^2}{2m} \, |\Psi\rangle \geqslant \frac{3}{5}\left(\frac{3\pi}{2\underline{q}}\right)^{2/3}\left(\frac{\hbar^2}{2m}\right) \int \mathrm{d}^3\mathbf{x} \; [\rho(\mathbf{x})]^{5/3}. \tag{2.373}$$

From (2.365), we have

$$\sum_{i=1}^{N}\sum_{j=1}^{k} \langle\Psi| \, \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \, |\Psi\rangle = \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x} \; \rho(\mathbf{x}) \, \frac{Z_j e^2}{|\mathbf{x} - \mathbf{R}_j|}. \tag{2.374}$$

From (2.123), we also have

$$\langle\Psi| \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} \, |\Psi\rangle = e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x}) \, \rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}. \tag{2.375}$$

By using (2.370), as applied to the third term on the right-hand side of (2.320), we obtain

$$\langle\Psi| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \, |\Psi\rangle \geqslant \langle\Psi| \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} \, |\Psi\rangle$$

$$- \langle\Psi| \frac{e^2}{2} \int d^3\mathbf{x}\, d^3\mathbf{x}' \, \frac{\rho(\mathbf{x})\, \rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \, |\Psi\rangle$$

$$- \langle\Psi| \frac{16\underline{q}\hbar^2}{10\pi^2 m\beta} \left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \int d^3\mathbf{x}\, \rho^{5/3}(\mathbf{x}) \, |\Psi\rangle$$

$$+ \langle\Psi| \, \beta N E_{\mathrm{TF}}(1) \, |\Psi\rangle \, . \tag{2.376}$$

Substitute (2.375) into the right-hand side of (2.376), to obtain

$$\langle\Psi| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \, |\Psi\rangle \geqslant e^2 \int d^3\mathbf{x}' \int d^3\mathbf{x} \, \frac{\rho(\mathbf{x})\, \rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

$$- \frac{e^2}{2} \int d^3\mathbf{x}\, d^3\mathbf{x}' \, \frac{\rho(\mathbf{x})\, \rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \, \langle\Psi|\Psi\rangle$$

$$- \frac{16\underline{q}\hbar^2}{10\pi^2 m\beta} \left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \int d^3\mathbf{x}\, \rho^{5/3}(\mathbf{x}) \, \langle\Psi|\Psi\rangle$$

$$+ \beta N E_{\mathrm{TF}}(1) \, \langle\Psi|\Psi\rangle \, . \tag{2.377}$$

From (2.377), for the Coulomb potential energy of repulsion part of the electrons

$$\langle\Psi| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \, |\Psi\rangle \geqslant \frac{e^2}{2} \int d^3\mathbf{x}' \int d^3\mathbf{x} \, \frac{\rho(\mathbf{x})\, \rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

$$- \frac{16\underline{q}\hbar^2}{10\pi^2 m\beta} \left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \int d^3\mathbf{x}\, \rho^{5/3}(\mathbf{x})$$

$$+ \beta N E_{\mathrm{TF}}(1). \tag{2.378}$$

Substitute (2.373), (2.374) and (2.378) into the right-hand side of (2.320), to obtain

$$\langle\Psi| \, H \, |\Psi\rangle \geqslant \frac{3}{5} \left(\frac{3\pi}{2\underline{q}}\right)^{2/3} \left(\frac{\hbar^2}{2m}\right) \int d^3\mathbf{x} \, [\rho(\mathbf{x})]^{5/3} - \sum_{j=1}^{k} \int d^3\mathbf{x}\, \rho(\mathbf{x}) \, \frac{Z_j e^2}{|\mathbf{x} - \mathbf{R}_j|}$$

$$+\frac{e^2}{2}\int d^3\mathbf{x}'\int d^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

$$-\frac{16\underline{q}\hbar^2}{10\pi^2 m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\int d^3\mathbf{x}\,\rho^{5/3}(\mathbf{x})$$

$$+\beta N E_{\mathrm{TF}}(1)+\sum_{i<j}^{k}\frac{Z_i Z_j e^2}{|\mathbf{R}_i-\mathbf{R}_j|}. \tag{2.379}$$

Consider the first term and the third term on the right-hand side of (2.379), to giving

$$\left[\frac{3}{5}\left(\frac{3\pi}{2\underline{q}}\right)^{2/3}\left(\frac{\hbar^2}{2m}\right)-\frac{16\underline{q}\hbar^2}{10\pi^2 m\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\right]\int d^3\mathbf{x}\;[\rho(\mathbf{x})]^{5/3}$$

$$=\left[\frac{3}{5}\left(\frac{3\pi}{2\underline{q}}\right)^{2/3}\left(\frac{\hbar^2}{2m}\right)-\frac{16\underline{q}}{5\pi^2\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\left(\frac{\hbar^2}{2m}\right)\right]\int d^3\mathbf{x}\;[\rho(\mathbf{x})]^{5/3}$$

$$=\left[\frac{3}{5}\left(\frac{3\pi}{2\underline{q}}\right)^{2/3}-\frac{16\underline{q}}{5\pi^2\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\right]\left(\frac{\hbar^2}{2m}\right)\int d^3\mathbf{x}\;[\rho(\mathbf{x})]^{5/3}$$

$$=\frac{16\underline{q}}{5\pi^2\beta'}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\left(\frac{\hbar^2}{2m}\right)\int d^3\mathbf{x}\;[\rho(\mathbf{x})]^{5/3} \tag{2.380}$$

where we have set

$$\left[\frac{3}{5}\left(\frac{3\pi}{2\underline{q}}\right)^{2/3}-\frac{16\underline{q}}{5\pi^2\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\right]=\frac{16\underline{q}}{5\pi^2\beta'}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \tag{2.381}$$

To obtain β, we rewrite (2.381) as

$$\frac{1}{\beta'}=\frac{\left[\frac{3}{5}\left(\frac{3\pi}{2\underline{q}}\right)^{2/3}-\frac{16\underline{q}}{5\pi^2\beta}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}\right]}{\frac{16\underline{q}}{5\pi^2}\left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3}}$$

$$=\frac{3}{5}\left(\frac{3\pi}{2\underline{q}}\right)^{2/3}\frac{5\pi^2}{16\underline{q}}\left(\frac{4\underline{q}}{3\pi^2}\right)^{5/3}-\frac{1}{\beta}$$

$$= \left(\frac{3\pi}{2\underline{q}}\right)^{2/3} \frac{3\pi^2}{16\underline{q}} \left(\frac{4\underline{q}}{3\pi^2}\right)^{5/3} - \frac{1}{\beta}$$

$$= \left(\frac{3\pi}{2\underline{q}}\right)^{2/3} \frac{1}{4} \left(\frac{4\underline{q}}{3\pi^2}\right)^{2/3} - \frac{1}{\beta}$$

$$= \left(\frac{3\pi}{2\underline{q}}\right)^{2/3} \frac{1}{4} \left(\frac{2\underline{q}}{3\pi}\right)^{2/3} \left(\frac{2}{\pi}\right)^{2/3} - \frac{1}{\beta}$$

$$= \left(\frac{1}{4\pi}\right)^{2/3} - \frac{1}{\beta}. \tag{2.382}$$

For a positive β' we must choose $\beta > (4\pi)^{2/3}$.

Substitute (2.381) into the right-hand side of (2.380), to obtain

$$\langle\Psi|\, H\,|\Psi\rangle \geqslant \frac{16\underline{q}}{5\pi^2\beta'} \left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \left(\frac{\hbar^2}{2m}\right) \int \mathrm{d}^3\mathbf{x}\, \rho^{5/3}(\mathbf{x}) - \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, \frac{Z_j e^2}{|\mathbf{x} - \mathbf{R}_j|}$$

$$+ \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\, \rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} + \sum_{i<j}^{k} \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|}$$

$$+ \beta N E_{\mathrm{TF}}(1). \tag{2.383}$$

Using (2.368), with β replaced by β', we obtain

$$\frac{16\underline{q}\hbar^2}{10\pi^2 m\beta'} \left(\frac{3\pi^2}{4\underline{q}}\right)^{5/3} \int \mathrm{d}^3\mathbf{x}\, \left[\rho(\mathbf{x})\right]^{5/3} - \sum_{j=1}^{k} Z_j\, e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|}$$

$$+ \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \rho(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \rho(\mathbf{x}') + \sum_{i<j}^{k} \frac{Z_i Z_j\, e^2}{|\mathbf{R}_i - \mathbf{R}_j|}$$

$$\geqslant \beta' E_{\mathrm{TF}}(1) \sum_{i=1}^{k} Z_i^{7/3}. \tag{2.384}$$

Substitute (2.384) into the right-hand side of (2.382), to obtain

$$\langle\Psi|\, H \,|\Psi\rangle \geqslant \beta' E_{\mathrm{TF}}(1) \sum_{i=1}^{k} Z_i^{7/3} + \beta N E_{\mathrm{TF}}(1). \tag{2.385}$$

Substitute (2.382) into the right-hand side of (2.385), to get

$$\langle\Psi|\, H \,|\Psi\rangle \geqslant E_{TF}(1) \left[\beta N + \frac{\sum\limits_{i=1}^{k} Z_i^{7/3}}{\left(\dfrac{1}{4\pi}\right)^{2/3} - \dfrac{1}{\beta}} \right]. \tag{2.386}$$

Optimizing over β, we obtain

$$\beta = (4\pi)^{2/3} \left[1 + \left(\frac{\sum\limits_{i=1}^{k} Z_i^{7/3}}{N} \right)^{1/2} \right] \tag{2.387}$$

giving finally a Lieb-Thirring bound

$$\langle\Psi|\, H \,|\Psi\rangle \geqslant E_{TF}(1)(4\pi)^{2/3} N \left[1 + \left(\sum_{i=1}^{k} \frac{Z_i^{7/3}}{N} \right)^{1/2} \right]^2 \tag{2.388}$$

where

$$E_{\mathrm{TF}}(1) = -\, 0.68060 \left(\frac{2q}{3\pi} \right)^{2/3} \left(\frac{2me^4}{\hbar^2} \right) \tag{2.389}$$

If Z corresponds to the nucleus with the maximum charge, in units of $|e|$, then

$$\sum_{i=1}^{k} Z_i^{7/3} \leqslant Z^{4/3} \sum_{i=1}^{k} Z_i = N Z^{4/3}. \tag{2.390}$$

Substitute (2.389) and (2.390) into the right-hand side of (2.388), giving for the ground-state energy E_N the explicit lower bound

$$E_N \geqslant -0.68060\,(4\pi)^{2/3}\left(\frac{2q}{3\pi}\right)^{2/3}\left(\frac{2me^4}{\hbar^2}\right)N\left[1+Z^{2/3}\right]^2 \tag{2.391}$$

where we have used the fact that Ψ is arbitrary and hence (2.387) is true for the ground-state as well. The numerical factor $0.68060(4\pi)^{2/3}$ can be further decreased by methods developed by Laptev, Weidl (1999). This, however, does not change the conclusion reached in this work.

CHAPTER III

RIGOROUS UPPER BOUNDS FOR THE GROUND-STATE ENERGY OF MATTER

3.1 Introduction

In this chapter we derive two upper bounds for the exact ground-state energy both involving a single power of $N-$the number of electrons in matter. The first bound (Sect. 3.2) is based on the following construction. We consider the N electrons localized in N non-overlapping ordered boxes, with the k nuclei placed at the centers of the first k boxes with appropriate choices of trial wavefunctions for the N electrons. The second bound (Sect. 3.4) is based on considering infinitely separated N clusters : k hydrogenic atoms, each in its ground-state, with nuclear charges $Z_1|e|,\dots,Z_k|e|$ each having one electron, and $(N-k)$ free electrons with vanishingly small kinetic energies. For this latter bound we need several estimates involving hydrogenic wavefunctions in their ground states. These detailed estimates are given in turn is Sect. 3.3.

3.2 Upper Bound for the Exact Ground-State Energy of Matter I

A quick and rather conservative upper bound for E_N may be derived by considering the following determinantal function

$$\Psi(\mathbf{r}_1\sigma_1,\dots,\mathbf{r}_N\sigma_N)=\frac{1}{\sqrt{N!}}\det\left[\psi_j(\mathbf{r},\sigma)\right] \tag{3.1}$$

for $j,k=1,\dots,N$, with matrix elements specified by the couple (j,k) and where

$$\psi_j(\mathbf{r},\sigma)=\psi\left(\mathbf{r}-\mathbf{L}^{(j)}\right)\chi_j(\sigma),\quad j=1,\dots,N. \tag{3.2}$$

Each orbital occurring in(3.1) is product of a spatial state $\psi(\mathbf{r})$, and a spin state $\chi(\sigma)$. Since orbitals of different spin are automatically orthogonal, Eq.(3.1) reduces to the condition that space orbitals corresponding to the same spin function be orthonormal. This assures that the wavefunction is normalized

$$\begin{aligned}\langle\Psi|\Psi\rangle &= \sum_{\sigma_1,\ldots,\sigma_N}^{n} \int \mathrm{d}^3\mathbf{r}_1, \mathrm{d}^3\mathbf{r}_2 ... \mathrm{d}^3\mathbf{r}_N \; \Psi^*(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, ..., \mathbf{r}_N\sigma_N) \; \Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, ..., \mathbf{r}_N\sigma_N) \\ &= \sum_{\sigma_1,\ldots,\sigma_N}^{n} \int \mathrm{d}^3\mathbf{r}_1, \mathrm{d}^3\mathbf{r}_2 ... \mathrm{d}^3\mathbf{r}_N \, |\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, ..., \mathbf{r}_N\sigma_N)|^2 \\ &= 1 \end{aligned} \tag{3.3}$$

with normalized spin functions $\chi_j(\sigma)$

$$\sum_\sigma \chi_i^*(\sigma)\,\chi_j(\sigma) = \delta_{ij}. \tag{3.4}$$

We choose the following localized single-particle trial wave function consistent with above construction by placing the N negatively charged particles in boxes of sides $2L \times 2L \times 2L$:

$$\psi(\mathbf{r}) = \prod_i \left(\frac{1}{\sqrt{L}} \cos\left(\frac{\pi x_i}{2L}\right)\right), \quad |x_i| \leqslant L. \tag{3.5}$$

$i = 1, 2, 3$, and is zero otherwise, $\mathbf{r} = (x_1, x_2, x_3)$. We choose the vectors $\mathbf{L}_1, \ldots, \mathbf{L}_N$ as follows

$$\mathbf{L}^{(j)} = jD(1,1,1), \quad j = 1, \ldots, N \tag{3.6}$$

where D is a constant and to ensure that all boxes are non-overlapping, we may choose

$$4L < D. \tag{3.7}$$

On the other hand, we place the k nuclei at the centers of the first k boxes, i.e., at $\mathbf{L}^{(1)}, \ldots, \mathbf{L}^{(k)}$ and hence we have $\mathbf{R}_j = \mathbf{L}^{(j)}$, with $j = 1, \ldots, k$. There are no nuclei in the remaining $(N-k)$ boxes, centered at $(\mathbf{L}^{(k+1)}, \ldots, \mathbf{L}^{(N)})$. All the boxes are of sides $2L \times 2L \times 2L$.

It is easy to see that the intervals : $\{jD - L \leqslant x_i \leqslant jD + L\}$, for $j = 1, \ldots, N$, are disjoint, for each $i = 1, 2, 3$, and the functions $\psi(\mathbf{r} - \mathbf{L}^{(j)})$ are then non-overlapping, and orthogonal with respect to *each* of the components x_i of $\mathbf{r}$. This construction consists of conveniently placing the k nuclei at $\mathbf{L}^{(1)}, \ldots, \mathbf{L}^{(k)}$ and one electron in each one of the k boxes with centers at $\mathbf{L}^{(1)}, \ldots, \mathbf{L}^{(k)}$. One electron is also placed in each of the remaining $(N-k)$ nuclei-free boxes with center at $\mathbf{L}^{(k+1)}, \ldots, \mathbf{L}^{(N)}$. The Coulomb potential being of long range, interactions occur between particles in the different boxes as well.

By using (3.2), for example, with $j, k = 1, 2, \ldots$, we obtain

$$\psi_1(\mathbf{r}_1, \sigma_1) = \psi\left(\mathbf{r}_1 - \mathbf{L}^{(1)}\right) \chi_1(\sigma), \tag{3.8a}$$

$$\psi_2(\mathbf{r}_2, \sigma_2) = \psi\left(\mathbf{r}_2 - \mathbf{L}^{(1)}\right) \chi_2(\sigma), \tag{3.8b}$$

$$\vdots$$

$$\psi_j(\mathbf{r}, \sigma) = \psi\left(\mathbf{r} - \mathbf{L}^{(j)}\right) \chi_j(\sigma), \tag{3.8c}$$

where

$$\mathbf{r}_k = (x_1^{(k)}, x_2^{(k)}, x_3^{(k)}). \tag{3.9}$$

By using (3.5), we obtain from (3.8), for $j = 1, 2, \ldots$ that

$$\psi(\mathbf{r}_1 - \mathbf{L}^{(1)}) = \frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x_1^{(1)} - L_1^{(1)}\right]}{2L}\right)\right] \frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x_2^{(1)} - L_2^{(1)}\right]}{2L}\right)\right]$$

$$\times \frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x_3^{(1)}-L_3^{(1)}\right]}{2L}\right)\right], \tag{3.10a}$$

$$\psi(\mathbf{r}_2-\mathbf{L}^{(2)}) = \frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x_1^{(2)}-L_1^{(2)}\right]}{2L}\right)\right]\frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x_2^{(2)}-L_2^{(2)}\right]}{2L}\right)\right]$$

$$\times \frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x_3^{(2)}-L_3^{(1)}\right]}{2L}\right)\right], \tag{3.10b}$$

$$\psi(\mathbf{r}_3-\mathbf{L}^{(3)}) = \frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x_1^{(3)}-L_1^{(3)}\right]}{2L}\right)\right]\frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x_2^{(3)}-L_2^{(3)}\right]}{2L}\right)\right]$$

$$\times \frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x_3^{(3)}-L_3^{(3)}\right]}{2L}\right)\right], \tag{3.10c}$$

$$\vdots$$

$$\psi(\mathbf{r}-\mathbf{L}^{(j)}) = \frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x^{(1)}-L_1^{(j)}\right]}{2L}\right)\right]\frac{1}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x^{(1)}-L_2^{(j)}\right]}{2L}\right)\right]$$

$$\times \frac{j}{\sqrt{L}}\left[\cos\left(\frac{\pi\left[x^{(1)}-L_3^{(1)}\right]}{2L}\right)\right]. \tag{3.10d}$$

From (3.10), we can rewrite the latter as

$$\psi(\mathbf{r}-\mathbf{L}^{(j)}) = \prod_i\left(\frac{1}{\sqrt{L}}\cos\left(\frac{\pi\left[x_i-L_i^{(j)}\right]}{2L}\right)\right), \quad |x_i-L_i^{(j)}| \leqslant L. \tag{3.11}$$

To obtain the upper bound we are seeking, we consider the expectation value of the Hamiltonian H with respect to anti-symmetric and normalized wavefunctions in

(3.1) defined through (3.3)–(3.7)

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{i=1}^{N} \sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{r}_i - \mathbf{R}_j|} + \sum_{i<j}^{k} \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{3.12}$$

where N is number of electrons and k is number of nuclei.

From (3.1) and (3.12), we obtain

$$\langle\Psi| H |\Psi\rangle = \langle\Psi| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} |\Psi\rangle + \langle\Psi| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} |\Psi\rangle - \langle\Psi| \sum_{i=1}^{N} \sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} |\Psi\rangle + \langle\Psi| \sum_{i<j}^{k} \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|} |\Psi\rangle \tag{3.13}$$

For example, for $N = 2$, by using (3.1), we obtain the anti-symmetric wavefunction

$$\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_1(\mathbf{r}_1, \sigma_1) & \psi_1(\mathbf{r}_2, \sigma_2) \\ \psi_2(\mathbf{r}_1, \sigma_1) & \psi_2(\mathbf{r}_2, \sigma_2) \end{vmatrix} \tag{3.14}$$

and can rewrite (3.14) as

$$\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \frac{1}{\sqrt{2}} \left[\psi_1(\mathbf{r}_1, \sigma_1)\, \psi_2(\mathbf{r}_2, \sigma_2) - \psi_2(\mathbf{r}_1, \sigma_1)\, \psi_1(\mathbf{r}_2, \sigma_2)\right] \tag{3.15}$$

By using (3.8) and (3.11), we obtain

$$\psi_1(\mathbf{r}_1, \sigma_1)\, \psi_2(\mathbf{r}_2, \sigma_2) = \chi_1(\sigma_1)\, \chi_2(\sigma_2) \left(\prod_{1}^{3} \left[\frac{1}{\sqrt{L}} \cos\left(\frac{\pi \left[x_i^{(1)} - L_i^{(1)}\right]}{2L} \right) \right] \right) \times \left(\prod_{1}^{3} \left[\frac{1}{\sqrt{L}} \cos\left(\frac{\pi \left[x_i^{(2)} - L_i^{(2)}\right]}{2L} \right) \right] \right) \tag{3.16}$$

and

$$\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2) = \chi_2(\sigma_1)\chi_1(\sigma_2)\left(\prod_1^3\left[\frac{1}{\sqrt{L}}\cos\left(\frac{\pi\left[x_i^{(1)}-L_i^{(2)}\right]}{2L}\right)\right]\right)$$
$$\times\left(\prod_1^3\left[\frac{1}{\sqrt{L}}\cos\left(\frac{\pi\left[x_i^{(2)}-L_i^{(1)}\right]}{2L}\right)\right]\right). \qquad (3.17)$$

To obtain the kinetic energy part on the first term on the right-hand side of (3.13), for example, for $N = 2$, we obtain

$$\langle\Psi|\sum_{i=1}^{2}\frac{\mathbf{p}_i^2}{2m}|\Psi\rangle = \langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle + \langle\Psi|\frac{\mathbf{p}_2^2}{2m}|\Psi\rangle \qquad (3.18)$$

where

$$\frac{\mathbf{p}_1^2}{2m} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x_1^{(1)\,2}} + \frac{\partial^2}{\partial x_2^{(1)\,2}} + \frac{\partial^2}{\partial x_3^{(1)\,2}}\right], \qquad (3.19a)$$

$$\frac{\mathbf{p}_2^2}{2m} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x_1^{(2)\,2}} + \frac{\partial^2}{\partial x_2^{(2)\,2}} + \frac{\partial^2}{\partial x_3^{(2)\,2}}\right]. \qquad (3.19b)$$

Hence we have

$$\frac{\partial^2}{\partial x_1^2}\cos\left(\frac{\pi\left[x_1-L_1^{(1)}\right]}{2L}\right) = -\left(\frac{\pi}{2L}\right)^2\cos\left(\frac{\pi\left[x_1-L_1^{(1)}\right]}{2L}\right), \qquad (3.20a)$$

$$\frac{\partial^2}{\partial x_2^2}\cos\left(\frac{\pi\left[x_2-L_2^{(1)}\right]}{2L}\right) = -\left(\frac{\pi}{2L}\right)^2\cos\left(\frac{\pi\left[x_2-L_2^{(1)}\right]}{2L}\right), \qquad (3.20b)$$

$$\frac{\partial^2}{\partial x_3^2}\cos\left(\frac{\pi\left[x_3-L_1^{(1)}\right]}{2L}\right) = -\left(\frac{\pi}{2L}\right)^2\cos\left(\frac{\pi\left[x_3-L_3^{(1)}\right]}{2L}\right). \qquad (3.20c)$$

By using (3.20) and from (3.15)–(3.19), we obtain

$$
\begin{aligned}
\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle =& \frac{\mathbf{p}_1^2}{2m}\left|\frac{1}{\sqrt{2}}\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_1,\sigma_1)-\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2)\right]\right\rangle \\
=& -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x_1^{(1)\,2}}+\frac{\partial^2}{\partial x_2^{(1)\,2}}+\frac{\partial^2}{\partial x_3^{(1)\,2}}\right]\frac{1}{\sqrt{2}}\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2) \\
&+\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x_1^{(1)\,2}}+\frac{\partial^2}{\partial x_2^{(1)\,2}}+\frac{\partial^2}{\partial x_3^{(1)\,2}}\right]\frac{1}{\sqrt{2}}\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2). \qquad (3.21)
\end{aligned}
$$

By applying (3.20) to the first term on the right-hand side of (3.21), we obtain

$$
\begin{aligned}
&-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x_1^{(1)\,2}}+\frac{\partial^2}{\partial x_2^{(1)\,2}}+\frac{\partial^2}{\partial x_3^{(1)\,2}}\right]\frac{1}{\sqrt{2}}\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2) \\
&=\frac{\hbar^2}{2m}\left[\left(\frac{\pi}{2L}\right)^2+\left(\frac{\pi}{2L}\right)^2+\left(\frac{\pi}{2L}\right)^2\right]\frac{1}{\sqrt{2}}\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2) \\
&=\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\frac{1}{\sqrt{2}}\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2). \qquad (3.22)
\end{aligned}
$$

By applying (3.20) to the second term on the right-hand side of (3.21), we obtain

$$
\begin{aligned}
&\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x_1^{(1)\,2}}+\frac{\partial^2}{\partial x_2^{(1)\,2}}+\frac{\partial^2}{\partial x_3^{(1)\,2}}\right]\frac{1}{\sqrt{2}}\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2) \\
&=\frac{\hbar^2}{2m}\left[-\left(\frac{\pi}{2L}\right)^2-\left(\frac{\pi}{2L}\right)^2-\left(\frac{\pi}{2L}\right)^2\right]\frac{1}{\sqrt{2}}\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2) \\
&=-\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\frac{1}{\sqrt{2}}\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2). \qquad (3.23)
\end{aligned}
$$

Substitute (3.22) and (3.23) into the right-hand side of (3.21), to obtain

$$
\begin{aligned}
\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle =& \frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\frac{1}{\sqrt{2}}\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2)-\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\frac{1}{\sqrt{2}}\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2) \\
=& \frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\frac{1}{\sqrt{2}}\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2)-\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2)\right]
\end{aligned}
$$

$$=\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2|\Psi\rangle\,. \tag{3.24}$$

From (3.24), we obtain that

$$\begin{aligned}\langle\Psi|\,\frac{\mathbf{p}_1^2}{2m}\,|\Psi\rangle &= \langle\Psi|\,\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2|\Psi\rangle \\ &= \frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\langle\Psi|\Psi\rangle \\ &= \frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2. \end{aligned}\tag{3.25}$$

By using (3.20) and from (3.15)–(3.19), we obtain

$$\begin{aligned}\frac{\mathbf{p}_2^2}{2m}\,|\Psi\rangle =& \frac{\mathbf{p}_2^2}{2m}\left|\frac{1}{\sqrt{2}}\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_1,\sigma_1)-\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2)\right]\right\rangle \\ =& -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x_1^{(2)\,2}}+\frac{\partial^2}{\partial x_2^{(2)\,2}}+\frac{\partial^2}{\partial x_3^{(2)\,2}}\right]\frac{1}{\sqrt{2}}\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2) \\ &+\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x_1^{(2)\,2}}+\frac{\partial^2}{\partial x_2^{(2)\,2}}+\frac{\partial^2}{\partial x_3^{(2)\,2}}\right]\frac{1}{\sqrt{2}}\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2). \end{aligned}\tag{3.26}$$

By applying (3.20) to the first term on the right-hand side of (3.26), we obtain

$$\begin{aligned}&-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x_1^{(2)\,2}}+\frac{\partial^2}{\partial x_2^{(2)\,2}}+\frac{\partial^2}{\partial x_3^{(2)\,2}}\right]\frac{1}{\sqrt{2}}\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2) \\ &=\frac{\hbar^2}{2m}\left[\left(\frac{\pi}{2L}\right)^2+\left(\frac{\pi}{2L}\right)^2+\left(\frac{\pi}{2L}\right)^2\right]\frac{1}{\sqrt{2}}\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2) \\ &=\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\frac{1}{\sqrt{2}}\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2). \end{aligned}\tag{3.27}$$

By applying (3.20) to the second term on the right-hand side of (3.26), we obtain

$$\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x_1^{(2)\,2}}+\frac{\partial^2}{\partial x_2^{(2)\,2}}+\frac{\partial^2}{\partial x_3^{(2)\,2}}\right]\frac{1}{\sqrt{2}}\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2)$$

$$=\frac{\hbar^2}{2m}\left[-\left(\frac{\pi}{2L}\right)^2-\left(\frac{\pi}{2L}\right)^2-\left(\frac{\pi}{2L}\right)^2\right]\frac{1}{\sqrt{2}}\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2)$$

$$=-\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\frac{1}{\sqrt{2}}\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2). \tag{3.28}$$

Substitute (3.27) and (3.28) into the right-hand side of (3.26), to obtain

$$\frac{\mathbf{p}_2^2}{2m}\left|\Psi\right\rangle=\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\frac{1}{\sqrt{2}}\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2)-\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\frac{1}{\sqrt{2}}\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2)$$

$$=\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\frac{1}{\sqrt{2}}\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\psi_2(\mathbf{r}_2,\sigma_2)-\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2)\right]$$

$$=\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\left|\Psi\right\rangle. \tag{3.29}$$

From (3.29), we obtain that

$$\left\langle\Psi\right|\frac{\mathbf{p}_2^2}{2m}\left|\Psi\right\rangle=\left\langle\Psi\right|\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\left|\Psi\right\rangle$$

$$=\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2\left\langle\Psi|\Psi\right\rangle$$

$$=\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2. \tag{3.30}$$

Substitute (3.25) and (3.28) into the right-hand side of (3.18), to obtain for the kinetic energy part for $N=2$:

$$\left\langle\Psi\right|\sum_{i=1}^{2}\frac{\mathbf{p}_i^2}{2m}\left|\Psi\right\rangle=\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2+\frac{3\hbar^2}{2m}\left(\frac{\pi}{2L}\right)^2$$

$$=2\left(\frac{3\hbar^2}{2m}\right)\left(\frac{\pi}{2L}\right)^2. \tag{3.31}$$

The analysis for arbitrary N is similar, by well know standard techniques (Bethe and

Jackiw, 1986, p.56), and we can write the kinetic energy part for N particles

$$\langle\Psi|\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}|\Psi\rangle = N\left(\frac{3\hbar^2}{2m}\right)\left(\frac{\pi}{2L}\right)^2. \tag{3.32}$$

To obtain the bound of electron-electron interaction, first we derive a lower bound for $|\mathbf{r}_i-\mathbf{r}_j|$, by using (3.6). We rewrite

$$(1,1,1) = 1\widehat{\mathbf{x}}_1 + 1\widehat{\mathbf{x}}_2 + 1\widehat{\mathbf{x}}_3, \tag{3.33a}$$

$$|(1,1,1)| = \sqrt{3}, \tag{3.33b}$$

$$|\mathbf{L}^{(j)}| = jD\sqrt{3}. \tag{3.33c}$$

with the $\widehat{\mathbf{x}}_i$ as unit vectors.

By using (3.33), we obtain

$$|\mathbf{L}^{(1)}| = D\sqrt{3}, \tag{3.34a}$$

$$|\mathbf{L}^{(2)}| = 2D\sqrt{3}, \tag{3.34b}$$

$$|\mathbf{L}^{(3)}| = 3D\sqrt{3}. \tag{3.34c}$$

and

$$|\mathbf{L}^{(1)}-\mathbf{L}^{(2)}| = D\sqrt{3}, \tag{3.35a}$$

$$|\mathbf{L}^{(1)}-\mathbf{L}^{(3)}| = 2D\sqrt{3}, \tag{3.35b}$$

$$|\mathbf{L}^{(1)}-\mathbf{L}^{(j)}| = (j-1)D\sqrt{3}, \tag{3.35c}$$

$$|\mathbf{L}^{(i)}-\mathbf{L}^{(j)}| \geqslant D\sqrt{3}\,,\ j>i \tag{3.35d}$$

From (3.35), we obtain the inequality

$$|\mathbf{L}^{(i)} - \mathbf{L}^{(j)}| \geqslant D\sqrt{3}. \tag{3.36}$$

Since the boxes are non-overlapping, we have from (3.33)–(3.36) , with boxes of sides $2L \times 2L \times 2L$. Due to the localizations of the functions $\psi_j(\mathbf{r}, \sigma)$, as described above, the electrons are well separated, and we may write

$$|\mathbf{r}_1 - \mathbf{r}_2| \geqslant |\mathbf{L}^{(1)} - \mathbf{L}^{(2)}| - 2\sqrt{3}\,L = D\sqrt{3} - 2\sqrt{3}\,L, \tag{3.37a}$$

$$|\mathbf{r}_1 - \mathbf{r}_3| \geqslant |\mathbf{L}^{(1)} - \mathbf{L}^{(3)}| - 2\sqrt{3}\,L = 2D\sqrt{3} - 2\sqrt{3}\,L, \tag{3.37b}$$

$$|\mathbf{r}_1 - \mathbf{r}_j| \geqslant |\mathbf{L}^{(1)} - \mathbf{L}^{(j)}| - 2\sqrt{3}\,L = (j-1)D\sqrt{3} - 2\sqrt{3}\,L, \tag{3.37c}$$

$$|\mathbf{r}_i - \mathbf{r}_j| \geqslant |\mathbf{L}^{(i)} - \mathbf{L}^{(j)}| - 2\sqrt{3}\,L = (j-i)D\sqrt{3} - 2\sqrt{3}\,L. \tag{3.37d}$$

From (3.37), we obtain

$$|\mathbf{r}_i - \mathbf{r}_j| \geqslant D\sqrt{3} - 2\sqrt{3}\,L. \tag{3.38}$$

Substitute (3.7) into the right-hand side of inequality (3.8), to obtain

$$|\mathbf{r}_i - \mathbf{r}_j| \geqslant D\sqrt{3} - 2\sqrt{3}\,\frac{D}{4}$$

$$= \frac{\sqrt{3}\,D}{2} = \frac{\sqrt{3}}{\sqrt{2}}\frac{D}{\sqrt{2}}$$

$$|\mathbf{r}_i - \mathbf{r}_j| \geqslant \frac{D}{\sqrt{2}} \tag{3.39}$$

and can rewrite (3.39) as

$$\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \leqslant \frac{\sqrt{2}}{D}. \tag{3.40}$$

By using (3.40), we rewrite the second term on the right-hand side of (3.13) as

$$\langle\Psi|\sum_{i<j}^{N}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}|\Psi\rangle=\sum_{i<j}^{N}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}\langle\Psi|\Psi\rangle$$

$$=\sum_{i<j}^{N}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}$$

$$\leqslant\frac{e^2\sqrt{2}}{D}\sum_{i<j}^{N}(1). \tag{3.41}$$

To obtain the bound of nuclei-electrons interaction, we use the conservative bound

$$-\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_je^2}{|\mathbf{r}_i-\mathbf{R}_j|}\leqslant-\sum_{i=1}^{k}\sum_{j=1}^{k}\frac{Z_je^2}{|\mathbf{r}_i-\mathbf{R}_j|}$$

$$\leqslant-\sum_{i=1}^{k}\frac{Z_ie^2}{|\mathbf{r}_i-\mathbf{R}_i|}$$

$$=-\sum_{i=1}^{k}\frac{Z_ie^2}{|\mathbf{r}_i-\mathbf{L}^{(i)}|}$$

$$\therefore\quad-\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_je^2}{|\mathbf{r}_i-\mathbf{R}_j|}\leqslant-\sum_{i=1}^{k}\frac{Z_ie^2}{|\mathbf{r}_i-\mathbf{L}^{(i)}|}. \tag{3.42}$$

Substitute (3.42) into the third term on the right-hand side of (3.13), to obtain

$$-\langle\Psi|\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_je^2}{|\mathbf{x}_i-\mathbf{R}_j|}|\Psi\rangle\leqslant-\langle\Psi|\sum_{i=1}^{k}\frac{Z_ie^2}{|\mathbf{r}_i-\mathbf{L}^{(i)}|}|\Psi\rangle. \tag{3.43}$$

From (3.1), (3.2) and (3.11), we obtain

$$\langle\Psi|\sum_{i=1}^{k}\frac{Z_ie^2}{|\mathbf{r}_i-\mathbf{L}^{(i)}|}|\Psi\rangle=\sum_{i=1}^{k}Z_ie^2\langle\Psi|\frac{1}{|\mathbf{r}_i-\mathbf{L}^{(i)}|}|\Psi\rangle$$

$$= \sum_{i=1}^{k} Z_i e^2 \int \mathrm{d}^3\mathbf{r}\, \frac{\psi_i^2(\mathbf{r}_i, \sigma_i)}{|\mathbf{r}_i - \mathbf{L}^{(i)}|}$$

$$= \sum_{i=1}^{k} Z_i e^2 \int \mathrm{d}^3\mathbf{r}\, \frac{\psi^2(\mathbf{r})}{|\mathbf{r}|} \tag{3.44}$$

with the spin normalization condition. Since $|x_i| < L$, $\mathbf{r} = \mathbf{x}_1 + \mathbf{x}_2 + \mathbf{x}_3$ and $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2 + \mathbf{L}_3$, we obtain

$$|\mathbf{r}| \leqslant |\mathbf{L}|$$

$$|\mathbf{r}| \leqslant \sqrt{L^2 + L^2 + L^2}$$

$$|\mathbf{r}| \leqslant \sqrt{3}\, L \tag{3.45}$$

where $|\mathbf{L}_1| = |\mathbf{L}_2| = |\mathbf{L}_3| = L$. We can rewrite (3.45) as

$$\frac{1}{|\mathbf{r}|} \geqslant \frac{1}{\sqrt{3}\, L}. \tag{3.46}$$

Substitute (3.46) into the right-hand side of (3.44), to obtain

$$\langle\Psi| \sum_{i=1}^{k} \frac{Z_i e^2}{|\mathbf{r}_i - \mathbf{L}^{(i)}|} |\Psi\rangle \geqslant \frac{1}{\sqrt{3}\, L} \sum_{i=1}^{k} Z_i e^2$$

$$= \frac{N e^2}{\sqrt{3}\, L}$$

$$\therefore \quad \langle\Psi| \sum_{i=1}^{k} \frac{Z_i e^2}{|\mathbf{r}_i - \mathbf{L}^{(i)}|} |\Psi\rangle \geqslant \frac{N e^2}{\sqrt{3}\, L} \tag{3.47}$$

with the normalization wavefunction condition $\int \mathrm{d}^3\mathbf{r}\, |\psi(\mathbf{r})|^2 = 1$ and $\sum_{i=1}^{k} Z_i = N$.

Multiply (3.47) by -1, to reverse the function of the inequality giving

$$-\langle\Psi|\sum_{i=1}^{k}\frac{Z_i e^2}{|\mathbf{r}_i-\mathbf{L}^{(i)}|}|\Psi\rangle \leqslant -\frac{Ne^2}{\sqrt{3}\,L}. \tag{3.48}$$

Substitute (3.48) into (3.43), to obtain the following upper bound for the nuclei-electrons interaction part :

$$-\langle\Psi|\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_j e^2}{|\mathbf{r}_i-\mathbf{R}_j|}|\Psi\rangle \leqslant -\frac{Ne^2}{\sqrt{3}\,L}. \tag{3.49}$$

To obtain an upper bound for the nuclei-nuclei interaction part, first we have to bound $|\mathbf{R}_i-\mathbf{R}_j|$. By using (3.6), we may choose

$$\mathbf{R}_j=\mathbf{L}^{(j)} \tag{3.50}$$

for $j=1,\ldots,k$.

Substitute (3.50) into the left-hand side of (3.36), to obtain

$$|\mathbf{R}_i-\mathbf{R}_j| \geqslant D\sqrt{3}\ \ ,i\neq j \tag{3.51}$$

and we can rewrite (3.51) as

$$\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|} \leqslant \frac{1}{D\sqrt{3}} \tag{3.52}$$

for $i\neq j$.

Substitute (3.52) into the fourth term on the right-hand side of (3.13), to obtain

$$\langle\Psi|\sum_{i<j}^{k}\frac{Z_iZ_j e^2}{|\mathbf{R}_i-\mathbf{R}_j|}|\Psi\rangle \leqslant \frac{e^2}{D\sqrt{3}}\sum_{i<j}^{k}Z_iZ_j \tag{3.53}$$

with the normalization wavefunction condition $\langle\Psi|\Psi\rangle=1$.

Substitute (3.32), (3.41), (3.49) and (3.53) into the right-hand side of (3.13), to

obtain

$$\langle\Psi|\,H\,|\Psi\rangle \leqslant N\left(\frac{3\hbar^2}{2m}\right)\left(\frac{\pi}{2L}\right)^2 + \frac{e^2\sqrt{2}}{D}\sum_{i<j}^{N}(1) - \frac{Ne^2}{\sqrt{3}\,L} + \frac{e^2}{D\sqrt{3}}\sum_{i<j}^{k} Z_i Z_j. \qquad (3.54)$$

By optimizing (3.54) over L, we obtain for the latter

$$L = \frac{3\sqrt{3}}{4}\left(\frac{\pi^2\hbar^2}{me^2}\right). \qquad (3.55)$$

Substitute (3.55) into the right-hand side of (3.54), to obtain

$$\langle\Psi|\,H\,|\Psi\rangle \leqslant -\frac{4}{9\pi^2}\left(\frac{me^4}{2\hbar^2}\right)N + \frac{e^2}{D}\left[\sqrt{2}\sum_{i<j}^{N}(1) + \frac{1}{\sqrt{3}}\sum_{i<j}^{k} Z_i Z_j\right]. \qquad (3.56)$$

We may choose D large enough to make the second term as small as we please in comparison to the first one (e.g., equal to $0.00031(me^2/2\hbar^2)N$) to obtain

$$\langle\Psi|\,H\,|\Psi\rangle \leqslant -0.0450\left(\frac{me^4}{2\hbar^2}\right)N. \qquad (3.57)$$

3.3 Basic Estimates Involving the Hydrogen Atom Wavefunction in the Ground-State

In this section we provide basic estimates involving the hydrogen atom wavefunction in the ground-state by considering the following determinantal function in (3.1) with normalized wavefunction and normalized spin functions $\chi_j(\sigma)$ and $\mathbf{r}_i$ is vector from the origin to electron e_i. Set $\mathbf{L}$, $\mathbf{L}'$ are vector from the origin to nucleus $Z|e|$ and $Z'|e|$ localization,

$$\mathbf{L} = L_0\mathbf{n}$$

$$\mathbf{L}' = L_0\mathbf{n}'$$

$$
\begin{aligned}
\mathbf{L}_1 =& L_0\mathbf{n}_1 \\
\mathbf{L}_2 =& L_0\mathbf{n}_2 \\
&\vdots \\
\mathbf{L}_i =& L_0\mathbf{n}_i
\end{aligned} \tag{3.58}
$$

with $L_0 = L_0'$ gives

$$\mathbf{L} - \mathbf{L}' = \mathbf{L_0} = L_0(\mathbf{n} - \mathbf{n}'), \tag{3.59a}$$

$$\mathbf{L}' - \mathbf{L} = \mathbf{L_0'} = L_0(\mathbf{n}' - \mathbf{n}), \tag{3.59b}$$

where L_0, L_0', are a constant.

The $\psi\left(\mathbf{r}-\mathbf{L}_j\right)$ are the hydrogen atom wavefunctions in the ground-state. These estimates will be then used to derive another upper bound to E_N. Consider the hydrogen atom wavefunction in the ground-state :

$$\psi\left(\mathbf{r}-\mathbf{L}_j\right) = \frac{\beta^{3/2}}{\sqrt{\pi}} \mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}_j|} \tag{3.60}$$

where

$$\beta = \frac{me^2}{\hbar^2} \tag{3.61}$$

and $1/\beta$ is the Bohr radius $\hbar^2/me^2$.

From (3.58), for H in (1.1), we obtain

$$\langle\Psi| H |\Psi\rangle = \langle\Psi| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} |\Psi\rangle - \langle\Psi| \sum_{i=1}^{N} \sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{r}_i - \mathbf{R}_j|} |\Psi\rangle$$

$$+\langle\Psi|\sum_{i<j}^{N}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}|\Psi\rangle+\langle\Psi|\sum_{i<j}^{k}\frac{Z_iZ_je^2}{|\mathbf{R}_i-\mathbf{R}_j|}|\Psi\rangle\,. \tag{3.62}$$

For $k = 1$, and noting that the hydrogen atom has 1 proton consisting the nucleus, $N = 1$ electron. In this case, we can ignore the third and the fourth term in the right-hand side of (3.62), and we obtain the expectation value of the Hamiltonian H for a hydrogen atom :

$$\begin{aligned}\langle\Psi|\,H\,|\Psi\rangle &= \langle\Psi|\sum_{i=1}^{1}\frac{\mathbf{p}_i^2}{2m}|\Psi\rangle-\langle\Psi|\sum_{i=1}^{1}\sum_{j=1}^{1}\frac{Z_je^2}{|\mathbf{r}_i-\mathbf{R}_j|}|\Psi\rangle\\ &= \langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle-\langle\Psi|\frac{Z_1e^2}{|\mathbf{r}_1-\mathbf{R}_1|}|\Psi\rangle\end{aligned} \tag{3.63}$$

where for the hydrogen atom ($k = 1$ and $N = 1$)

$$\Psi(\mathbf{r}_1,\sigma_1)=\psi_1(\mathbf{r}_1,\sigma_1)=\psi\left(\mathbf{r}_1-\mathbf{L}_1\right)\chi_1(\sigma)=\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\chi_1(\sigma). \tag{3.64}$$

We introduce the expectation value of kinetic energy as :

$$\langle\Psi|\frac{\mathbf{p}^2}{2m}|\Psi\rangle=\frac{\hbar^2}{2m}\int\mathrm{d}^3\mathbf{r}\;(\nabla\Psi^*(\mathbf{r}))\cdot(\nabla\Psi(\mathbf{r})) \tag{3.65}$$

and the expectation value of the potential as

$$\langle\Psi|\frac{1}{|\mathbf{r}|}|\Psi\rangle=\int\mathrm{d}^3\mathbf{r}\;\Psi^*(\mathbf{r})\frac{1}{|\mathbf{r}|}\Psi(\mathbf{r})\;\;,\;|\mathbf{r}|=r \tag{3.66}$$

with the wavefunction and spin normalization condition.

$$\langle\Psi(\mathbf{r},\sigma)|\Psi(\mathbf{r},\sigma)\rangle=1, \tag{3.67}$$

and with $\psi(\mathbf{r})$, $\mathbf{r}=\mathbf{r}_1-\mathbf{L}_1$, denoting the $\mathbf{r}$-dependent part in (3.64),

$$\langle\psi(\mathbf{r})|\psi(\mathbf{r})\rangle=\int\mathrm{d}^3\mathbf{r}\;|\psi(\mathbf{r})|^2=1, \tag{3.68a}$$

$$\sum_{\sigma} \chi_i^*(\sigma)\, \chi_j(\sigma) = 1, \tag{3.68b}$$

$$\nabla(r,\theta,\varphi) = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \varphi}, \tag{3.68c}$$

$$\int \mathrm{d}^3\mathbf{r}\,(.) = \int_0^\infty \int_0^\pi \int_0^{2\pi} r^2 \sin\theta \,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\varphi\,(.)\,. \tag{3.68d}$$

By substituting (3.64) into the right-hand side of (3.63), and using (3.60) and (3.65)–(3.68), we obtain for the expectation value of the kinetic energy of the hydrogen atom

$$\begin{aligned}
\langle\Psi|\,\frac{\mathbf{p}_1^2}{2m}\,|\Psi\rangle =& \frac{\hbar^2}{2m}\int \mathrm{d}^3\mathbf{r}_1\,\left(\nabla\Psi^*(\mathbf{r}_1,\sigma_1)\right)\cdot\left(\nabla\Psi(\mathbf{r}_1,\sigma_1)\right) \\
=& \frac{\hbar^2}{2m}\int \mathrm{d}^3\mathbf{r}_1\,\left(\nabla\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right)\cdot\left(\nabla\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right)\chi^*(\sigma)\,\chi(\sigma) \\
=& \frac{\hbar^2}{2m}\left(\frac{\beta^{3/2}}{\sqrt{\pi}}\right)^2\int \mathrm{d}^3\mathbf{r}_1\,\left(\nabla\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right)\cdot\left(\nabla\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right) \\
=& \frac{\hbar^2}{2m}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_1\,\left(\nabla\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right)\cdot\left(\nabla\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right).
\end{aligned} \tag{3.69}$$

Let $\mathbf{R} = \mathbf{r}_1 - \mathbf{L}_1$ and $|\mathbf{R}| = R$, then (3.69) becomes

$$\langle\Psi|\,\frac{\mathbf{p}_1^2}{2m}\,|\Psi\rangle = \frac{\hbar^2}{2m}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{R}\,\left(\nabla_R\,\mathrm{e}^{-\beta|R|}\right)\cdot\left(\nabla_R\,\mathrm{e}^{-\beta|R|}\right). \tag{3.70}$$

Consider the right-hand side of (3.70), by using (3.68), to obtain

$$\begin{aligned}
\nabla_R\,\mathrm{e}^{-\beta|R|} =& \hat{R}\frac{\partial}{\partial R}\left[\mathrm{e}^{-\beta R}\right] + \hat{\theta}\frac{1}{R}\frac{\partial}{\partial\theta}\left[\mathrm{e}^{-\beta R}\right] \\
=& -\beta\,\mathrm{e}^{-\beta R}\hat{R}
\end{aligned} \tag{3.71}$$

and

$$\nabla_R \,\mathrm{e}^{-\beta|R|} \cdot \nabla_R \,\mathrm{e}^{-\beta|R|} = \left(-\beta \,\mathrm{e}^{-\beta R}\right) \hat{R} \cdot \left(-\beta \,\mathrm{e}^{-\beta R}\right) \hat{R}$$

$$= \beta^2 \,\mathrm{e}^{-2\beta R}. \tag{3.72}$$

Substitute (3.72) into the right-hand side of (3.70), then use (3.68), to obtain

$$\langle\Psi| \frac{\mathbf{p}_1^2}{2m} |\Psi\rangle = \frac{\hbar^2}{2m} \frac{\beta^3}{\pi} \int \mathrm{d}^3\mathbf{R} \left(\nabla_R \,\mathrm{e}^{-\beta|R|}\right) \cdot \left(\nabla_R \,\mathrm{e}^{-\beta|R|}\right)$$

$$= \frac{\hbar^2}{2m} \frac{\beta^5}{\pi} \int_0^\infty \int_0^\pi \int_0^{2\pi} \mathrm{d}R \,\mathrm{d}\theta \,\mathrm{d}\varphi \; R^2 \,\mathrm{e}^{-2\beta R} \sin\theta$$

$$= \frac{\hbar^2}{2m} \frac{\beta^5}{\pi} 4\pi \int_0^\infty \mathrm{d}R \, R^2 \,\mathrm{e}^{-2\beta R}$$

$$= \frac{2\hbar^2 \beta^5}{m} \int_0^\infty \mathrm{d}R \, R^2 \,\mathrm{e}^{-2\beta R}. \tag{3.73}$$

Now let $u = 2\beta$, to rewrite the integral term on the right-hand side of (3.73) as

$$\int_0^\infty \mathrm{d}R \, R^2 \,\mathrm{e}^{-2\beta R} = \int_0^\infty \mathrm{d}R \, R^2 \,\mathrm{e}^{-uR}$$

$$= \frac{\partial^2}{\partial u^2} \int_0^\infty \mathrm{d}R \,\mathrm{e}^{-uR}$$

$$= \frac{\partial^2}{\partial u^2} \left[-\frac{\mathrm{e}^{-uR}}{u} \Big|_0^\infty \right]$$

$$= \frac{\partial^2}{\partial u^2} \left[0 - \left(-\frac{1}{u} \right) \right]$$

$$= \frac{\partial^2}{\partial u^2} \left(\frac{1}{u} \right)$$

$$= \frac{2}{u^3}$$

$$=\frac{1}{4\beta^3}. \tag{3.74}$$

Substitute (3.74) into the right-hand side of (3.73), to obtain for the expectation value of kinetic energy of the hydrogen atom

$$\begin{aligned}\langle\Psi|\,\frac{\mathbf{p}_1^2}{2m}\,|\Psi\rangle =&\frac{2\hbar^2\beta^5}{m}\int_0^\infty \mathrm{d}R\,R^2\,\mathrm{e}^{-2\beta R}\\ =&\frac{2\hbar^2\beta^5}{m}\frac{1}{4\beta^3}\\ =&\frac{\hbar^2\beta^2}{2m}.\end{aligned} \tag{3.75}$$

For the second term on the right-hand side of (3.63), the expectation value of nucleus-electron interaction, Set $\mathbf{R}=\mathbf{L}$, to obtain

$$\begin{aligned}-\langle\Psi|\,\frac{Z_1e^2}{|\mathbf{r}_1-\mathbf{R}_1|}\,|\Psi\rangle =& -\langle\Psi|\,\frac{Z_1e^2}{|\mathbf{r}_1-\mathbf{L}_1|}\,|\Psi\rangle\\ =& -Z_1e^2\int \mathrm{d}^3\mathbf{r}_1\,\Psi^*(\mathbf{r}_1,\sigma_1)\cdot\frac{1}{|\mathbf{r}_1-\mathbf{L}_1|}\Psi(\mathbf{r}_1,\sigma_1)\\ =& -Z_1e^2\int \mathrm{d}^3\mathbf{r}_1\,\psi^*(\mathbf{r}_1-\mathbf{L}_1)\cdot\frac{1}{|\mathbf{r}_1-\mathbf{L}_1|}\,(\psi(\mathbf{r}_1-\mathbf{L}_1))\,\chi^*(\sigma)\,\chi(\sigma)\\ =& -Z_1e^2\int \mathrm{d}^3\mathbf{r}_1\,\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\cdot\frac{1}{|\mathbf{r}_1-\mathbf{L}_1|}\,\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\\ =& -\frac{Z_1e^2\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_1\frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_1|}.\end{aligned} \tag{3.76}$$

where $\mathbf{L}_1=\mathbf{R}_1$ is vector going from the origin to the nucleus of charge $Z_1|e|$.

Let $\mathbf{D}=\mathbf{r}_1-\mathbf{L}_1$ and $|\mathbf{D}|=D$, then substitute into the right-hand side of (3.76), to obtain

$$-\langle\Psi|\,\frac{Z_1e^2}{|\mathbf{r}_1-\mathbf{R}_1|}\,|\Psi\rangle = -\frac{Z_1e^2\beta^3}{\pi}\int \mathrm{d}^3\mathbf{D}\frac{\mathrm{e}^{-2\beta|\mathbf{D}|}}{|\mathbf{D}|}$$

$$= -\frac{Z_1 e^2 \beta^3}{\pi} \int_0^\infty \mathrm{d}D \, \frac{D^2 \mathrm{e}^{-2\beta D}}{D} \int_0^\pi \int_0^{2\pi} \mathrm{d}\theta \, \sin\theta \mathrm{d}\varphi$$

$$= -\frac{Z_1 e^2 \beta^3}{\pi}(4\pi) \int_0^\infty \mathrm{d}D \, D\mathrm{e}^{-2\beta D}$$

$$= -4Z_1 e^2 \beta^3 \left(\frac{\mathrm{e}^{-2\beta D}}{-2\beta} \left[D - \frac{1}{-2\beta} \right] \right) \Bigg|_0^\infty$$

$$= -4Z_1 e^2 \beta^3 \left(-\frac{1}{4\beta^2} \right)$$

$$= -Z_1 e^2 \beta$$

$$\therefore \quad -\langle \Psi | \frac{Z_1 e^2}{|\mathbf{r}_1 - \mathbf{R}_1|} | \Psi \rangle = -Z_1 e^2 \beta. \tag{3.77}$$

Substitute (3.75) and (3.77) into the right-hand side of (3.63), to obtain

$$\langle \Psi | H | \Psi \rangle = \frac{\hbar^2 \beta^2}{2m} - Z_1 e^2 \beta. \tag{3.78}$$

With β as defined in (3.61), we obtain the following for the ground-state energy of a hydrogen atom as

$$\langle \Psi | H | \Psi \rangle = \frac{\hbar^2}{2m} \left(\frac{me^2}{\hbar^2} \right)^2 - Z_1 e^2 \left(\frac{me^2}{\hbar^2} \right)$$

$$= -\frac{me^4}{2m}$$

$$\langle \Psi | H | \Psi \rangle = -\frac{me^4}{2\hbar^2} \quad , Z_1 = 1 \tag{3.79}$$

as expected.

For $k = 2$, $Z_1 + Z_2 = 2$, gives $Z_1 = Z_2 = 1$, $N = 2$, giving

$$\langle \Psi | H | \Psi \rangle = \langle \Psi | \sum_{i=1}^{2} \frac{\mathbf{p}_i^2}{2m} | \Psi \rangle - \langle \Psi | \sum_{i=1}^{2} \sum_{j=1}^{2} \frac{Z_j e^2}{|\mathbf{r}_i - \mathbf{R}_j|} | \Psi \rangle$$

$$+ \langle\Psi| \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} |\Psi\rangle + \langle\Psi| \frac{Z_1 Z_2 e^2}{|\mathbf{R}_1 - \mathbf{R}_2|} |\Psi\rangle \tag{3.80}$$

where the anti-symmetric wavefunction for $k = 2$ is given by

$$\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_1(\mathbf{r}_1, \sigma_1) & \psi_1(\mathbf{r}_2, \sigma_2) \\ \psi_2(\mathbf{r}_1, \sigma_1) & \psi_2(\mathbf{r}_2, \sigma_2) \end{vmatrix} \tag{3.81}$$

which can be rewritten as

$$\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \frac{1}{\sqrt{2}} \left[\psi_1(\mathbf{r}_1, \sigma_1)\, \psi_2(\mathbf{r}_2, \sigma_2) - \psi_2(\mathbf{r}_1, \sigma_1)\, \psi_1(\mathbf{r}_2, \sigma_2)\right] \tag{3.82}$$

and as before we have the hydrogen atom wavefunction :

$$\psi\left(\mathbf{r} - \mathbf{L}\right) = \frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}|}. \tag{3.83}$$

From (3.59) and (3.82), we obtain

$$\psi_1(\mathbf{r}_1, \sigma_1) = \psi\left(\mathbf{r}_1 - \mathbf{L}_1\right) \chi_1(\sigma) = \frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \chi_1(\sigma_1), \tag{3.84a}$$

$$\psi_1(\mathbf{r}_2, \sigma_2) = \psi\left(\mathbf{r}_2 - \mathbf{L}_1\right) \chi_2(\sigma) = \frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \chi_2(\sigma_2), \tag{3.84b}$$

$$\psi_2(\mathbf{r}_1, \sigma_1) = \psi\left(\mathbf{r}_1 - \mathbf{L}_2\right) \chi_2(\sigma) = \frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \chi_1(\sigma_1), \tag{3.84c}$$

$$\psi_2(\mathbf{r}_2, \sigma_2) = \psi\left(\mathbf{r}_2 - \mathbf{L}_2\right) \chi_2(\sigma) = \frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \chi_2(\sigma_2). \tag{3.84d}$$

Substitute (3.84) into the first term on the right-hand side of (3.82), to obtain

$$\psi_1(\mathbf{r}_1, \sigma_1)\, \psi_2(\mathbf{r}_2, \sigma_2) = \frac{\beta^3}{\pi}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \chi_1(\sigma_1)\, \chi_2(\sigma_2). \tag{3.85}$$

Substitute (3.84) into the second term on the right-hand side of (3.82), to obtain

$$\psi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2) = \frac{\beta^3}{\pi}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\chi_1(\sigma_2)\,\chi_2(\sigma_1) \tag{3.86}$$

then substitute (3.85) and (3.86) into the right-hand side of (3.82), to obtain for the anti-symmetric wavefunction of hydrogen atom with $k=2$

$$\Psi(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2) = \frac{\beta^3}{\pi\sqrt{2}}\Big[\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\chi_1(\sigma_1)\,\chi_2(\sigma_2)$$
$$-\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\chi_1(\sigma_2)\,\chi_2(\sigma_1)\Big]\,. \tag{3.87}$$

From (3.80), the expectation value of kinetic energy for $k=N=2$ is

$$\langle\Psi|\sum_{i=1}^{2}\frac{\mathbf{p}_i^2}{2m}|\Psi\rangle = \langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle + \langle\Psi|\frac{\mathbf{p}_2^2}{2m}|\Psi\rangle \tag{3.88}$$

where

$$\langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle = \langle\Psi|\,T_1\,|\Psi\rangle = \frac{\hbar^2}{2m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\left[\nabla_1\Psi^*\right]\cdot\left[\nabla_1\Psi\right], \tag{3.89a}$$

$$\langle\Psi|\frac{\mathbf{p}_2^2}{2m}|\Psi\rangle = \langle\Psi|\,T_2\,|\Psi\rangle = \frac{\hbar^2}{2m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\left[\nabla_2\Psi^*\right]\cdot\left[\nabla_2\Psi\right], \tag{3.89b}$$

and from (3.68c), for no φ dependence and $\hat{\theta}\cdot\hat{\mathbf{r}}=0$, gives

$$\nabla(r_1,\theta) = \hat{r}_1\frac{\partial}{\partial r_1} + \hat{\theta}\frac{1}{r_1}\frac{\partial}{\partial\theta}, \tag{3.90a}$$

$$\nabla(r_2,\theta) = \hat{r}_2\frac{\partial}{\partial r_2} + \hat{\theta}\frac{1}{r_2}\frac{\partial}{\partial\theta}. \tag{3.90b}$$

Substitute (3.87) into (3.89), to obtain

$$\nabla_1\Psi = \frac{\beta^3}{\pi\sqrt{2}}\Big[\chi_1(\sigma_1)\,\chi_2(\sigma_2)\,\nabla_1\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right)$$

$$-\chi_2(\sigma_1)\,\chi_1(\sigma_2)\,\nabla_1\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right)\Big]$$

$$= C_1\left[\chi_a\,\nabla_1\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right)\right.$$

$$\left.-\chi_b\,\nabla_1\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right)\right] \tag{3.91}$$

and

$$\nabla_1\Psi^* = C_1^*\left[\chi_a^*\,\nabla_1\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right)^*\right.$$

$$\left.-\chi_b^*\,\nabla_1\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right)^*\right] \tag{3.92}$$

where

$$C_1 = \frac{\beta^3}{\pi\sqrt{2}} = C_1^*, \tag{3.93a}$$

$$\chi_a = \chi_1(\sigma_1)\,\chi_2(\sigma_2), \tag{3.93b}$$

$$\chi_b = \chi_2(\sigma_1)\,\chi_1(\sigma_2). \tag{3.93c}$$

From (3.4), (3.91) and (3.92), we obtain

$$\nabla_1\Psi^*\cdot\nabla_1\Psi$$

$$= \left\{\frac{\beta^3}{\pi\sqrt{2}}\frac{\beta^3}{\pi\sqrt{2}}\right\}$$

$$\times\left[\chi_a^*\,\nabla_1\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right)^* - \chi_b^*\,\nabla_1\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right)^*\right]$$

$$\cdot\left[\chi_a\,\nabla_1\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right) - \chi_b\,\nabla_1\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right)\right]$$

$$= \left\{\frac{\beta^3}{\pi\sqrt{2}}\frac{\beta^3}{\pi\sqrt{2}}\right\}$$

$$\times \Big\{ [\chi_a^* \cdot \chi_a] \Big[\nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right)^* \cdot \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right) \Big]$$

$$+ [\chi_b^* \cdot \chi_b] \Big[\nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right)^* \cdot \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right) \Big]$$

$$- [\chi_a^* \cdot \chi_b] \Big[\nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right)^* \cdot \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right) \Big]$$

$$- [\chi_b^* \cdot \chi_a] \Big[\nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right)^* \cdot \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right) \Big] \Big\}$$

$$= \left\{ \frac{\beta^3}{\pi\sqrt{2}} \frac{\beta^3}{\pi\sqrt{2}} \right\}$$

$$\times \left\{ \delta_{aa} \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right) \cdot \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right) \right.$$

$$+ \delta_{bb} \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right) \cdot \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right)$$

$$\left. -2\delta_{ab} \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right) \cdot \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right) \right\} . \qquad (3.94)$$

Substitute (3.94) into (3.89a), to obtain

$$\langle \Psi | \frac{\mathbf{p}_1^2}{2m} | \Psi \rangle = \frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \; [\nabla_1 \Psi^*(\mathbf{r})] \cdot [\nabla_1 \Psi(\mathbf{r})]$$

$$= \frac{\hbar^2}{2m} \frac{\beta^3}{2\pi} \frac{\beta^3}{\pi} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2$$

$$\times \left\{ \delta_{aa} \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right) \cdot \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right) \right.$$

$$+ \delta_{bb} \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right) \cdot \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right)$$

$$\left. -2\delta_{ab} \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right) \cdot \nabla_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right) \right\}$$

$$= \frac{\hbar^2}{2m} \frac{\beta^3}{2\pi} \left\{ \int \mathrm{d}^3\mathbf{r}_1 \, \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \cdot \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \right.$$

$$\times \int \mathrm{d}^3\mathbf{r}_2 \left| \frac{\beta^{3/2}}{\sqrt{\pi}} \; \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right|^2 \delta_{aa}$$

$$
\begin{aligned}
&+ \int \mathrm{d}^3\mathbf{r}_1 \, \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \cdot \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \\
&\quad \times \int \mathrm{d}^3\mathbf{r}_2 \left| \frac{\beta^{3/2}}{\sqrt{\pi}} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right|^2 \delta_{bb} \\
&- 2\,\delta_{ab} \int \mathrm{d}^3\mathbf{r}_1 \, \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \cdot \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \\
&\quad \times \left(\frac{\beta^3}{\pi}\right) \int \mathrm{d}^3\mathbf{r}_2 \left(\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right) \left(\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right) \Bigg\} \\
=&\frac{\hbar^2}{2m}\frac{\beta^3}{2\pi} \Bigg\{ \int \mathrm{d}^3\mathbf{r}_1 \, \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \cdot \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \\
&+ \int \mathrm{d}^3\mathbf{r}_1 \, \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \cdot \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \\
&- 2\delta_{ab} \int \mathrm{d}^3\mathbf{r}_1 \, \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \cdot \nabla_1 \, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \\
&\quad \times \left(\frac{\beta^3}{\pi}\right) \int \mathrm{d}^3\mathbf{r}_2 \left(\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right) \left(\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right) \Bigg\}
\end{aligned} \tag{3.95}
$$

where

$$
\int \mathrm{d}^3\mathbf{r}_2 \left| \frac{\beta^{3/2}}{\sqrt{\pi}} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \right|^2 \delta_{aa} =1, \tag{3.96a}
$$

$$
\int \mathrm{d}^3\mathbf{r}_2 \left| \frac{\beta^{3/2}}{\sqrt{\pi}} \, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right|^2 \delta_{bb} =1. \tag{3.96b}
$$

To evaluate the integrals in (3.95), we set $\mathbf{R}_i = \mathbf{r}_i - \mathbf{L}$, for $\mathbf{L} = \mathbf{L}'$:

$$
\int \mathrm{d}^3\mathbf{r}_i \, \nabla_i \mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|} \cdot \nabla_i \mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|} = \int \mathrm{d}^3\mathbf{R}_i \, \nabla_i \mathrm{e}^{-\beta|\mathbf{R}|} \cdot \nabla_i \mathrm{e}^{-\beta|\mathbf{R}|} \tag{3.97}
$$

where $\mathbf{L}'$ is vector from the origin to nucleus $Z'|e|$.

In reference to the right-hand side of (3.97), we have

$$
\nabla_{r_i} \left(\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}\right) =\nabla_{R_i} \left(\mathrm{e}^{-\beta|\mathbf{R}_i|}\right)
$$

$$=\hat{R}\frac{\partial}{\partial R_i}\left(\mathrm{e}^{-\beta R_i}\right)$$

$$=-\beta\,\mathrm{e}^{-\beta R_i}\hat{R}. \tag{3.98}$$

By using (3.98), we obtain for the dot product :

$$\begin{aligned}\nabla_{r_i}\left(\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}\right)\cdot\nabla_{r_i}\left(\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}\right) =&\nabla_{R_i}\left(\mathrm{e}^{-\beta|\mathbf{R}_i|}\right)\cdot\nabla_{R_i}\left(\mathrm{e}^{-\beta|\mathbf{R}_i|}\right)\\ =&\left(-\beta\,\mathrm{e}^{-\beta R_i}\right)\hat{R}\cdot\left(-\beta\,\mathrm{e}^{-\beta R_i}\right)\hat{R}\\ =&\beta^2\mathrm{e}^{-2\beta R_i}.\end{aligned} \tag{3.99}$$

Substitute (3.99) into (3.97), for $\mathbf{L}=\mathbf{L}'$, to obtain

$$\begin{aligned}\int \mathrm{d}^3\mathbf{r}_i\,\nabla_i\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}\cdot\nabla_i\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|} =&\int \mathrm{d}^3\mathbf{R}_i\,\beta^2\mathrm{e}^{-2\beta R_i}\\ =&\beta^2\int_0^\infty\int_0^\pi\int_0^{2\pi}\mathrm{d}R_i\,\mathrm{d}\theta\,\mathrm{d}\varphi\;R_i^2\,\mathrm{e}^{-2\beta R_i}\sin\theta\\ =&\beta^2(4\pi)\int_0^\infty\mathrm{d}R_i\,R_i^2\,\mathrm{e}^{-2\beta R_i}\\ =&\beta^2(4\pi)\int_0^\infty\mathrm{d}R\,R^2\,\mathrm{e}^{-uR}\qquad,u=2\beta\\ =&\beta^2(4\pi)\frac{\partial^2}{\partial u^2}\int_0^\infty\mathrm{d}R\,\mathrm{e}^{-uR}\\ =&\beta^2(4\pi)\frac{\partial^2}{\partial u^2}\left[-\frac{\mathrm{e}^{-uR}}{u}\Big|_0^\infty\right]\\ =&\beta^2(4\pi)\frac{\partial^2}{\partial u^2}\left[0-\left(-\frac{1}{u}\right)\right]\\ =&\beta^2(4\pi)\frac{\partial^2}{\partial u^2}\left(\frac{1}{u}\right)\end{aligned}$$

$$=\beta^2(4\pi)\frac{2}{u^3}$$

$$=\beta^2(4\pi)\frac{1}{4\beta^3}$$

$$=\frac{\pi}{\beta}$$

$$\therefore \quad \int d^3\mathbf{r}_i\, \nabla_i e^{-\beta|\mathbf{r}_i-\mathbf{L}|}\cdot\nabla_i e^{-\beta|\mathbf{r}_i-\mathbf{L}|} = \frac{\pi}{\beta}. \tag{3.100}$$

For $\mathbf{L} \neq \mathbf{L}'$, we obtain

$$\nabla_i e^{-\beta|\mathbf{r}_i-\mathbf{L}|} = \nabla_i e^{-\beta\sqrt{r_i^2-2r_iL\cos\theta+L^2}}$$

$$= \left(\hat{r}\frac{\partial}{\partial r_i}+\hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta}\right)e^{-\beta\sqrt{r_i^2-2r_iL\cos\theta+L^2}}$$

$$= -\beta\left[\frac{(r_i-L\cos\theta)\,\hat{r}}{\sqrt{r_i^2-2r_iL\cos\theta+L^2}}+\frac{L\sin\theta\,\hat{\theta}}{\sqrt{r_i^2-2r_iL\cos\theta+L^2}}\right]$$

$$\times\, e^{-\beta\sqrt{r_i^2-2r_iL\cos\theta+L^2}}$$

$$= -\beta\left[\frac{(r_i-L\cos\theta)\,\hat{r}}{|\mathbf{r}_i-\mathbf{L}|}+\frac{L\sin\theta\,\hat{\theta}}{|\mathbf{r}_i-\mathbf{L}|}\right]e^{-\beta|\mathbf{r}_i-\mathbf{L}|}. \tag{3.101}$$

From (3.101), we replace $\mathbf{L}$ by $\mathbf{L}'$, to obtain

$$\nabla_i e^{-\beta|\mathbf{r}_i-\mathbf{L}'|} = -\beta\left[\frac{(r_i-L'\cos\theta)\,\hat{r}}{|\mathbf{r}_i-\mathbf{L}'|}+\frac{L'\sin\theta\,\hat{\theta}}{|\mathbf{r}_i-\mathbf{L}'|}\right]e^{-\beta|\mathbf{r}_i-\mathbf{L}'|}. \tag{3.102}$$

By using (3.97), from (3.101) and (3.102), we obtain

$$\int d^3\mathbf{r}_i\, \nabla_i e^{-\beta|\mathbf{r}_i-\mathbf{L}|}\cdot\nabla_i e^{-\beta-\beta|\mathbf{r}_i-\mathbf{L}'|}$$

$$=\beta^2\int d^3\mathbf{r}_i\left[\frac{(r_i-L\cos\theta)\,\hat{r}}{|\mathbf{r}_i-\mathbf{L}|}+\frac{L\sin\theta\,\hat{\theta}}{|\mathbf{r}_i-\mathbf{L}|}\right]e^{-\beta|\mathbf{r}_i-\mathbf{L}|}$$

$$\cdot \left[\frac{(r_i - L' \cos\theta)\,\hat{r}}{|\mathbf{r}_i - \mathbf{L'}|} + \frac{L' \sin\theta\,\hat{\theta}}{|\mathbf{r}_i - \mathbf{L}'|}\right] \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|}$$

$$=\beta^2 \int \mathrm{d}^3\mathbf{r}_i \left[\frac{(r_i - L\cos\theta)(r_i - L'\cos\theta)}{|\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i - \mathbf{L}'|} + \frac{L\sin\theta\,L'\sin\theta}{|\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i - \mathbf{L}|}\right]$$

$$\times\, \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|}$$

$$=\beta^2 \int \mathrm{d}^3\mathbf{r}_i \left[\frac{\mathbf{r}_i \cdot (\mathbf{r}_i - \mathbf{L})\,\mathbf{r}_i \cdot (\mathbf{r}_i - \mathbf{L}')}{r_i^2\,|\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i - \mathbf{L}'|} + \frac{LL'\sin\theta\,\sin\theta}{|\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i - \mathbf{L}|}\right]$$

$$\times\, \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|}$$

$$\leqslant\beta^2 \int \mathrm{d}^3\mathbf{r}_i \left[\frac{|\mathbf{r}_i||\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i||\mathbf{r}_i - \mathbf{L}'|}{r_i^2\,|\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i - \mathbf{L}'|} + \frac{LL'\sin\theta\,\sin\theta}{|\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i - \mathbf{L}|}\right] \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|}$$

$$\leqslant\beta^2 \int \mathrm{d}^3\mathbf{r}_i \left[\frac{|\mathbf{r}_i||\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i||\mathbf{r}_i - \mathbf{L}'|}{r_i^2\,|\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i - \mathbf{L}'|} + \frac{LL'}{|\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i - \mathbf{L}|}\right] \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|}$$

$$=\beta^2 \int \mathrm{d}^3\mathbf{r}_i \left[1 + \frac{LL'}{|\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i - \mathbf{L}|}\right] \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|}$$

$$=\beta^2 \int \mathrm{d}^3\mathbf{r}_i \left[\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|} + \frac{LL'}{|\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i - \mathbf{L}|}\,\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|}\right]$$

$$=\beta^2 \int \mathrm{d}^3\mathbf{r}_i\, \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|}$$

$$+\,\beta^2 \int \mathrm{d}^3\mathbf{r}_i \frac{LL'}{|\mathbf{r}_i - \mathbf{L}|\,|\mathbf{r}_i - \mathbf{L}|}\,\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|} \tag{3.103}$$

where

$$\mathbf{r}_i \cdot (\mathbf{r}_i - \mathbf{L}) = |\mathbf{r}_i||\mathbf{r}_i - \mathbf{L}|\cos\theta_i$$

$$\leqslant |\mathbf{r}_i||\mathbf{r}_i - \mathbf{L}|, \tag{3.104a}$$

$$LL'\sin\theta\sin\theta \leqslant LL'. \tag{3.104b}$$

Let $\mathbf{r}_i - \mathbf{L} = \mathbf{R}_i$, $\mathrm{d}^3\mathbf{r}_i = \mathrm{d}^3(\mathbf{R}_i + \mathbf{L}) = \mathrm{d}^3\mathbf{R}_i$, substitute into the right-hand side of (3.103), to obtain

$$\begin{aligned}
\beta^2 \int \mathrm{d}^3\mathbf{r}_i\, \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|} =& \beta^2 \int \mathrm{d}^3\mathbf{R}_i\, \mathrm{e}^{-\beta|\mathbf{R}_i|}\mathrm{e}^{-\beta|\mathbf{R}_i + \mathbf{L} - \mathbf{L}'|} \\
=& \beta^2 \int \mathrm{d}^3\mathbf{R}_i\, \mathrm{e}^{-\beta|\mathbf{R}_i|}\mathrm{e}^{-\beta|\mathbf{R}_i - \mathbf{L}_0|} \\
\leqslant& \beta^2 \int \mathrm{d}^3\mathbf{R}_i\, \mathrm{e}^{-\beta|\mathbf{R}_i|}\mathrm{e}^{-\beta|R_i - L_0|} \\
=& \beta^2 \int_0^\infty \mathrm{d}R_i\, R_i^2\, \mathrm{e}^{-\beta R_i}\mathrm{e}^{-\beta|R_i - L_0|} \int_0^\pi \int_0^{2\pi} \mathrm{d}\theta_i\, \mathrm{d}\varphi_i\, \sin\theta_i \\
=& \beta^2(4\pi) \int_0^\infty \mathrm{d}R_i\, R_i^2\, \mathrm{e}^{-\beta R_i}\mathrm{e}^{-\beta|R_i - L_0|} \\
=& \beta^2(4\pi) \int_0^{L_0} \mathrm{d}R_i\, R_i^2\, \mathrm{e}^{-\beta R_i}\mathrm{e}^{-\beta(L_0 - R_i)} \\
&+ \beta^2(4\pi) \int_{L_0}^\infty \mathrm{d}R_i\, R_i^2\, \mathrm{e}^{-\beta R_i}\mathrm{e}^{-\beta(R_i - L_0)} \\
=& \beta^2(4\pi)\, \mathrm{e}^{-\beta L_0} \int_0^{L_0} \mathrm{d}R_i\, R_i^2 \\
&+ \beta^2(4\pi)\, \mathrm{e}^{\beta L_0} \int_{L_0}^\infty \mathrm{d}R_i\, R_i^2\, \mathrm{e}^{-2\beta R_i} \\
=& \beta^2(4\pi)\, \mathrm{e}^{-\beta L_0} \frac{L_0^3}{3} \\
&+ \beta^2(4\pi)\, \mathrm{e}^{\beta L_0} \frac{\partial^2}{\partial u^2} \int_{L_0}^\infty \mathrm{d}R_i\, \mathrm{e}^{-uR_i} \qquad , u = 2\beta \\
=& \beta^2(4\pi)\, \mathrm{e}^{-\beta L_0} \frac{L_0^3}{3} + \beta^2(4\pi)\, \mathrm{e}^{\beta L_0} \frac{\partial^2}{\partial u^2} \left[- \frac{\mathrm{e}^{-uR}}{u} \bigg|_{L_0}^{\infty} \right]
\end{aligned} \tag{3.105}$$

where

$$\mathbf{L}_0 = \mathbf{L}' - \mathbf{L}, \tag{3.106a}$$

$$|\mathbf{R}_i - \mathbf{L}_0| = \sqrt{R_i^2 - 2\mathbf{R}_i\mathbf{L} + L_0^2} \geqslant \sqrt{R_i^2 - 2R_iL + L_0^2}, \tag{3.106b}$$

$$\mathrm{e}^{-\beta|\mathbf{R}_i - \mathbf{L}_0|} \leqslant \mathrm{e}^{-\beta|R_i - L_0|}. \tag{3.106c}$$

Consider the second term on the right-hand side of (3.105), to obtain

$$\begin{aligned}
\mathrm{e}^{\beta L_0}\frac{\partial^2}{\partial u^2}\left[-\frac{\mathrm{e}^{-uR}}{u}\Bigg|_{L_0}^{\infty}\right] =& \mathrm{e}^{\beta L_0}\frac{\partial^2}{\partial u^2}\left[\frac{\mathrm{e}^{-uL_0}}{u}\right] \\
=& \mathrm{e}^{\beta L_0}\left[\frac{2}{u^3}\,\mathrm{e}^{-uL_0} + \frac{2L_0}{u^2}\,\mathrm{e}^{-uL_0} + \frac{L_0^2}{u}\,\mathrm{e}^{-uL_0}\right] \\
=& \mathrm{e}^{\beta L_0}\left[\frac{2}{(2\beta)^3}\,\mathrm{e}^{-2\beta L_0} + \frac{2L_0}{(2\beta)^2}\,\mathrm{e}^{-2\beta L_0} + \frac{L_0^2}{2\beta}\,\mathrm{e}^{-2\beta L_0}\right] \\
=& \mathrm{e}^{-\beta L_0}\left[\frac{1}{4\beta^3} + \frac{L_0}{2\beta^2} + \frac{L_0^2}{2\beta}\right]
\end{aligned} \tag{3.107}$$

Substitute into the right-hand side of (3.105), to obtain

$$\beta^2\int \mathrm{d}^3\mathbf{r}_i\,\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|} \leqslant \beta^2(4\pi)\,\mathrm{e}^{-\beta L_0}\frac{L_0^3}{3} + \beta^2(4\pi)\mathrm{e}^{-\beta L_0}\left[\frac{1}{4\beta^3} + \frac{L_0}{2\beta^2} + \frac{L_0^2}{2\beta}\right]. \tag{3.108}$$

Consider the second term on the right-hand side of (3.103), let $\mathbf{r}_i - \mathbf{L} = \mathbf{R}_i$, $\mathrm{d}^3\mathbf{r}_i = \mathrm{d}^3(\mathbf{R}_i + \mathbf{L}) = \mathrm{d}^3\mathbf{R}_i$, and use (3.106), to obtain

$$\begin{aligned}
\beta^2\int \mathrm{d}^3\mathbf{r}_i\frac{LL'\,\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}}{|\mathbf{r}_i-\mathbf{L}|\,|\mathbf{r}_i-\mathbf{L}|} =& \beta^2\int \mathrm{d}^3\mathbf{R}_i\frac{LL'\,\mathrm{e}^{-\beta|\mathbf{R}_i|}\mathrm{e}^{-\beta|\mathbf{R}_i-\mathbf{L}_0|}}{|\mathbf{R}_i|\,|\mathbf{R}_i-\mathbf{L}_0|} \\
\leqslant& \beta^2\int \mathrm{d}^3\mathbf{R}_i\frac{LL'\,\mathrm{e}^{-\beta R_i}\mathrm{e}^{-\beta|R_i-L_0|}}{R_i\,|\mathbf{R}_i-\mathbf{L}_0|}.
\end{aligned} \tag{3.109}$$

By using the expansion

$$\frac{1}{|\mathbf{R}_i - \mathbf{L}_0|} = \sum_{\ell=0}^{\infty} \left(\frac{R_{i<}}{R_{i>}}\right)^{\ell} \frac{1}{R_{i>}} P_\ell(\cos\theta) \tag{3.110}$$

and

$$\int \mathrm{d}\Omega\, P_\ell(\cos\theta) = 4\pi\delta_{\ell 0} \tag{3.111}$$

where $\sum_{\ell=0}^{\infty} t^\ell P_\ell(\cos\theta) = \left(\sqrt{1+t^2-2t\cos\theta}\right)^{-1}$ and $R_i = \max[L_0, R_i]$.

Substitute (3.111) into the right-hand side of inequality (3.109), we obtain

$$\begin{aligned}
&\beta^2 \int \mathrm{d}^3\mathbf{r}_i \frac{LL'\,\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}}{|\mathbf{r}_i-\mathbf{L}|\,|\mathbf{r}_i-\mathbf{L}|} \\
&\qquad \leqslant \beta^2 \int \mathrm{d}^3\mathbf{R}_i \frac{LL'\,\mathrm{e}^{-\beta R_i}\mathrm{e}^{-\beta|R_i-L_0|}}{R_i\,|\mathbf{R}_i-\mathbf{L}_0|} \\
&\qquad = \beta^2 \int \mathrm{d}^3\mathbf{R}_i \frac{LL'\,\mathrm{e}^{-\beta R_i}\mathrm{e}^{-\beta|R_i-L_0|}}{R_i} \sum_{\ell=0}^{\infty} \left(\frac{R_{i<}}{R_{i>}}\right)^{\ell} \frac{1}{R_{i>}} P_\ell(\cos\theta) \\
&\qquad = \beta^2 \int_0^{\infty} \mathrm{d}R_i \frac{R_i^2 LL'\,\mathrm{e}^{-\beta R_i}\mathrm{e}^{-\beta|R_i-L_0|}}{R_i} \\
&\qquad\qquad \times \int \mathrm{d}\Omega \sum_{\ell=0}^{\infty} \left(\frac{R_{i<}}{R_{i>}}\right)^{\ell} \frac{1}{R_{i>}} P_\ell(\cos\theta).
\end{aligned} \tag{3.112}$$

By using (3.110), with $\ell = 0$, as applied to the right-hand side of inequality (3.112), we obtain

$$\begin{aligned}
&\beta^2 \int \mathrm{d}^3\mathbf{r}_i \frac{LL'\,\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}}{|\mathbf{r}_i-\mathbf{L}|\,|\mathbf{r}_i-\mathbf{L}|} \\
&\qquad \leqslant 4\pi\beta^2 \int_0^{\infty} \mathrm{d}R_i \frac{R_i LL'\,\mathrm{e}^{-\beta R_i}\mathrm{e}^{-\beta|R_i-L_0|}}{R_{i>}} \\
&\qquad = 4\pi\beta^2 \int_0^{L_0} \mathrm{d}R_i \frac{R_i LL'\,\mathrm{e}^{-\beta R_i}\mathrm{e}^{-\beta(L_0-R_i)}}{L_0}
\end{aligned}$$

$$
\begin{aligned}
&+ 4\pi\beta^2 \int_{L_0}^{\infty} \mathrm{d}R_i \frac{R_i L L' \,\mathrm{e}^{-\beta R_i} \mathrm{e}^{-\beta(R_i - L_0)}}{R} \\
=& \frac{4\pi L L' \beta^2}{L_0} \mathrm{e}^{-\beta L_0} \int_0^{L_0} \mathrm{d}R_i \, R_i + 4\pi\beta^2 L L' \mathrm{e}^{\beta L_0} \int_{L_0}^{\infty} \mathrm{d}R_i \,\mathrm{e}^{-2\beta R_i} \\
=& \frac{4\pi L L' \beta^2}{L_0} \frac{L_0^2}{2} \mathrm{e}^{-\beta L_0} + 4\pi\beta^2 L L' \mathrm{e}^{\beta L_0} \left(-\frac{\mathrm{e}^{-2\beta R_i}}{2\beta} \right) \Bigg|_{L_0}^{\infty} \\
=& \frac{4\pi\beta^2 L L' L_0}{2} \mathrm{e}^{-\beta L_0} + \frac{4\pi\beta L L'}{2} \mathrm{e}^{-\beta L_0}. \qquad (3.113)
\end{aligned}
$$

From (3.113), we obtain the inequality

$$
\beta^2 \int \mathrm{d}^3\mathbf{r}_i \frac{L L' \,\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|} \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|}}{|\mathbf{r}_i - \mathbf{L}| \, |\mathbf{r}_i - \mathbf{L}|} \leqslant \left(\frac{4\pi\beta^2 L L' L_0}{2} + \frac{4\pi\beta L L'}{2} \right) \mathrm{e}^{-\beta L_0}. \qquad (3.114)
$$

By substituting (3.108) and (3.114) into the right-hand side of inequality (3.103), we obtain

$$
\begin{aligned}
&\int \mathrm{d}^3\mathbf{r}_i \, \nabla_i \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|} \cdot \nabla_i \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|} \\
&= \beta^2 \int \mathrm{d}^3\mathbf{r}_i \,\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|} \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|} + \beta^2 \int \mathrm{d}^3\mathbf{r}_i \frac{L L'}{|\mathbf{r}_i - \mathbf{L}| \, |\mathbf{r}_i - \mathbf{L}|} \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}|} \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|} \\
&\leqslant \beta^2 (4\pi) \,\mathrm{e}^{-\beta L_0} \frac{L_0^3}{3} + \beta^2 (4\pi) \,\mathrm{e}^{-\beta L_0} \left[\frac{1}{4\beta^3} + \frac{L_0}{2\beta^2} + \frac{L_0^2}{2\beta} \right] + \frac{4\pi\beta^2 L L' L_0}{2} \mathrm{e}^{-\beta L_0} \\
&\quad + \frac{4\pi\beta L L'}{2} \mathrm{e}^{-\beta L_0} \\
&= 4\pi \mathrm{e}^{-\beta L_0} \left[\beta^2 \frac{L_0^3}{3} + \beta^2 \left[\frac{1}{4\beta^3} + \frac{L_0}{2\beta^2} + \frac{L_0^2}{2\beta} \right] + \frac{\beta^2 L L' L_0}{2} + \frac{\beta L L'}{2} \right] \\
&= 4\pi \mathrm{e}^{-\beta L_0} \left[\beta^2 \frac{L_0^3}{3} + \frac{1}{4\beta} + \frac{L_0}{2} + \frac{\beta L_0^2}{2} + \frac{\beta^2 L L' L_0}{2} + \frac{\beta L L'}{2} \right]. \qquad (3.115)
\end{aligned}
$$

Also

$$\begin{aligned}
\int \mathrm{d}^3\mathbf{r}_i \left(\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}\right) \left(\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}\right) &= \int_0^\infty \mathrm{d}^3\mathbf{R}_i \,\mathrm{e}^{-\beta|\mathbf{R}_i|}\,\mathrm{e}^{-\beta|\mathbf{R}_i-\mathbf{L}_0|} \\
&\leqslant \int_0^\infty \mathrm{d}^3\mathbf{R}_i \,\mathrm{e}^{-\beta R_i}\,\mathrm{e}^{-\beta|R_i-L_0|} \\
&=4\pi \int_0^\infty \mathrm{d}R_i\, R_i^2\,\mathrm{e}^{-\beta R_i}\mathrm{e}^{-\beta|R_i-L_0|} \\
&=4\pi \mathrm{e}^{-\beta L_0} \int_0^{L_0} \mathrm{d}R_i\, R_i^2 \\
&\quad + 4\pi \mathrm{e}^{\beta L_0} \int_{L_0}^\infty \mathrm{d}R_i\, R_i^2\,\mathrm{e}^{-2\beta R_i} \\
&=4\pi \mathrm{e}^{-\beta L_0}\frac{L_0^3}{2} + 4\pi \mathrm{e}^{-\beta L_0}\left[\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right] \\
&=4\pi \mathrm{e}^{-\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]
\end{aligned}$$

$$\therefore \quad \int \mathrm{d}^3\mathbf{r}_i \left(\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}\right) \left(\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}\right) \leqslant 4\pi \mathrm{e}^{-\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]. \qquad (3.116)$$

From (3.100), for $\mathbf{L} = \mathbf{L}'$, we have the useful expression

$$\int \mathrm{d}^3\mathbf{r}_i\, \nabla_i \mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|} \cdot \nabla_i \mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|} = \frac{\pi}{\beta}. \qquad (3.117)$$

For $\mathbf{L} \neq \mathbf{L}'$, from (3.115) we have

$$\begin{aligned}
&\int \mathrm{d}^3\mathbf{r}_i\, \nabla_i \mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|} \cdot \nabla_i \mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|} \\
&\qquad \leqslant 4\pi \mathrm{e}^{-\beta L_0}\left[\beta^2\frac{L_0^3}{3}+\frac{1}{4\beta}+\frac{L_0}{2}+\frac{\beta L_0^2}{2}+\frac{\beta^2 LL' L_0}{2}+\frac{\beta LL'}{2}\right] \qquad (3.118)
\end{aligned}$$

and from (3.116), we have

$$\int \mathrm{d}^3\mathbf{r}_i \left(\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}\right) \left(\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}\right) \leqslant 4\pi\mathrm{e}^{-\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]. \tag{3.119}$$

By using (3.117), and from (3.95), with $i=1$ and $\mathbf{L}_1=\mathbf{L}$, we obtain

$$\int \mathrm{d}^3\mathbf{r}_1\, \nabla_1\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\cdot\nabla_1\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} = \frac{\pi}{\beta}. \tag{3.120}$$

By using (3.117), and from (3.95), with $i=1$ and $\mathbf{L}_2=\mathbf{L}$, we obtain

$$\int \mathrm{d}^3\mathbf{r}_1\, \nabla_1\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\cdot\nabla_1\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} = \frac{\pi}{\beta}. \tag{3.121}$$

By using (3.118) and (3.119), from (3.95), with $i=1$, $\mathbf{L}_1=\mathbf{L}$ and $\mathbf{L}_2=\mathbf{L}'$, we obtain

$$\begin{aligned} &2\int \mathrm{d}^3\mathbf{r}_1\, \nabla_1 \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\cdot\nabla_1\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \\ &\qquad \leqslant 8\pi\mathrm{e}^{-\beta L_0}\left[\frac{\beta^2 L_0^3}{3}+\frac{1}{4\beta}+\frac{L_0}{2}+\frac{\beta L_0^2}{2}+\frac{\beta^2 LL' L_0}{2}+\frac{\beta LL'}{2}\right] \end{aligned} \tag{3.122}$$

and with $i=2$, $\mathbf{L}_1=\mathbf{L}$ and $\mathbf{L}_2=\mathbf{L}'$, we obtain

$$\int \mathrm{d}^3\mathbf{r}_2 \left(\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right) \left(\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right) \leqslant 4\pi\mathrm{e}^{-\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]. \tag{3.123}$$

By substituting (3.120), (3.121), (3.122) and (3.123) into the right-hand side of (3.95), we obtain

$$\begin{aligned} &\langle\Psi|\,\frac{\mathbf{p}_1^2}{2m}\,|\Psi\rangle \\ &\leqslant \frac{\hbar^2}{2m}\frac{\beta^3}{2\pi}\left\{\frac{\pi}{\beta}+\frac{\pi}{\beta}-8\pi\mathrm{e}^{-\beta L_0}\left[\frac{\beta^2 L_0^3}{3}+\frac{1}{4\beta}+\frac{L_0}{2}+\frac{\beta L_0^2}{2}+\frac{\beta^2 LL' L_0}{2}+\frac{\beta LL'}{2}\right]\right. \end{aligned}$$

$$\times \left(\frac{\beta^3}{\pi}\right) 4\pi \mathrm{e}^{-\beta L_0} \left[\frac{L_0^3}{2} + \frac{1}{\beta^3} + \frac{L_0}{2\beta^2} + \frac{L_0^2}{2\beta}\right]\Bigg\}$$

$$= \frac{\hbar^2\beta^2}{2m} + \mathrm{e}^{-2\beta L_0}\frac{\hbar^2}{2m}\frac{\beta^3}{2}\Bigg\{32\left[\frac{\beta^2 L_0^3}{3} + \frac{1}{4\beta} + \frac{L_0}{2} + \frac{\beta L_0^2}{2} + \frac{\beta^2 LL' L_0}{2} + \frac{\beta LL'}{2}\right]$$

$$\times \left(\frac{\beta^3}{\pi}\right)\left[\frac{L_0^3}{2} + \frac{1}{\beta^3} + \frac{L_0}{2\beta^2} + \frac{L_0^2}{2\beta}\right]\Bigg\}. \tag{3.124}$$

From (3.124), taking the limit $L_0 \to \infty$, we obtain

$$\langle\Psi|\,\frac{\mathbf{p}_1^2}{2m}\,|\Psi\rangle \leqslant \frac{\hbar^2\beta^2}{2m}. \tag{3.125}$$

By using (3.89) and (3.95), we replace ∇_1 by ∇_2, to obtain

$$\langle\Psi|\,\frac{\mathbf{p}_2^2}{2m}\,|\Psi\rangle = \frac{\hbar^2}{2m}\int \mathrm{d}^3\mathbf{r}_2\,\mathrm{d}^3\mathbf{r}_1\;[\nabla_2\Psi^*(\mathbf{r})]\cdot[\nabla_2\Psi(\mathbf{r})]$$

$$= \frac{\hbar^2}{2m}\frac{\beta^3}{2\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2$$

$$\times \Big\{\delta_{aa}\nabla_2\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right)\cdot\nabla_2\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right)$$

$$+ \delta_{bb}\nabla_2\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right)\cdot\nabla_2\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right)$$

$$-2\delta_{ab}\nabla_2\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right)\cdot\nabla_2\left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right)\Big\}$$

$$= \frac{\hbar^2}{2m}\frac{\beta^3}{2\pi}\Bigg\{\int \mathrm{d}^3\mathbf{r}_2\,\nabla_2\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\cdot\nabla_2\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}$$

$$\times \int \mathrm{d}^3\mathbf{r}_1\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\;\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right|^2\delta_{aa}$$

$$+ \int \mathrm{d}^3\mathbf{r}_2\,\nabla_2\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\cdot\nabla_2\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}$$

$$\times \int \mathrm{d}^3\mathbf{r}_1\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right|^2\delta_{bb}$$

$$- 2\,\delta_{ab} \int \mathrm{d}^3\mathbf{r}_2\, \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \cdot \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}$$

$$\times \left(\frac{\beta^3}{\pi}\right) \int \mathrm{d}^3\mathbf{r}_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right) \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right)\Bigg\}$$

$$= \frac{\hbar^2}{2m}\frac{\beta^3}{2\pi} \Bigg\{ \int \mathrm{d}^3\mathbf{r}_2\, \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \cdot \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}$$

$$+ \int \mathrm{d}^3\mathbf{r}_2\, \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \cdot \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}$$

$$- 2\,\delta_{ab} \int \mathrm{d}^3\mathbf{r}_2\, \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \cdot \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}$$

$$\times \left(\frac{\beta^3}{\pi}\right) \int \mathrm{d}^3\mathbf{r}_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right) \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right)\Bigg\}. \qquad (3.126)$$

By using (3.117), from (3.126), with $i = 2$ and $\mathbf{L}_2 = \mathbf{L}$, we obtain

$$\int \mathrm{d}^3\mathbf{r}_2\, \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \cdot \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} = \frac{\pi}{\beta}. \qquad (3.127)$$

By using (3.117), and from (3.91), with $i = 2$ and $\mathbf{L}_1 = \mathbf{L}$, we obtain

$$\int \mathrm{d}^3\mathbf{r}_2\, \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \cdot \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} = \frac{\pi}{\beta}. \qquad (3.128)$$

By using (3.118) and (3.119), from (3.126), with $i = 1$, $\mathbf{L}_1 = \mathbf{L}$ and $\mathbf{L}_2 = \mathbf{L}'$, we obtain

$$2 \int \mathrm{d}^3\mathbf{r}_2\, \nabla_2 \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \cdot \nabla_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}$$

$$\leqslant 8\pi \mathrm{e}^{-\beta L_0} \left[\frac{\beta^2 L_0^3}{3} + \frac{1}{4\beta} + \frac{L_0}{2} + \frac{\beta L_0^2}{2} + \frac{\beta^2 L L' L_0}{2} + \frac{\beta L L'}{2}\right] \qquad (3.129)$$

and with $i = 1$, $\mathbf{L}_1 = \mathbf{L}$ and $\mathbf{L}_2 = \mathbf{L}'$, we obtain

$$\int \mathrm{d}^3\mathbf{r}_1 \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right) \left(\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right) \leqslant 4\pi \mathrm{e}^{-\beta L_0} \left[\frac{L_0^3}{2} + \frac{1}{\beta^3} + \frac{L_0}{2\beta^2} + \frac{L_0^2}{2\beta}\right]. \qquad (3.130)$$

By substituting (3.127), (3.128), (3.129) and (3.130) into the right-hand side of (3.126), we obtain

$$\begin{aligned}
&\langle\Psi|\,\frac{\mathbf{p}_2^2}{2m}\,|\Psi\rangle \\
&\leqslant \frac{\hbar^2}{2m}\frac{\beta^3}{2\pi}\left\{\frac{\pi}{\beta}+\frac{\pi}{\beta}-8\pi\mathrm{e}^{-\beta L_0}\left[\frac{\beta^2 L_0^3}{3}+\frac{1}{4\beta}+\frac{L_0}{2}+\frac{\beta L_0^2}{2}+\frac{\beta^2 LL' L_0}{2}+\frac{\beta LL'}{2}\right]\right. \\
&\qquad\left.\times\left(\frac{\beta^3}{\pi}\right)4\pi\mathrm{e}^{-\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]\right\} \\
&=\frac{\hbar^2\beta^2}{2m}+\mathrm{e}^{-2\beta L_0}\frac{\hbar^2}{2m}\frac{\beta^3}{2}\left\{32\left[\frac{\beta^2 L_0^3}{3}+\frac{1}{4\beta}+\frac{L_0}{2}+\frac{\beta L_0^2}{2}+\frac{\beta^2 LL' L_0}{2}+\frac{\beta LL'}{2}\right]\right. \\
&\qquad\left.\times\left(\frac{\beta^3}{\pi}\right)\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]\right\}. \qquad (3.131)
\end{aligned}$$

From (3.131), by taking the limit $L_0 \to \infty$, we obtain

$$\langle\Psi|\,\frac{\mathbf{p}_2^2}{2m}\,|\Psi\rangle \leqslant \frac{\hbar^2\beta^2}{2m}. \qquad (3.132)$$

From (3.125) and (3.132), we obtain the expectation value of kinetic energy of hydrogen atom for $k = N = 2$

$$\begin{aligned}
\langle\Psi|\sum_{i=1}^{2}\frac{\mathbf{p}_i^2}{2m}\,|\Psi\rangle &= \langle\Psi|\,\frac{\mathbf{p}_1^2}{2m}\,|\Psi\rangle+\langle\Psi|\,\frac{\mathbf{p}_2^2}{2m}\,|\Psi\rangle \\
&\leqslant 2\,\frac{\hbar^2\beta^2}{2m}. \qquad (3.133)
\end{aligned}$$

From (3.75) and (3.133), we imply that the expectation value of kinetic energy of hydrogen atom for k nuclei with N electrons is

$$\begin{aligned}
\langle\Psi|\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}\,|\Psi\rangle &= \langle\Psi|\,\frac{\mathbf{p}_1^2}{2m}\,|\Psi\rangle+\langle\Psi|\,\frac{\mathbf{p}_2^2}{2m}\,|\Psi\rangle+\ldots+\langle\Psi|\,\frac{\mathbf{p}_N^2}{2m}\,|\Psi\rangle \\
&\leqslant \frac{\hbar^2\beta^2}{2m}\,N. \qquad (3.134)
\end{aligned}$$

To obtain the bound of nucleus-electron interaction, we define the vector from the origin to the nuclei of charges $Z_i|e|$ by choosing

$$\mathbf{L}_i = \mathbf{R}_i. \tag{3.135}$$

For $k > 1$, a similar analysis as for $k = 2$ and $N = 2$, first substitute into the second term on the right-hand side of (3.80), to obtain

$$\begin{aligned} -\langle\Psi| \sum_{i=1}^{2}\sum_{j=1}^{2} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} |\Psi\rangle = &-\langle\Psi| \frac{Z_1 e^2}{|\mathbf{r}_1 - \mathbf{L}_1|} |\Psi\rangle - \langle\Psi| \frac{Z_2 e^2}{|\mathbf{r}_2 - \mathbf{L}_2|} |\Psi\rangle \\ &-\langle\Psi| \frac{Z_1 e^2}{|\mathbf{r}_2 - \mathbf{L}_1|} |\Psi\rangle - \langle\Psi| \frac{Z_2 e^2}{|\mathbf{r}_1 - \mathbf{L}_2|} |\Psi\rangle . \end{aligned} \tag{3.136}$$

Consider the first term on the right-hand side of the inequality (3.136), to obtain

$$\begin{aligned} -\langle\Psi| \frac{Z_1 e^2}{|\mathbf{r}_1 - \mathbf{R}_1|} |\Psi\rangle &= -\langle\Psi| \frac{Z_1 e^2}{|\mathbf{r}_1 - \mathbf{L}_1|} |\Psi\rangle \\ &= -Z_1 e^2 \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \Psi^*(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) \frac{1}{|\mathbf{r}_1 - \mathbf{L}_1|} \Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2). \end{aligned} \tag{3.137}$$

Substitute (3.93b), (3.93b), (3.68b) and (3.87) into the inequality (3.137), to obtain

$$\begin{aligned} -\langle\Psi| \frac{Z_1 e^2}{|\mathbf{r}_1 - \mathbf{R}_1|} |\Psi\rangle &= -Z_1 e^2 \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \Psi^*(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) \frac{1}{|\mathbf{r}_1 - \mathbf{L}_1|} \Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) \\ &= -\frac{Z_1 e^2 \beta^3}{\pi\sqrt{2}} \frac{\beta^3}{\pi\sqrt{2}} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2 \\ &\quad \times \Bigg[[\chi_a^* \cdot \chi_a]\, \mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_1|}\, \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_2|} \frac{\mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_1|}\, \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_2|}}{|\mathbf{r}_1 - \mathbf{L}_1|} \\ &\qquad + [\chi_b^* \cdot \chi_b]\, \mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_2|}\, \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_1|} \frac{\mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_2|}\, \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_1|}}{|\mathbf{r}_1 - \mathbf{L}_1|} \end{aligned}$$

$$
\begin{aligned}
&-2\left[\chi_a^* \cdot \chi_b\right] \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|} \frac{\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_1|}\Bigg] \\
=& -\frac{Z_1 e^2 \beta^3}{2\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\delta_{aa}\, \mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_1|}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \\
& -\frac{Z_1 e^2 \beta^3}{2\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\delta_{bb}\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_2|}}{|\mathbf{r}_1-\mathbf{L}_1|}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \\
& +\left[\frac{Z_1 e^2 \beta^3}{\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_1\, \frac{\delta_{ab}\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_1|}\right. \\
& \qquad \left. \times \int \mathrm{d}^3\mathbf{r}_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right] \\
=& -\frac{Z_1 e^2 \beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_1|}\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right|^2 \delta_{aa} \\
& -\frac{Z_1 e^2 \beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_2|}}{|\mathbf{r}_1-\mathbf{L}_1|}\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right|^2 \delta_{bb} \\
& +\left[\frac{Z_1 e^2 \beta^3}{\pi}\frac{\beta^3}{\pi}\delta_{ab}\int \mathrm{d}^3\mathbf{r}_1\, \frac{\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_1|}\right. \\
& \qquad \left. \times \int \mathrm{d}^3\mathbf{r}_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right]. \\
=& -\frac{Z_1 e^2 \beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_1|} - \frac{Z_1 e^2 \beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_2|}}{|\mathbf{r}_1-\mathbf{L}_1|} \\
& +\delta_{ab}\left[\frac{Z_1 e^2 \beta^3}{\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_1\, \frac{\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_1|}\right. \\
& \qquad \left. \times \int \mathrm{d}^3\mathbf{r}_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right].
\end{aligned} \tag{3.138}
$$

To obtain above, we introduce the basic following integral for $\mathbf{L} = \mathbf{L}'$, and set $\mathbf{R} = \mathbf{r}_i - \mathbf{L}$

$$
\int \mathrm{d}^3\mathbf{r}_i\, \frac{\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}\, \mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}}{|\mathbf{r}_i-\mathbf{L}|} = \int \mathrm{d}^3\mathbf{r}_i\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_i-\mathbf{L}|}}{|\mathbf{r}_i-\mathbf{L}|}
$$

$$
\begin{aligned}
&= \int \mathrm{d}^3\mathbf{R}\, \frac{\mathrm{e}^{-2\beta|\mathbf{R}|}}{|\mathbf{R}|} \\
&= \int_0^\infty \mathrm{d}R\, \frac{R^2 \mathrm{e}^{-2\beta R}}{R} \int_0^\pi \int_0^{2\pi} \mathrm{d}\theta\, \sin\theta \mathrm{d}\varphi \\
&=(4\pi) \int_0^\infty \mathrm{d}R\, R\mathrm{e}^{-2\beta R} \\
&=4\pi \left(\frac{\mathrm{e}^{-2\beta R}}{-2\beta} \left[R - \frac{1}{-2\beta} \right] \right) \Bigg|_0^\infty \\
&=0 - 4\pi \left(-\frac{1}{4\beta^2} \right) \\
&=\frac{\pi}{\beta^2}
\end{aligned}
\tag{3.139}
$$

and for $\mathbf{L} \neq \mathbf{L}'$, we obtain

$$
\begin{aligned}
\int \mathrm{d}^3\mathbf{r}_i\, \frac{\mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|}\, \mathrm{e}^{-\beta|\mathbf{r}_i - \mathbf{L}'|}}{|\mathbf{r}_i - \mathbf{L}|} &= \int \mathrm{d}^3\mathbf{r}_i\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_i - \mathbf{L}'|}}{|\mathbf{r}_i - \mathbf{L}|} \\
&= \int \mathrm{d}^3\mathbf{R}_i\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_i - \mathbf{L}'|}}{|\mathbf{R}_i|} \quad , \qquad \mathbf{R}_i = \mathbf{r}_i - \mathbf{L} \\
&= \int \mathrm{d}^3\mathbf{R}_i\, \frac{\mathrm{e}^{-2\beta|\mathbf{R}_i + \mathbf{L} - \mathbf{L}'|}}{|\mathbf{R}_i|} \;,\;\; \mathbf{r}_i - \mathbf{L}' = \mathbf{R}_i + \mathbf{L} - \mathbf{L}' \\
&= \int \mathrm{d}^3\mathbf{R}_i\, \frac{\mathrm{e}^{-2\beta|\mathbf{R}_i + \mathbf{L}_0'|}}{|\mathbf{R}_i|} \quad , \qquad \mathbf{L}_0' = \mathbf{L} + \mathbf{L}' \\
&\geqslant \int \mathrm{d}^3\mathbf{R}_i\, \frac{\mathrm{e}^{-2\beta\left|R_i + L_0'\right|}}{R_i} \\
&= \int_0^\infty \mathrm{d}R_i\; R_i\, \mathrm{e}^{-2\beta|R_i + L_0'|} \int_0^\pi \int_0^{2\pi} \mathrm{d}\theta\, \mathrm{d}\varphi\, \sin\theta \\
&=4\pi \int_0^\infty \mathrm{d}R_i\; R_i\, \mathrm{e}^{-2\beta|R_i + L_0'|} \\
&=4\pi \mathrm{e}^{-2\beta L_0'} \int_0^\infty \mathrm{d}R_i\; R_i\, \mathrm{e}^{-2\beta R_i}
\end{aligned}
$$

$$=4\pi\,\mathrm{e}^{-2\beta L_0'}\left(\frac{\mathrm{e}^{-2\beta R_i}}{-2\beta}\left[R_i+\frac{1}{2\beta}\right]\Bigg|_0^\infty\right)$$

$$=-\,4\pi\,\mathrm{e}^{-2\beta L_0'}\left(\frac{1}{2\beta}\left[\frac{1}{2\beta}\right]\right)$$

$$=-\,4\pi\,\mathrm{e}^{-2\beta L_0'}\frac{1}{4\beta^2}$$

$$=-\,\mathrm{e}^{-2\beta L_0'}\frac{\pi}{\beta^2}\qquad,|\mathbf{L}_0'|=|\mathbf{L}-\mathbf{L}'|=|-\mathbf{L}_0|$$

$$=-\,\mathrm{e}^{-2\beta L_0}\frac{\pi}{\beta^2}\qquad,L_0'=L_0$$

$$\therefore\quad\int \mathrm{d}^3\mathbf{r}_i\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}\,\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}}{|\mathbf{r}_i-\mathbf{L}|}>0. \tag{3.140}$$

which vanishes very rapidly for $L_0\to\infty$.

From the inequality (3.140), we obviously have

$$-\int \mathrm{d}^3\mathbf{r}_i\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}\,\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}}{|\mathbf{r}_i-\mathbf{L}|}<0. \tag{3.141}$$

for $L_0\to\infty$, to write this as a limit

$$\lim_{L_0\to\infty}\left[-\int \mathrm{d}^3\mathbf{r}_i\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}\,\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}}{|\mathbf{r}_i-\mathbf{L}|}\right]=0. \tag{3.142}$$

In the other case for $\mathbf{L}\neq\mathbf{L}'$

$$\int \mathrm{d}^3\mathbf{r}_i\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}\,\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}}{|\mathbf{r}_i-\mathbf{L}|}=\int \mathrm{d}^3\mathbf{R}_i\,\frac{\mathrm{e}^{-\beta|\mathbf{R}_i|}}{|\mathbf{R}_i|}\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|},\quad \mathbf{R}_i=\mathbf{r}_i-\mathbf{L}$$

$$=\int \mathrm{d}^3\mathbf{R}_i\,\frac{\mathrm{e}^{-\beta|\mathbf{R}_i|}}{|\mathbf{R}_i|}\mathrm{e}^{-\beta|\mathbf{R}_i+\mathbf{L}-\mathbf{L}'|},\quad \mathbf{r}_i-\mathbf{L}'=\mathbf{R}_i+\mathbf{L}-\mathbf{L}'$$

$$=\int \mathrm{d}^3\mathbf{R}_i\,\frac{\mathrm{e}^{-\beta|\mathbf{R}_i|}}{|\mathbf{R}_i|}\mathrm{e}^{-\beta|\mathbf{R}_i-\mathbf{L}_0|},\quad \mathbf{L}_0=\mathbf{L}'-\mathbf{L}. \tag{3.143}$$

By using (3.106), applied to the right-hand side of (3.143), we obtain

$$
\begin{aligned}
\int \mathrm{d}^3\mathbf{r}_i \, \frac{\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}\,\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}}{|\mathbf{r}_i-\mathbf{L}|} &= \int \mathrm{d}^3\mathbf{R}_i \, \frac{\mathrm{e}^{-\beta|\mathbf{R}_i|}}{|\mathbf{R}_i|}\mathrm{e}^{-\beta|\mathbf{R}_i-\mathbf{L}_0|} \\
&\leqslant \int \mathrm{d}^3\mathbf{R}_i \, \frac{\mathrm{e}^{-\beta|\mathbf{R}_i|}\,\mathrm{e}^{-\beta|R_i-L_0|}}{|\mathbf{R}_i|} \\
&= \int_0^\infty \int_0^\pi \int_0^{2\pi} \mathrm{d}R_i\,\mathrm{d}\theta\,\mathrm{d}\varphi\, R_i^2 \sin\theta \, \frac{\mathrm{e}^{-\beta R_i}\,\mathrm{e}^{-\beta|R_i-L_0|}}{R_i} \\
&=4\pi \int_0^\infty \mathrm{d}R_i\, R_i\, \mathrm{e}^{-\beta R_i}\,\mathrm{e}^{-\beta|R_i-L_0|} \\
&=4\pi \int_0^{L_0} \mathrm{d}R_i\, R_i\, \mathrm{e}^{-\beta R_i}\,\mathrm{e}^{-\beta(L_0-R_i)} \\
&\quad + 4\pi \int_{L_0}^\infty \mathrm{d}R_i\, R_i\, \mathrm{e}^{-\beta R_i}\,\mathrm{e}^{-\beta(R_i-L_0)} \\
&=4\pi\mathrm{e}^{-\beta L_0} \int_0^{L_0} \mathrm{d}R_i\, R_i + 4\pi\mathrm{e}^{\beta L_0} \int_{L_0}^\infty \mathrm{d}R_i\, R_i\, \mathrm{e}^{-2\beta R_i} \\
&=4\pi\mathrm{e}^{-\beta L_0}\frac{L_0^2}{2} + 4\pi\,\mathrm{e}^{\beta L_0}\left(\frac{\mathrm{e}^{-2\beta R_i}}{-2\beta}\left[R_i+\frac{1}{2\beta}\right]\Bigg|_{L_0}^{\infty}\right) \\
&=4\pi\mathrm{e}^{-\beta L_0}\frac{L_0^2}{2} + 4\pi\,\mathrm{e}^{\beta L_0}\left(\frac{\mathrm{e}^{-2\beta L_0}}{2\beta}\left[L_0+\frac{1}{2\beta}\right]\right) \\
&=4\pi\mathrm{e}^{-\beta L_0}\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right]. \qquad (3.144)
\end{aligned}
$$

From (3.139), (3.142) and (3.144) we can rewrite as

$$
-\int \mathrm{d}^3\mathbf{r}_i \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_i-\mathbf{L}|}}{|\mathbf{r}_i-\mathbf{L}|} = -\frac{\pi}{\beta^2} \qquad (3.145a)
$$

$$
-\int \mathrm{d}^3\mathbf{r}_i \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_i-\mathbf{L}'|}}{|\mathbf{r}_i-\mathbf{L}|} <0 \qquad (3.145b)
$$

$$
\int \mathrm{d}^3\mathbf{r}_i \, \frac{\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}'|}\,\mathrm{e}^{-\beta|\mathbf{r}_i-\mathbf{L}|}}{|\mathbf{r}_i-\mathbf{L}|} \leqslant 4\pi\mathrm{e}^{-\beta L_0}\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right]. \qquad (3.145c)
$$

By using the integral in (3.145a), with $i = 1$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{r}_i = \mathbf{r}_1$, as applied to the first term on the right-hand side of inequality (3.138), with normalized wavefunction, gives

$$-\frac{Z_1 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1 \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1 - \mathbf{L}_1|}}{|\mathbf{r}_1 - \mathbf{L}_1|} = -\frac{Z_1 e^2 \beta}{2}. \tag{3.146}$$

By using the integration in (3.145b), set $i = 1$, $\mathbf{L} = \mathbf{L}_1$, $\mathbf{L}' = \mathbf{L}_2$ and $\mathbf{r}_i = \mathbf{r}_1$, as applied to the second term on the right-hand side of inequality (3.138), with normalized wavefunction, for $L_0 \to \infty$, we obtain

$$\begin{aligned}-\frac{Z_1 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1 \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1 - \mathbf{L}_2|}}{|\mathbf{r}_1 - \mathbf{L}_1|} =& \frac{Z_1 e^2 \beta^3}{2\pi} \left(-\int \mathrm{d}^3\mathbf{r}_1 \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1 - \mathbf{L}_2|}}{|\mathbf{r}_1 - \mathbf{L}_1|} \right) \\ <& \frac{Z_1 e^2 \beta^3}{2\pi} (0) \\ =& 0. \end{aligned} \tag{3.147}$$

We also have the following obvious inequality

$$-\frac{Z_1 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1 \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1 - \mathbf{L}_2|}}{|\mathbf{r}_1 - \mathbf{L}_1|} \leqslant 0. \tag{3.148}$$

By using (3.119), with $i = 2$, $\mathbf{r}_i = \mathbf{r}_2$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{L}' = \mathbf{L}_2$, as applied to the third term on the right-hand side of (3.138), we obtain

$$\int \mathrm{d}^3\mathbf{r}_2 \, \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_1|} \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_2|} < 4\pi \mathrm{e}^{-\beta L_0} \left[\frac{L_0^3}{2} + \frac{1}{\beta^3} + \frac{L_0}{2\beta^2} + \frac{L_0^2}{2\beta} \right] \tag{3.149}$$

and by using (3.145c), with $i = 1$, $\mathbf{r}_i = \mathbf{r}_1$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{L}' = \mathbf{L}_2$, as applied to the third term on the right-hand side of (3.138), we obtain

$$\int \mathrm{d}^3\mathbf{r}_1 \, \frac{\mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_1|}}{|\mathbf{r}_1 - \mathbf{L}_1|} \leqslant 4\pi \mathrm{e}^{-\beta L_0} \left[\frac{L_0^2}{2} + \frac{L_0}{2\beta} + \frac{1}{4\beta^2} \right]. \tag{3.150}$$

Substitute (3.149) and (3.150) into the third term on the right-hand side of (3.138), we obtain

$$\frac{Z_1e^2\beta^3}{\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_1\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_1|}\int \mathrm{d}^3\mathbf{r}_2\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}$$
$$\leqslant 16Z_1e^2\beta^3\mathrm{e}^{-2\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right]. \qquad (3.151)$$

By substituting (3.146), (3.148) and (3.151) into the right-hand side of (3.138), we obtain

$$-\langle\Psi|\,\frac{Z_1e^2}{|\mathbf{r}_1-\mathbf{R}_1|}\,|\Psi\rangle\leqslant-\frac{Z_1e^2\beta}{2}+0$$
$$+\,16Z_1e^2\beta^3\,\delta_{ab}\,\mathrm{e}^{-2\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]$$
$$\times\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right]. \qquad (3.152)$$

From (3.152), by taking the limit $L_0\to\infty$ we may write

$$-\langle\Psi|\,\frac{Z_1e^2}{|\mathbf{r}_1-\mathbf{R}_1|}\,|\Psi\rangle\leqslant-\frac{Z_1e^2\beta}{2}. \qquad (3.153)$$

By referring (3.138), consider the second term on the right-hand side of (3.136), to obtain

$$-\langle\Psi|\,\frac{Z_2e^2}{|\mathbf{r}_2-\mathbf{R}_2|}\,|\Psi\rangle=-\frac{Z_2e^2\beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_2|}\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right|^2\delta_{aa}$$
$$-\frac{Z_2e^2\beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_1|}}{|\mathbf{r}_2-\mathbf{L}_2|}\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right|^2\delta_{bb}$$
$$+\,\delta_{ab}\left[\frac{Z_2e^2\beta^3}{\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_2|}\right.$$

$$\times \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\Bigg] . \tag{3.154}$$

By using the integration in (3.145a), with $i = 2$, $\mathbf{L} = \mathbf{L}_2$ and $\mathbf{r}_i = \mathbf{r}_2$, as applied to the first term on the right-hand side of inequality (3.154), with normalized wavefunction, we obtain

$$\begin{aligned} -\frac{Z_2 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_2|} \left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right|^2 \delta_{aa} \\ = -\frac{Z_2 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_2|} \\ = -\frac{Z_2 e^2 \beta^3}{2\pi} \frac{\pi}{\beta^2} \\ = -\frac{Z_2 e^2 \beta}{2}. \end{aligned} \tag{3.155}$$

From (3.155), we obtain

$$-\frac{Z_2 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_2|} \left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right|^2 \delta_{aa} = -\frac{Z_2 e^2 \beta}{2}. \tag{3.156}$$

By using the integration in (3.145b), with $i = 2$, $\mathbf{L} = \mathbf{L}_2$, $\mathbf{L}' = \mathbf{L}_1$ and $\mathbf{r}_i = \mathbf{r}_2$, as applied to the second term on the right-hand side of inequality (3.154), with normalized wavefunction, we obtain

$$\begin{aligned} -\frac{Z_2 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_1|}}{|\mathbf{r}_2-\mathbf{L}_2|} \left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right|^2 \delta_{bb} \\ = -\frac{Z_2 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_1|}}{|\mathbf{r}_2-\mathbf{L}_2|} \\ = \frac{Z_2 e^2 \beta^3}{2\pi} \left(-\int \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_1|}}{|\mathbf{r}_2-\mathbf{L}_2|}\right) \\ \leqslant \frac{Z_2 e^2 \beta^3}{2\pi} (0) \end{aligned}$$

$$=0. \tag{3.157}$$

From (3.157), we obtain the inequality

$$-\frac{Z_2 e^2 \beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_1|}}{|\mathbf{r}_2-\mathbf{L}_2|}\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right|^2\delta_{bb}\leqslant 0. \tag{3.158}$$

By using (3.119), with $i = 1$, $\mathbf{r}_i = \mathbf{r}_1$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{L}' = \mathbf{L}_2$, as applied to the third term on the right-hand side of (3.154), we obtain

$$\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\leqslant 4\pi\mathrm{e}^{-\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right] \tag{3.159}$$

and by using (3.145c), set $i = 2$, $\mathbf{r}_2 = \mathbf{r}_i$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{L}' = \mathbf{L}_2$, then apply to the third term on the right-hand side of (3.154), we obtain

$$\int \mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_2|}\leqslant 4\pi\mathrm{e}^{-\beta L_0}\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right]. \tag{3.160}$$

Substitute (3.159) and (3.160) into the third term on the right-hand side of (3.154), to obtain

$$\begin{aligned}\frac{Z_2 e^2\beta^3}{\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_2|}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}&\\ \leqslant 16 Z_2 e^2\beta^3\mathrm{e}^{-2\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right].&\end{aligned} \tag{3.161}$$

By substituting (3.156), (3.158) and (3.161) into the right-hand side of (3.154), we obtain

$$-\langle\Psi|\,\frac{Z_2 e^2}{|\mathbf{r}_2-\mathbf{R}_2|}\,|\Psi\rangle$$

$$\leqslant -\frac{Z_2 e^2\beta}{2}+0$$

$$+\,\delta_{ab}16Z_2e^2\beta^3\mathrm{e}^{-2\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right]. \qquad (3.162)$$

From (3.162), by taking the limit $L_0 \to \infty$, we have the inequality

$$-\left\langle\Psi\right|\frac{Z_2e^2}{|\mathbf{r}_2-\mathbf{R}_2|}\left|\Psi\right\rangle \leqslant -\frac{Z_2e^2\beta}{2}. \qquad (3.163)$$

By referring (3.137)–(3.153), consider the third term on the right-hand side of (3.136), to obtain

$$\begin{aligned}
-\left\langle\Psi\right|\frac{Z_1e^2}{|\mathbf{r}_2-\mathbf{R}_1|}\left|\Psi\right\rangle = &-\frac{Z_1e^2\beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_1|}\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right|^2\delta_{aa}\\
&-\frac{Z_1e^2\beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_1|}}{|\mathbf{r}_2-\mathbf{L}_1|}\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right|^2\delta_{bb}\\
&+\delta_{ab}\left[\frac{Z_1e^2\beta^3}{\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_1|}\right.\\
&\qquad\left.\times\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right]. \qquad (3.164)
\end{aligned}$$

By using the integration in (3.145b), with $i=2$, $\mathbf{L}=\mathbf{L}_2$, $\mathbf{L}'=\mathbf{L}_1$ and $\mathbf{r}_i=\mathbf{r}_2$, as applied to the first term on the right-hand side of inequality (3.164), with normalized wavefunction, we obtain

$$\begin{aligned}
-\frac{Z_1e^2\beta^3}{2\pi}&\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_1|}\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right|^2\delta_{aa}\\
&= -\frac{Z_1e^2\beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_1|}\\
&=\frac{Z_1e^2\beta^3}{2\pi}\left(-\int \mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_1|}\right)\\
&\leqslant\frac{Z_1e^2\beta^3}{2\pi}(0)
\end{aligned}$$

$$=0. \tag{3.165}$$

From (3.165), we obtain the inequality

$$-\frac{Z_1 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_1|} \left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\right|^2 \delta_{aa} \leqslant 0. \tag{3.166}$$

By using the integration in (3.145a), with $i = 2$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{r}_i = \mathbf{r}_2$, as applied to the second term on the right-hand side of inequality (3.164), with normalized wavefunction, we obtain

$$\begin{aligned}
-\frac{Z_1 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_1|}}{|\mathbf{r}_2-\mathbf{L}_1|} \left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right|^2 \delta_{bb}& \\
&= -\frac{Z_1 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_1|}}{|\mathbf{r}_2-\mathbf{L}_1|} \\
&= -\frac{Z_1 e^2 \beta^3}{2\pi} \frac{\pi}{\beta^2} \\
&= -\frac{Z_1 e^2 \beta}{2}.
\end{aligned} \tag{3.167}$$

From (3.167), we obtain

$$-\frac{Z_1 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_1|}}{|\mathbf{r}_2-\mathbf{L}_1|} \left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right|^2 \delta_{bb} = -\frac{Z_1 e^2 \beta}{2}. \tag{3.168}$$

By using (3.119), with $i = 1$, $\mathbf{r}_i = \mathbf{r}_1$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{L}' = \mathbf{L}_2$, as applied to the third term on the right-hand side of (3.164), we obtain

$$\int \mathrm{d}^3\mathbf{r}_1\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|} \leqslant 4\pi \mathrm{e}^{-\beta L_0} \left[\frac{L_0^3}{2} + \frac{1}{\beta^3} + \frac{L_0}{2\beta^2} + \frac{L_0^2}{2\beta}\right] \tag{3.169}$$

and by using (3.145c), with $i = 2$, $\mathbf{r}_i = \mathbf{r}_2$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{L}' = \mathbf{L}_2$, as applied to the third term on the right-hand side of (3.164), we obtain

$$\int \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_1|} \leqslant 4\pi\mathrm{e}^{-\beta L_0}\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right]. \tag{3.170}$$

Substitute (3.169) and (3.170) into the third term on the right-hand side of (3.164), to obtain

$$\frac{Z_1e^2\beta^3}{\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}}{|\mathbf{r}_2-\mathbf{L}_1|}\int \mathrm{d}^3\mathbf{r}_1\, \mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}$$
$$\leqslant \delta_{ab}\,16Z_1e^2\beta^3\mathrm{e}^{-2\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right]. \tag{3.171}$$

By substituting (3.166), (3.168) and (3.171) into the right-hand side of (3.164), we obtain

$$-\langle\Psi|\,\frac{Z_1e^2}{|\mathbf{r}_2-\mathbf{R}_1|}\,|\Psi\rangle$$
$$\leqslant -\frac{Z_1e^2\beta}{2}+0$$
$$+\,16Z_1e^2\beta^3\mathrm{e}^{-2\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right]. \tag{3.172}$$

From (3.172), by taking the limit $L_0 \to \infty$, we have

$$-\langle\Psi|\,\frac{Z_1e^2}{|\mathbf{r}_2-\mathbf{R}_1|}\,|\Psi\rangle \leqslant -\frac{Z_1e^2\beta}{2}. \tag{3.173}$$

By referring (3.137)–(3.153), consider the fourth term on the right-hand side of (3.136), to obtain

$$-\langle\Psi|\,\frac{Z_2e^2}{|\mathbf{r}_1-\mathbf{R}_2|}\,|\Psi\rangle = -\frac{Z_2e^2\beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_2|}\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right|^2\delta_{aa}$$

$$
\begin{aligned}
&-\frac{Z_2 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_2|}}{|\mathbf{r}_1-\mathbf{L}_2|} \left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right|^2 \delta_{bb} \\
&+\delta_{ab} \left[\frac{Z_2 e^2 \beta^3}{\pi} \frac{\beta^3}{\pi} \int \mathrm{d}^3\mathbf{r}_1\, \frac{\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_2|} \right. \\
&\quad \left. \times \int \mathrm{d}^3\mathbf{r}_2\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right]. \qquad (3.174)
\end{aligned}
$$

By using the integration in (3.145b), with $i = 1$, $\mathbf{L} = \mathbf{L}_2$, $\mathbf{L}' = \mathbf{L}_1$ and $\mathbf{r}_i = \mathbf{r}_1$, as applied to the first term on the right-hand side of inequality (3.164), with normalized wavefunction, we obtain

$$
\begin{aligned}
-\frac{Z_2 e^2 \beta^3}{2\pi} &\int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_2|} \left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right|^2 \delta_{aa} \\
&= -\frac{Z_2 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_2|} \\
&= \frac{Z_2 e^2 \beta^3}{2\pi} \left(-\int \mathrm{d}^3\mathbf{r}_1\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_2|}\right) \\
&\leqslant \frac{Z_2 e^2 \beta^3}{2\pi} (0) \\
&= 0. \qquad (3.175)
\end{aligned}
$$

We also have the following obvious inequality

$$
-\frac{Z_2 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_2|} \left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right|^2 \delta_{aa} \leqslant 0. \qquad (3.176)
$$

By using the integration in (3.145a), with $i = 1$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{r}_i = \mathbf{r}_1$, as applied to the second term on the right-hand side of inequality (3.174), with normalized wavefunction, we obtain

$$
-\frac{Z_2 e^2 \beta^3}{2\pi} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_2|}}{|\mathbf{r}_1-\mathbf{L}_2|} \left|\frac{\beta^{3/2}}{\sqrt{\pi}}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right|^2 \delta_{bb}
$$

$$= -\frac{Z_2e^2\beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_2|}}{|\mathbf{r}_1-\mathbf{L}_2|}$$

$$= -\frac{Z_2e^2\beta^3}{2\pi}\frac{\pi}{\beta^2}$$

$$= -\frac{Z_2e^2\beta}{2}. \tag{3.177}$$

From (3.177), we obtain

$$-\frac{Z_2e^2\beta^3}{2\pi}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_2|}}{|\mathbf{r}_1-\mathbf{L}_2|}\left|\frac{\beta^{3/2}}{\sqrt{\pi}}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\right|^2\delta_{bb} = -\frac{Z_2e^2\beta}{2}. \tag{3.178}$$

By using (3.119), with $i = 2$, $\mathbf{r}_i = \mathbf{r}_2$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{L}' = \mathbf{L}_2$, as applied to the third term on the right-hand side of (3.174), we obtain

$$\int \mathrm{d}^3\mathbf{r}_2\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|} \leqslant 4\pi\mathrm{e}^{-\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]. \tag{3.179}$$

and by using (3.145c), with $i = 1$, $\mathbf{r}_i = \mathbf{r}_1$, $\mathbf{L} = \mathbf{L}_1$ and $\mathbf{L}' = \mathbf{L}_2$, as applied to the third term on the right-hand side of (3.174), we obtain

$$\int \mathrm{d}^3\mathbf{r}_1\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_2|} \leqslant 4\pi\mathrm{e}^{-\beta L_0}\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right]. \tag{3.180}$$

Substitute (3.179) and (3.180) into the third term on the right-hand side of (3.174), to obtain

$$\begin{aligned}\frac{Z_2e^2\beta^3}{\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_1\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_2|}\int \mathrm{d}^3\mathbf{r}_2\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}&\\ \leqslant \delta_{ab}\,16Z_2e^2\beta^3\mathrm{e}^{-2\beta L_0}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]\left[\frac{L_0^2}{2}+\frac{L_0}{2\beta}+\frac{1}{4\beta^2}\right].&\end{aligned} \tag{3.181}$$

By substituting (3.176), (3.178) and (3.181) into the right-hand side of (3.174), we

obtain

$$
\begin{aligned}
&- \langle\Psi| \frac{Z_2 e^2}{|\mathbf{r}_1 - \mathbf{R}_2|} |\Psi\rangle \\
&\quad \leqslant -\frac{Z_2 e^2 \beta}{2} + 0 \\
&\quad\quad + 16 Z_2 e^2 \beta^3 \mathrm{e}^{-2\beta L_0} \left[\frac{L_0^3}{2} + \frac{1}{\beta^3} + \frac{L_0}{2\beta^2} + \frac{L_0^2}{2\beta}\right] \left[\frac{L_0^2}{2} + \frac{L_0}{2\beta} + \frac{1}{4\beta^2}\right]. \qquad (3.182)
\end{aligned}
$$

From (3.182), by taking the limit $L_0 \to \infty$, we have

$$
- \langle\Psi| \frac{Z_2 e^2}{|\mathbf{r}_1 - \mathbf{R}_2|} |\Psi\rangle \leqslant -\frac{Z_2 e^2 \beta}{2}. \qquad (3.183)
$$

By substituting (3.153) and (3.163) into the right-hand side of (3.136), we obtain

$$
\begin{aligned}
- \langle\Psi| \sum_{i=1}^{2} \sum_{j=1}^{2} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} |\Psi\rangle &\leqslant -\frac{Z_1 e^2 \beta}{2} - \frac{Z_2 e^2 \beta}{2} - \frac{Z_1 e^2 \beta}{2} - \frac{Z_2 e^2 \beta}{2} \\
&= -\sum_{j=i}^{2} Z_j e^2 \beta \qquad , k = 2 \\
&= -\, 2\, e^2 \beta \qquad\qquad , Z_j = 1. \qquad (3.184)
\end{aligned}
$$

From (3.184), we obtain the following bound for the expectation value of the nucleus-electron interaction for the hydrogen atom

$$
- \langle\Psi| \sum_{i=1}^{2} \sum_{j=1}^{2} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} |\Psi\rangle \leqslant -2\, e^2 \beta. \qquad (3.185)
$$

From (3.77) and (3.185), have the following bound for the expectation value of the nucleus-electron interaction for k hydrogen atoms as

$$
- \langle\Psi| \sum_{i=1}^{N} \sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} |\Psi\rangle = -\sum_{j=i}^{k} Z_j e^2 \beta
$$

$$= - e^2 \beta N \tag{3.186}$$

where

$$\sum_{j=i}^{k} Z_j = N. \tag{3.187}$$

Consider the third term on the right-hand side of (3.80), the expectation value of electron-electron interaction for $k = 2$ hydrogen nuclei, we obtain

$$\begin{aligned}
\langle \Psi | \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} | \Psi \rangle =& e^2 \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \, \Psi^*(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \, \Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) \\
=& \frac{e^2\beta^3}{\pi\sqrt{2}} \frac{\beta^3}{\pi\sqrt{2}} \\
& \times \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \Bigg[\delta_{aa} \, \mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_2|} \frac{\mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_2|}}{|\mathbf{r}_1 - \mathbf{r}_2|} \\
& + \delta_{bb} \, \mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_1|} \frac{\mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_1|}}{|\mathbf{r}_1 - \mathbf{r}_2|} \\
& - 2 \, \delta_{ab} \, \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_1|} \, \mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_2|} \frac{\mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_1|}}{|\mathbf{r}_1 - \mathbf{r}_2|} \Bigg] \\
=& \delta_{aa} \frac{e^2\beta^3}{2\pi} \frac{\beta^3}{\pi} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1 - \mathbf{L}_1|}}{|\mathbf{r}_1 - \mathbf{r}_2|} \, \mathrm{e}^{-2\beta|\mathbf{r}_2 - \mathbf{L}_2|} \\
& + \delta_{bb} \frac{e^2\beta^3}{2\pi} \frac{\beta^3}{\pi} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1 - \mathbf{L}_2|}}{|\mathbf{r}_1 - \mathbf{r}_2|} \, \mathrm{e}^{-2\beta|\mathbf{r}_2 - \mathbf{L}_1|} \\
& - \delta_{ab} \Bigg[\frac{e^2\beta^3}{\pi} \frac{\beta^3}{\pi} \int \mathrm{d}^3\mathbf{r}_1 \, \frac{\mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_2|} \, \mathrm{e}^{-\beta|\mathbf{r}_1 - \mathbf{L}_1|}}{|\mathbf{r}_1 - \mathbf{r}_2|} \\
& \times \int \mathrm{d}^3\mathbf{r}_2 \, \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_1|} \mathrm{e}^{-\beta|\mathbf{r}_2 - \mathbf{L}_2|} \Bigg] \\
=& \delta_{aa} \frac{e^2\beta^3}{2\pi} \frac{\beta^3}{\pi} \int \mathrm{d}^3\mathbf{r}_2 \, \mathrm{e}^{-2\beta|\mathbf{r}_2 - \mathbf{L}_2|} \int \mathrm{d}^3\mathbf{r}_1 \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}_1 - \mathbf{L}_1|}}{|\mathbf{r}_1 - \mathbf{r}_2|}
\end{aligned}$$

$$+\,\delta_{bb}\frac{e^2\beta^3}{2\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_2\,\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_1|}\int \mathrm{d}^3\mathbf{r}_1\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}_1-\mathbf{L}_2|}}{|\mathbf{r}_1-\mathbf{r}_2|}$$

$$-\,\delta_{ab}\left[\frac{e^2\beta^3}{\pi}\frac{\beta^3}{\pi}\int \mathrm{d}^3\mathbf{r}_2\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_2|}\right.$$

$$\left.\times\int \mathrm{d}^3\mathbf{r}_1\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{r}_2|}\right]. \tag{3.188}$$

To evaluate (3.188), we introduce following variables :

$$\mathbf{R} = \mathbf{r}-\mathbf{L}, \tag{3.189a}$$

$$\mathbf{R}' = \mathbf{r}'-\mathbf{L}', \tag{3.189b}$$

$$\mathbf{L}_0 = \mathbf{L}'-\mathbf{L}, \tag{3.189c}$$

$$\mathbf{L}_0' = \mathbf{L}-\mathbf{L}', \tag{3.189d}$$

to obtain

$$\begin{aligned}
\int \mathrm{d}^3\mathbf{r}\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|} &= \int \mathrm{d}^3\mathbf{R}\,\frac{\mathrm{e}^{-2\beta|\mathbf{R}|}}{|\mathbf{R}+\mathbf{L}-\mathbf{R}'-\mathbf{L}'|}\\
&= \int \mathrm{d}^3\mathbf{R}\,\frac{\mathrm{e}^{-2\beta|\mathbf{R}|}}{|\mathbf{R}-\mathbf{R}'-\mathbf{L}_0|}\\
&= \int \mathrm{d}^3\mathbf{R}\,\frac{\mathrm{e}^{-2\beta|\mathbf{R}|}}{|\mathbf{R}-(\mathbf{R}'+\mathbf{L}_0)|}\\
&= \int \mathrm{d}^3\mathbf{R}\,\mathrm{e}^{-2\beta|\mathbf{R}|}\sum_{\ell=0}^{\infty}\left(\frac{R_<}{R_>}\right)^{\ell}\frac{1}{R_>}\,P_\ell(\cos\theta)\\
&= \int_0^\infty \mathrm{d}R\,\frac{R^2}{R_>}\,\mathrm{e}^{-2\beta|\mathbf{R}|}\int \mathrm{d}\Omega\,\sum_{\ell=0}^{\infty}\left(\frac{R_<}{R_>}\right)^{\ell}P_\ell(\cos\theta)\\
&= 4\pi\int_0^\infty \mathrm{d}R\,\frac{R^2}{R_>}\,\mathrm{e}^{-2\beta|\mathbf{R}|}
\end{aligned}$$

$$
\begin{aligned}
=&4\pi\int_0^{R'+L_0}\mathrm{d}R\,\frac{R^2}{R'+L_0}\,\mathrm{e}^{-2\beta R}+4\pi\int_{R'+L_0}^{\infty}\mathrm{d}R\,\frac{R^2}{R}\,\mathrm{e}^{-2\beta R}\\
=&\frac{4\pi}{R'+L_0}\int_0^{R'+L_0}\mathrm{d}R\,R^2\,\mathrm{e}^{-2\beta R}+4\pi\int_{R'+L_0}^{\infty}\mathrm{d}R\,R\,\mathrm{e}^{-2\beta R}\\
=&\frac{4\pi}{R'+L_0}\frac{\partial^2}{\partial u^2}\int_0^{R'+L_0}\mathrm{d}R\,\mathrm{e}^{-uR}\\
&+4\pi\int_{R'+L_0}^{\infty}\mathrm{d}R\,R\,\mathrm{e}^{-uR}\ \ ,u=2\beta
\end{aligned}\tag{3.190}
$$

where

$$
\frac{1}{|\mathbf{R}_i-(\mathbf{R}'+\mathbf{L}_0)|}=\sum_{\ell=0}^{\infty}\left(\frac{R_{i<}}{R_{i>}}\right)^{\ell}\frac{1}{R_{i>}}\,P_\ell(\cos\theta),\tag{3.191a}
$$

$$
R_>=\max(R,R'+L_0),\tag{3.191b}
$$

$$
\int\mathrm{d}\Omega\,P_\ell(\cos\theta)=4\pi\delta_{\ell 0}.\tag{3.191c}
$$

Consider the first term on the right-hand side of (3.190), we obtain

$$
\begin{aligned}
\frac{\partial^2}{\partial u^2}\int_0^{R'+L_0}\mathrm{d}R\,\mathrm{e}^{-uR}=&\frac{\partial^2}{\partial u^2}\left[-\frac{\mathrm{e}^{-uR}}{u}\bigg|_0^{R'+L_0}\right]\\
=&-\frac{\partial^2}{\partial u^2}\left[\frac{\mathrm{e}^{-u(R'+L_0)}}{u}-\frac{1}{u}\right].
\end{aligned}\tag{3.192}
$$

Since, taking the limit $L_0\to 0$ we have for (3.192)

$$
\frac{\partial^2}{\partial u^2}\int_0^{R'+L_0}\mathrm{d}R\,\mathrm{e}^{-uR}=\frac{2}{u}=\frac{1}{\beta}.\tag{3.193}
$$

Now consider the second term on the right-hand side of (3.190), to obtain

$$
\int_{R'+L_0}^{\infty}\mathrm{d}R\,R\,\mathrm{e}^{-2\beta R}=\left(-\frac{\mathrm{e}^{-2\beta R}}{2\beta}\left[R+\frac{1}{2\beta}\right]\right)\bigg|_{R'+L_0}^{\infty}
$$

$$=0-\left(-\frac{\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta}\left[(R'+L_0)+\frac{1}{2\beta}\right]\right)$$

$$=\frac{\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta}\left[(R'+L_0)+\frac{1}{2\beta}\right]$$

$$=\frac{(R'+L_0)\,\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta}+\frac{\mathrm{e}^{-2\beta(R'+L_0)}}{4\beta^2}. \tag{3.194}$$

Substitute (3.192) and (3.193) into the right-hand side of (3.190), for $L_0 \to \infty$, to obtain

$$\int \mathrm{d}^3\mathbf{r}\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|}=\frac{4\pi}{R'+L_0}\frac{\partial^2}{\partial u^2}\int_0^{R'+L_0}\mathrm{d}R\,\mathrm{e}^{-uR}$$
$$+4\pi\int_{R'+L_0}^{\infty}\mathrm{d}R\,R\,\mathrm{e}^{-2\beta R}$$
$$=\frac{4\pi}{\beta}\frac{1}{R'+L_0}+4\pi\left[\frac{(R'+L_0)\,\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta}+\frac{\mathrm{e}^{-2\beta(R'+L_0)}}{4\beta^2}\right]. \tag{3.195}$$

By using (3.189) and the integration from (3.194), for $L_0 \to \infty$, we obtain

$$\int \mathrm{d}^3\mathbf{r}'\,\mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}'|}\int \mathrm{d}^3\mathbf{r}\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|}$$
$$=\int \mathrm{d}^3\mathbf{R}'\,\mathrm{e}^{-2\beta|\mathbf{R}'|}\int \mathrm{d}^3\mathbf{r}\,\frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|}$$
$$=\frac{4\pi}{\beta}\int \mathrm{d}^3\mathbf{R}'\,\mathrm{e}^{-2\beta|\mathbf{R}'|}\frac{1}{R'+L_0}$$
$$+4\pi\int \mathrm{d}^3\mathbf{R}'\,\mathrm{e}^{-2\beta|\mathbf{R}'|}\left[\frac{(R'+L_0)\,\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta}+\frac{-\mathrm{e}^{2\beta(R'+L_0)}}{4\beta^2}\right]$$
$$=\frac{4\pi}{\beta}\int \mathrm{d}^3\mathbf{R}'\,\frac{\mathrm{e}^{-2\beta|\mathbf{R}'|}}{R'+L_0}$$

$$+ 4\pi \mathrm{e}^{-2\beta L_0} \int \mathrm{d}^3\mathbf{R}' \, \mathrm{e}^{-2\beta|\mathbf{R}'|} \left[\frac{(R' + L_0)\, \mathrm{e}^{-2\beta R'}}{2\beta} + \frac{\mathrm{e}^{-2\beta R'}}{4\beta^2} \right] . \tag{3.196}$$

For $L_0 \to \infty$, we can rewrite (3.196) as

$$\begin{aligned} \int \mathrm{d}^3\mathbf{r}' \, \mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}'|} \int \mathrm{d}^3\mathbf{r} \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|} =& \frac{4\pi}{\beta} \int \mathrm{d}^3\mathbf{R}' \, \frac{\mathrm{e}^{-2\beta|\mathbf{R}'|}}{R' + L_0} \\ =& \frac{4\pi}{\beta} \int_0^\infty \mathrm{d}R' \, \frac{R'^2}{R' + L_0} \, \mathrm{e}^{-2\beta R'} \int \mathrm{d}\Omega \\ =& \frac{16\pi^2}{\beta} \int_0^\infty \mathrm{d}R' \, \frac{R'^2}{R' + L_0} \, \mathrm{e}^{-2\beta R'} \\ =& 0 \end{aligned} \tag{3.197}$$

for $L_0 \to \infty$.

From (3.196), with $L_0 \to \infty$, we obtain

$$\int \mathrm{d}^3\mathbf{r}' \, \mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}'|} \int \mathrm{d}^3\mathbf{r} \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|} = 0. \tag{3.198}$$

In the other case, let $\mathbf{R}' = (\mathbf{r}' - \mathbf{L})$

$$\begin{aligned} &\int \mathrm{d}^3\mathbf{r}' \, \mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}|} \int \mathrm{d}^3\mathbf{r} \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}'|}}{|\mathbf{r}-\mathbf{r}'|} \\ &= \int \mathrm{d}^3\mathbf{R}' \, \mathrm{e}^{-2\beta|\mathbf{R}'|} \int \mathrm{d}^3\mathbf{r} \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}'|}}{|\mathbf{r}-\mathbf{R}'-\mathbf{L}|} \\ &= \int \mathrm{d}^3\mathbf{R}' \, \mathrm{e}^{-2\beta|\mathbf{R}'|} \int \mathrm{d}^3\mathbf{r} \, \frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}'|}}{|(\mathbf{r}-\mathbf{L})-\mathbf{R}'|} \\ &= \int \mathrm{d}^3\mathbf{r} \, \mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}'|} \int \mathrm{d}^3\mathbf{R}' \frac{\mathrm{e}^{-2\beta|\mathbf{R}'|}}{|\mathbf{R}'-\mathbf{A}|} \end{aligned} \tag{3.199}$$

with setting $\mathbf{A} = \mathbf{r} - \mathbf{L}$.

Consider the second term on the integral right-hand side of (3.199), to obtain

$$\int d^3\mathbf{R}' \frac{e^{-2\beta|\mathbf{R}'|}}{|\mathbf{R}'-\mathbf{A}|} = \int_0^\infty dR'\, R'^2 e^{-2\beta R'} \int d\Omega \sum_{\ell=0}^{\infty} \left(\frac{R'_<}{R'_>}\right)^\ell \frac{1}{R'_>} P_\ell(\cos\theta)$$

$$= 4\pi \int_0^\infty dR'\, e^{-2\beta R'} \frac{R'^2}{R'_>}$$

$$= \frac{4\pi}{A} \int_0^A dR'\, R'^2 e^{-2\beta R'} + 4\pi \int_A^\infty dR'\, R' e^{-2\beta R'}$$

$$= \frac{4\pi}{A} \frac{\partial^2}{\partial u^2} \int_0^A dR'\, e^{uR'} + 4\pi \frac{\partial}{\partial u} \int_A^\infty dR'\, e^{uR'} \quad , u = -2\beta$$

$$= \frac{4\pi}{A} \frac{e^{uR'}}{u} \left(R'^2 - \frac{2R'}{u} + \frac{2}{u^2}\right)\Bigg|_0^A + 4\pi \frac{e^{uR'}}{u} \left(R' - \frac{1}{u^2}\right)\Bigg|_A^\infty$$

$$= \frac{4\pi}{A} \left[\frac{e^{uA}}{u} \left(A^2 - \frac{2A}{u} + \frac{2}{u^2}\right) - \frac{2}{u^3}\right]$$

$$+ 4\pi \left[0 - \frac{e^{uA}}{u} \left(A - \frac{1}{u^2}\right)\right]$$

$$= \frac{4\pi}{A} \left[\frac{e^{uA}}{u} \left(A^2 - \frac{2A}{u} + \frac{2}{u^2}\right) - \frac{2}{u^3}\right]$$

$$- 4\pi \frac{e^{uA}}{u} \left(A - \frac{1}{u^2}\right)$$

$$= \frac{4\pi}{A} \frac{2}{8\beta^3} - \frac{4\pi}{A} \left[\frac{e^{-2\beta A}}{2\beta} \left(A^2 + \frac{2A}{2\beta} + \frac{2}{4\beta^2}\right)\right]$$

$$+ 4\pi \frac{e^{-2\beta A}}{2\beta} \left(A + \frac{1}{4\beta^2}\right)$$

$$= \frac{4\pi}{A} \frac{2}{8\beta^3} - \frac{4\pi e^{-2\beta A}}{2\beta} \left[\frac{1}{A} \left(A^2 + \frac{A}{\beta} + \frac{2}{4\beta^2}\right)\right]$$

$$+ \frac{4\pi e^{-2\beta A}}{2\beta} \left(A + \frac{1}{4\beta^2}\right)$$

$$= \frac{4\pi}{A} \frac{2}{8\beta^3} - \frac{4\pi e^{-2\beta A}}{2\beta} \left\{\left(A + \frac{1}{\beta} + \frac{1}{2A\beta^2}\right) + \left(A + \frac{1}{4\beta^2}\right)\right\}$$

$$\leqslant \frac{\pi}{\beta^3}\frac{1}{A} \tag{3.200}$$

substitute $A = |\mathbf{r} - \mathbf{L}|$ into the right-hand side of inequality (3.200), to obtain the inequality

$$\int \mathrm{d}^3\mathbf{R}' \frac{\mathrm{e}^{-2\beta|\mathbf{R}'|}}{|\mathbf{R}' - (\mathbf{r} - \mathbf{L})|} \leqslant \frac{\pi}{\beta^3}\frac{1}{|\mathbf{r} - \mathbf{L}|} \tag{3.201}$$

substitute (3.201) into (3.199), to obtain

$$\begin{aligned}
&\int \mathrm{d}^3\mathbf{r'}\, \mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}|} \int \mathrm{d}^3\mathbf{r}\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}'|}}{|\mathbf{r} - \mathbf{r}'|} \\
&\leqslant \frac{\pi}{\beta^3} \int \mathrm{d}^3\mathbf{r}\, \mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}'|} \frac{1}{|\mathbf{r} - \mathbf{L}|} \\
&= \frac{\pi}{\beta^3} \int \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-2\beta|\mathbf{R}|} \frac{1}{|\mathbf{R} + \mathbf{L}' - \mathbf{L}|} \quad , \mathbf{R} = \mathbf{r} - \mathbf{L}' \\
&= \frac{\pi}{\beta^3} \int \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-2\beta|\mathbf{R}|} \frac{1}{|\mathbf{R} - (\mathbf{L} - \mathbf{L}')|} \\
&= \frac{\pi}{\beta^3} \int \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-2\beta|\mathbf{R}|} \frac{1}{|\mathbf{R} - \mathbf{L}_0'|} \quad , \mathbf{L}_0' = \mathbf{L} - \mathbf{L}' \\
&= \frac{\pi}{\beta^3} \int_0^\infty \mathrm{d}R\, R^2\, \mathrm{e}^{-2\beta|\mathbf{R}|} \int \mathrm{d}\Omega \sum_{\ell=0}^{\infty} \left(\frac{R_<}{R_>}\right)^\ell \frac{1}{R_>} P_\ell(\cos\theta) \\
&= \frac{4\pi^2}{\beta^3} \int_0^\infty \mathrm{d}R\, \frac{R^2}{R_>}\, \mathrm{e}^{-2\beta R} \\
&= \frac{4\pi^2}{L_0'\beta^3} \int_0^{L_0'} \mathrm{d}R\, R^2\, \mathrm{e}^{-2\beta R} + \frac{4\pi^2}{\beta^3} \int_{L_0'}^\infty \mathrm{d}R\, R\, \mathrm{e}^{-2\beta R} \\
&= \frac{4\pi^2}{L_0'\beta^3} \frac{\partial^2}{\partial u^2} \int_0^{L_0'} \mathrm{d}R'\, \mathrm{e}^{uR'} + \frac{4\pi^2}{\beta^3} \frac{\partial}{\partial u} \int_{L_0'}^\infty \mathrm{d}R'\, \mathrm{e}^{uR'} \quad , u = -2\beta \\
&= \frac{4\pi^2}{L_0'\beta^3} \frac{\mathrm{e}^{uR'}}{u} \left(R'^2 - \frac{2R'}{u} + \frac{2}{u^2}\right)\Bigg|_0^{L_0'} + \frac{4\pi^2}{\beta^3} \frac{\mathrm{e}^{uR'}}{u} \left(R' - \frac{1}{u^2}\right)\Bigg|_{L_0'}^\infty
\end{aligned}$$

$$=\frac{4\pi^2}{L_0'\beta^3}\left[\frac{e^{uL_0'}}{u}\left({L_0'}^2-\frac{2L_0'}{u}+\frac{2}{u^2}\right)-\frac{2}{u^3}\right]+\frac{4\pi^2}{\beta^3}\left[0-\frac{e^{uL_0'}}{u}\left(L_0'-\frac{1}{u^2}\right)\right]$$

$$=\frac{4\pi^2}{L_0'\beta^3}\left[\frac{e^{uL_0'}}{u}\left({L_0'}^2-\frac{2L_0'}{u}+\frac{2}{u^2}\right)-\frac{2}{u^3}\right]-\frac{4\pi^2}{\beta^3}\frac{e^{uL_0'}}{u}\left(L_0'-\frac{1}{u^2}\right)$$

$$=\frac{\pi^2}{L_0'\beta^6}-\frac{4\pi^2}{L_0'\beta^3}\left[\frac{e^{-2\beta L_0'}}{2\beta}\left({L_0'}^2+\frac{2L_0'}{2\beta}+\frac{2}{4\beta^2}\right)\right]+\frac{4\pi^2}{\beta^3}\frac{e^{-2\beta L_0'}}{2\beta}\left(L_0'+\frac{1}{4\beta^2}\right)$$

$$=\frac{\pi^2}{L_0'\beta^6}-\frac{2\pi^2\, e^{-2\beta L_0'}}{\beta^4}\left[\frac{1}{L_0'}\left({L_0'}^2+\frac{L_0'}{\beta}+\frac{2}{4\beta^2}\right)\right]+\frac{2\pi^2\, e^{-2\beta L_0'}}{\beta^4}\left(L_0'+\frac{1}{4\beta^2}\right)$$

$$=\frac{\pi^2}{L_0'\beta^6}-\frac{2\pi^2\, e^{-2\beta L_0'}}{\beta^4}\left\{\left(L_0'+\frac{1}{\beta}+\frac{1}{2L_0'\beta^2}\right)+\left(L_0'+\frac{1}{4\beta^2}\right)\right\}$$

$$\leqslant\frac{\pi^2}{L_0'\beta^6} \qquad (3.202)$$

from (3.202), by taking the limit $L_0' \to \infty$, we obtain

$$\lim_{L_0\to\infty}\left[\int d^3\mathbf{r'}\, e^{-2\beta|\mathbf{r}'-\mathbf{L}|}\int d^3\mathbf{r}\,\frac{e^{-2\beta|\mathbf{r}-\mathbf{L}'|}}{|\mathbf{r}-\mathbf{r}'|}\right]=0. \qquad (3.203)$$

To obtain third term on the right-hand side of (3.188), consider the integral technic,

$$\int d^3\mathbf{r}\,\frac{e^{-\beta|\mathbf{r}-\mathbf{L}'|}\, e^{-\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|}$$

$$=\int d^3\mathbf{R}\,\frac{e^{-\beta|\mathbf{R}+\mathbf{L}-\mathbf{L}'|}\, e^{-\beta|\mathbf{R}|}}{|\mathbf{R}-(\mathbf{r}'-\mathbf{L})|}\quad,\mathbf{R}=\mathbf{r}-\mathbf{L}$$

$$=\int d^3\mathbf{R}\,\frac{e^{-\beta|\mathbf{R}+\mathbf{L}_0'|}\, e^{-\beta|\mathbf{R}|}}{|\mathbf{R}-(\mathbf{r}'-\mathbf{L})|}\quad,\mathbf{L}_0'=\mathbf{L}-\mathbf{L}'$$

$$\geqslant\int d^3\mathbf{R}\,\frac{e^{-\beta\left|R+L_0'\right|}\, e^{-\beta|\mathbf{R}|}}{|\mathbf{R}-\mathbf{B}|}\quad,\mathbf{B}=\mathbf{r}'-\mathbf{L}$$

$$=\int d^3\mathbf{R}\,\frac{e^{-\beta\left(R+L_0'\right)}\, e^{-\beta R}}{|\mathbf{R}-\mathbf{B}|}\quad,$$

$$=\mathrm{e}^{-\beta L_0'}\int_0^\infty \mathrm{d}R\, R^2\mathrm{e}^{-2\beta R}\int \mathrm{d}\Omega \sum_{\ell=0}^{\infty}\left(\frac{R_<}{R_>}\right)^\ell \frac{1}{R_>}\, P_\ell(\cos\theta)$$

$$=4\pi\, \mathrm{e}^{-\beta L_0'}\int_0^\infty \mathrm{d}R\, \mathrm{e}^{-2\beta R}\frac{R^2}{R_>}$$

$$=\frac{4\pi\, \mathrm{e}^{-\beta L_0'}}{B}\int_0^B \mathrm{d}R\, R^2\mathrm{e}^{-2\beta R} + 4\pi\, \mathrm{e}^{-\beta L_0'}\int_B^\infty \mathrm{d}R\, R\mathrm{e}^{-2\beta R}$$

$$=\frac{4\pi\, \mathrm{e}^{-\beta L_0'}}{B}\frac{\partial^2}{\partial u^2}\int_0^B \mathrm{d}R\, \mathrm{e}^{uR} + 4\pi\, \mathrm{e}^{-\beta L_0'}\frac{\partial}{\partial u}\int_B^\infty \mathrm{d}R\, \mathrm{e}^{uR} \quad , u=-2\beta$$

$$=\frac{4\pi\, \mathrm{e}^{-\beta L_0'}}{B}\,\frac{\mathrm{e}^{uR}}{u}\left(R^2-\frac{2R}{u}+\frac{2}{u^2}\right)\Bigg|_0^B + 4\pi\, \mathrm{e}^{-\beta L_0'}\,\frac{\mathrm{e}^{uR}}{u}\left(R-\frac{1}{u^2}\right)\Bigg|_B^\infty$$

$$=\frac{4\pi\, \mathrm{e}^{-\beta L_0'}}{B}\left[\frac{\mathrm{e}^{uB}}{u}\left(B^2-\frac{2B}{u}+\frac{2}{u^2}\right)-\frac{2}{u^3}\right]$$

$$-4\pi\, \mathrm{e}^{-\beta L_0'}\frac{\mathrm{e}^{uB}}{u}\left(B-\frac{1}{u^2}\right)$$

$$=\frac{4\pi\, \mathrm{e}^{-\beta L_0'}}{B}\frac{2}{8\beta^3}-\frac{4\pi\, \mathrm{e}^{-\beta L_0'}}{B}\left[\frac{\mathrm{e}^{-2\beta B}}{2\beta}\left(B^2+\frac{2B}{2\beta}+\frac{2}{4\beta^2}\right)\right]$$

$$+4\pi\, \mathrm{e}^{-\beta L_0'}\frac{\mathrm{e}^{-2\beta B}}{2\beta}\left(B+\frac{1}{4\beta^2}\right)$$

$$=\frac{4\pi\, \mathrm{e}^{-\beta L_0'}}{B}\frac{2}{8\beta^3}-\frac{4\pi\, \mathrm{e}^{-\beta L_0'}\, \mathrm{e}^{-2\beta B}}{2\beta}\left[\frac{1}{B}\left(B^2+\frac{B}{\beta}+\frac{2}{4\beta^2}\right)\right]$$

$$+\frac{4\pi\, \mathrm{e}^{-\beta L_0'}\, \mathrm{e}^{-2\beta B}}{2\beta}\left(B+\frac{1}{4\beta^2}\right)$$

$$=\frac{4\pi\, \mathrm{e}^{-\beta L_0'}}{B}\frac{2}{8\beta^3}-\frac{4\pi\, \mathrm{e}^{-\beta L_0'}\mathrm{e}^{-2\beta B}}{2\beta}\left\{\left(B+\frac{1}{\beta}+\frac{1}{2B\beta^2}\right)+\left(B+\frac{1}{4\beta^2}\right)\right\}$$

$$\geqslant-\frac{4\pi\, \mathrm{e}^{-\beta L_0'}\mathrm{e}^{-2\beta B}}{2\beta}\left\{\left(2B+\frac{1}{\beta}+\frac{1}{2B\beta^2}+\frac{1}{4\beta^2}\right)\right\} \tag{3.204}$$

where

$$|(\mathbf{R}+\mathbf{L})-\mathbf{r}'| = |\mathbf{r}'-(\mathbf{R}+\mathbf{L})| \tag{3.205}$$

Accordingly,

$$-\int d^3\mathbf{r}\,\frac{e^{-\beta|\mathbf{r}-\mathbf{L}'|}\,e^{-\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|} \leqslant \frac{4\pi\,e^{-\beta L_0'}e^{-2\beta B}}{2\beta}\left(2B+\frac{1}{\beta}+\frac{1}{2B\beta^2}+\frac{1}{4\beta^2}\right). \tag{3.206}$$

By using the inequality in (3.206) with $B = |\mathbf{r}'-\mathbf{L}|$, we obtain

$$\begin{aligned}
&-\int d^3\mathbf{r}'\,e^{-\beta|\mathbf{r}'-\mathbf{L}|}e^{-\beta|\mathbf{r}'-\mathbf{L}'|}\int d^3\mathbf{r}\,\frac{e^{-\beta|\mathbf{r}-\mathbf{L}'|}\,e^{-\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|}\\
&\quad\leqslant \int d^3\mathbf{r}'\,e^{-\beta|\mathbf{r}'-\mathbf{L}|}e^{-\beta|\mathbf{r}'-\mathbf{L}'|}\left[\frac{4\pi\,e^{-\beta L_0'}e^{-2\beta B}}{2\beta}\left(2B+\frac{1}{\beta}+\frac{1}{2B\beta^2}+\frac{1}{4\beta^2}\right)\right]\\
&\quad=\frac{4\pi\,e^{-\beta L_0'}}{2\beta}\int d^3\mathbf{r}'\,e^{-\beta|\mathbf{r}'-\mathbf{L}|}e^{-\beta|\mathbf{r}'-\mathbf{L}'|}\left[e^{-2\beta B}\left(2B+\frac{1}{\beta}+\frac{1}{2B\beta^2}+\frac{1}{4\beta^2}\right)\right]\\
&\quad=\frac{4\pi\,e^{-\beta L_0'}}{2\beta}\int d^3\mathbf{r}'\,e^{-2\beta|\mathbf{r}'-\mathbf{L}|}e^{-\beta|\mathbf{r}'-\mathbf{L}'|}\left[2|\mathbf{r}'-\mathbf{L}|+\frac{1}{\beta}+\frac{1}{2|\mathbf{r}'-\mathbf{L}|\beta^2}+\frac{1}{4\beta^2}\right]\\
&\quad=\frac{8\pi\,e^{-\beta L_0'}}{2\beta}\int d^3\mathbf{r}'\,e^{-2\beta|\mathbf{r}'-\mathbf{L}|}e^{-\beta|\mathbf{r}'-\mathbf{L}'|}|\mathbf{r}'-\mathbf{L}|\\
&\qquad+\frac{4\pi\,e^{-\beta L_0'}}{2\beta^2}\int d^3\mathbf{r}'\,e^{-2\beta|\mathbf{r}'-\mathbf{L}|}e^{-\beta|\mathbf{r}'-\mathbf{L}'|}\\
&\qquad+\frac{\pi\,e^{-\beta L_0'}}{\beta^3}\int d^3\mathbf{r}'\,e^{-2\beta|\mathbf{r}'-\mathbf{L}|}e^{-\beta|\mathbf{r}'-\mathbf{L}'|}\frac{1}{|\mathbf{r}'-\mathbf{L}|}\\
&\qquad+\frac{\pi\,e^{-\beta L_0'}}{2\beta^3}\int d^3\mathbf{r}'\,e^{-2\beta|\mathbf{r}'-\mathbf{L}|}e^{-\beta|\mathbf{r}'-\mathbf{L}'|}.
\end{aligned} \tag{3.207}$$

Consider the first term on the right-hand side of inequality (3.207), and let $\mathbf{R}' = \mathbf{r}'-\mathbf{L}$, to obtain

$$\frac{8\pi\,e^{-\beta L_0'}}{2\beta}\int d^3\mathbf{r}'\,e^{-2\beta|\mathbf{r}'-\mathbf{L}|}e^{-\beta|\mathbf{r}'-\mathbf{L}'|}|\mathbf{r}'-\mathbf{L}|$$

$$
\begin{aligned}
&= \frac{8\pi\, e^{-\beta L_0'}}{2\beta} \int d^3\mathbf{R}'\, |\mathbf{R}'|\, e^{-2\beta|\mathbf{R}'|} e^{-\beta|\mathbf{R}'-\mathbf{L}_0|} \\
&= \frac{8\pi\, e^{-\beta L_0'}}{2\beta} \int_0^\infty \int_0^\pi \int_0^{2\pi} dR'\, d\theta\, d\varphi\, R'^3 \sin\theta\, e^{-2\beta R'} e^{-\beta\sqrt{R'^2+L_0^2-2R'L_0\cos\theta}} \\
&\leqslant \frac{8\pi\, e^{-\beta L_0'}}{2\beta} \int_0^\infty \int_0^\pi \int_0^{2\pi} dR'\, d\theta\, d\varphi\, R'^3 \sin\theta\, e^{-2\beta R'} e^{-\beta\sqrt{R'^2+L_0^2-2R'L_0}} \\
&= \frac{8\pi\, e^{-\beta L_0'}}{2\beta} \int_0^\infty \int_0^\pi \int_0^{2\pi} dR'\, d\theta\, d\varphi\, R'^3 \sin\theta\, e^{-2\beta R'} e^{-\beta|R'-L_0|} \\
&= \frac{32\pi^2\, e^{-\beta L_0'}}{2\beta} \int_0^\infty dR'\, R'^3\, e^{-2\beta R'} e^{-\beta|R'-L_0|} \\
&= \frac{32\pi^2\, e^{-\beta L_0'}}{2\beta} \int_0^{L_0} dR'\, R'^3\, e^{-2\beta R'} e^{-\beta(L_0-R')} \\
&\quad + \frac{32\pi^2\, e^{-\beta L_0'}}{2\beta} \int_{L_0}^\infty dR'\, R'^3\, e^{-2\beta R'} e^{-\beta(R'-L_0)} \\
&= \frac{32\pi^2\, e^{-\beta(L_0'+L_0)}}{2\beta} \int_0^{L_0} dR'\, R'^3\, e^{-\beta R'} + \frac{32\pi^2\, e^{-\beta(L_0'-L_0)}}{2\beta} \int_{L_0}^\infty dR'\, R'^3\, e^{-3\beta R'} \\
&= \frac{32\pi^2\, e^{-2\beta L_0}}{2\beta} \int_0^{L_0} dR'\, R'^3\, e^{-\beta R'} + \frac{32\pi^2}{2\beta} \int_{L_0}^\infty dR'\, R'^3\, e^{-3\beta R'} \\
&= -\frac{32\pi^2\, e^{-2\beta L_0}}{2\beta} \left[e^{-\beta R'} \left(\frac{6+6\beta R'+3\beta^2R'^2+\beta^3R'^3}{\beta^4} \right) \right]_0^{L_0} \\
&\quad - \frac{32\pi^2}{2\beta} \left[e^{-3\beta R'} \left(\frac{2+6\beta R'+9\beta^2R'^2+9\beta^3R'^3}{27\beta^4} \right) \right]_{L_0}^\infty \\
&= -\frac{32\pi^2\, e^{-2\beta L_0}}{2\beta} \left[e^{-\beta L_0} \left(\frac{6+6\beta L_0+3\beta^2L_0^2+\beta^3L_0^3}{\beta^4} \right) - \frac{6}{\beta^4} \right] \\
&= \frac{32\pi^2\, e^{-2\beta L_0}}{2\beta} \frac{6}{\beta^4} - \frac{32\pi^2\, e^{-3\beta L_0}}{2\beta} \left(\frac{6+6\beta L_0+3\beta^2L_0^2+\beta^3L_0^3}{\beta^4} \right) \\
&\quad + \frac{32\pi^2 e^{-3\beta L_0}}{2\beta} \left(\frac{2+6\beta L_0+9\beta^2L_0^2+9\beta^3L_0^3}{27\beta^4} \right)
\end{aligned} \tag{3.208}
$$

where $\mathbf{L}_0', \mathbf{L}_0$ defined from (3.189) i.e,

$$\mathbf{L}_0' = -\,\mathbf{L}_0, \tag{3.209a}$$

$$L_0' = |\mathbf{L}_0'| = |-\mathbf{L}_0| = |\mathbf{L}_0| = L_0. \tag{3.209b}$$

From (3.208), we obtain the inequality

$$\begin{aligned}
&\frac{8\pi\,\mathrm{e}^{-\beta L_0'}}{2\beta}\int \mathrm{d}^3\mathbf{r}'\,\mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}'|}|\mathbf{r}'-\mathbf{L}| \\
&\qquad \leqslant \frac{32\pi^2\,\mathrm{e}^{-2\beta L_0}}{2\beta}\frac{6}{\beta^4} - \frac{32\pi^2\,\mathrm{e}^{-3\beta L_0}}{2\beta}\left(\frac{6+6\beta L_0+3\beta^2L_0^2+\beta^3L_0^3}{\beta^4}\right) \\
&\qquad\quad + \frac{32\pi^2\mathrm{e}^{-3\beta L_0}}{2\beta}\left(\frac{2+6\beta L_0+9\beta^2L_0^2+9\beta^3L_0^3}{27\beta^4}\right)
\end{aligned} \tag{3.210}$$

and for $L_0 \to \infty$, we have the limit

$$\lim_{L_0\to\infty}\left[\frac{8\pi\,\mathrm{e}^{-\beta L_0'}}{2\beta}\int \mathrm{d}^3\mathbf{r}'\,\mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}'|}|\mathbf{r}'-\mathbf{L}|\right] = 0. \tag{3.211}$$

Consider the second term on the right-hand side of inequality (3.207), let $\mathbf{R}' = \mathbf{r}' - \mathbf{L}$, we obtain

$$\begin{aligned}
&\frac{4\pi\,\mathrm{e}^{-\beta L_0'}}{2\beta^2}\int \mathrm{d}^3\mathbf{r}'\,\mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}'|} \\
&\qquad = \frac{4\pi\,\mathrm{e}^{-\beta L_0'}}{2\beta^2}\int \mathrm{d}^3\mathbf{R}'\,\mathrm{e}^{-2\beta|\mathbf{R}'|}\mathrm{e}^{-\beta|\mathbf{R}'-(\mathbf{L}'-\mathbf{L})|} \\
&\qquad = \frac{4\pi\,\mathrm{e}^{-\beta L_0'}}{2\beta^2}\int \mathrm{d}^3\mathbf{R}'\,\mathrm{e}^{-2\beta|\mathbf{R}'|}\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0|} \qquad ,\mathbf{L}_0 = \mathbf{L}'-\mathbf{L} \\
&\qquad = \frac{4\pi\,\mathrm{e}^{-\beta L_0'}}{2\beta^2}\int_0^\infty\int_0^\pi\int_0^{2\pi} \mathrm{d}R'\,\mathrm{d}\theta\,\mathrm{d}\varphi\,R'^2\sin\theta\,\mathrm{e}^{-2\beta R'}\mathrm{e}^{-\beta\sqrt{R'^2+L_0^2-2R'L_0\cos\theta}} \\
&\qquad \leqslant \frac{4\pi\,\mathrm{e}^{-\beta L_0'}}{2\beta^2}\int_0^\infty\int_0^\pi\int_0^{2\pi} \mathrm{d}R'\,\mathrm{d}\theta\,\mathrm{d}\varphi\,R'^2\sin\theta\,\mathrm{e}^{-2\beta R'}\mathrm{e}^{-\beta\sqrt{R'^2+L_0^2-2R'L_0}}
\end{aligned}$$

$$
\begin{aligned}
=&\frac{16\pi^2\,\mathrm{e}^{-\beta L_0'}}{2\beta^2}\int_0^\infty \mathrm{d}R'\,R'^2\,\mathrm{e}^{-\beta R'}\mathrm{e}^{-\beta|R'-L_0|}\\
=&\frac{16\pi^2\,\mathrm{e}^{-\beta L_0'}}{2\beta^2}\int_0^{L_0} \mathrm{d}R'\,R'^2\,\mathrm{e}^{-\beta R'}\mathrm{e}^{-\beta(L_0-R')}\\
&+\frac{16\pi^2\,\mathrm{e}^{-\beta L_0'}}{2\beta^2}\int_{L_0}^\infty \mathrm{d}R'\,R'^2\,\mathrm{e}^{-\beta R'}\mathrm{e}^{-\beta(R'-L_0)}\\
=&\frac{16\pi^2\,\mathrm{e}^{-\beta(L_0'+L_0)}}{2\beta^2}\int_0^{L_0} \mathrm{d}R'\,R'^2+\frac{16\pi^2\,\mathrm{e}^{-\beta(L_0'-L_0)}}{2\beta^2}\int_{L_0}^\infty \mathrm{d}R'\,R'^2\,\mathrm{e}^{-2\beta R'}\\
=&\frac{16\pi^2\,\mathrm{e}^{-2\beta L_0}}{2\beta^2}\int_0^{L_0} \mathrm{d}R'\,R'^2+\frac{16\pi^2}{2\beta^2}\int_{L_0}^\infty \mathrm{d}R'\,R'^2\,\mathrm{e}^{-2\beta R'}\quad ,L_0'=L_0\\
=&\frac{16\pi^2\,\mathrm{e}^{-2\beta L_0}}{2\beta^2}\left[\frac{R'^3}{3}\right]_0^{L_0}-\frac{16\pi^2}{2\beta^2}\left[\mathrm{e}^{-2\beta R'}\left(1+2\beta R'+2\beta^2R'^2\right)\right]_{L_0}^\infty\\
=&\frac{16\pi^2\,\mathrm{e}^{-2\beta L_0}}{2\beta^2}\frac{L_0^3}{2}+\frac{16\pi^2\,\mathrm{e}^{-2\beta L_0}}{2\beta^2}\left[\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]\\
=&\mathrm{e}^{-2\beta L_0}\frac{16\pi^2}{2\beta^2}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right].
\end{aligned}
\tag{3.212}
$$

From (3.212), we obtain the inequality

$$
\frac{4\pi\,\mathrm{e}^{-\beta L_0'}}{2\beta^2}\int \mathrm{d}^3\mathbf{r'}\,\mathrm{e}^{-2\beta|\mathbf{r'}-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r'}-\mathbf{L'}|}\leqslant \mathrm{e}^{-2\beta L_0}\frac{16\pi^2}{2\beta^2}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right] \tag{3.213}
$$

and for $L_0\to\infty$, we have the limit

$$
\lim_{L_0'\to\infty}\left[\frac{4\pi\,\mathrm{e}^{-\beta L_0'}}{2\beta^2}\int \mathrm{d}^3\mathbf{r'}\,\mathrm{e}^{-2\beta|\mathbf{r'}-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r'}-\mathbf{L'}|}\right]=0. \tag{3.214}
$$

Consider the third term on the right-hand side of inequality (3.207), let $\mathbf{R}'=\mathbf{r}'-\mathbf{L}$, to obtain

$$
\frac{\pi\,\mathrm{e}^{-\beta L_0'}}{\beta^3}\int \mathrm{d}^3\mathbf{r'}\,\mathrm{e}^{-2\beta|\mathbf{r'}-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r'}-\mathbf{L'}|}\frac{1}{|\mathbf{r'}-\mathbf{L}|}
$$

$$\leqslant \mathrm{e}^{-2\beta L_0}\left\{\frac{4\pi^2}{\beta^5}-\frac{4\pi^2\,\mathrm{e}^{-\beta L_0}\,(1+2\beta L_0)}{\beta^5}+\frac{4\pi^2\,\mathrm{e}^{-\beta L_0}\,(1+3\beta L_0)}{9\beta^5}\right\} \tag{3.215}$$

and for $L_0 \to \infty$, we have the limit

$$\lim_{L_0\to\infty}\left[\frac{\pi\,\mathrm{e}^{-\beta L_0'}}{\beta^3}\int \mathrm{d}^3\mathbf{r}'\,\mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}'|}\frac{1}{|\mathbf{r}'-\mathbf{L}|}\right]=0. \tag{3.216}$$

Consider the fourth term on the right-hand side of inequality (3.207), by using the inequality (3.213), to obtain

$$\frac{\pi\,\mathrm{e}^{-\beta L_0'}}{2\beta^3}\int \mathrm{d}^3\mathbf{r}'\,\mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}'|}\leqslant \mathrm{e}^{-2\beta L_0}\frac{4\pi^2}{2\beta^3}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right] \tag{3.217}$$

and for $L_0 \to \infty$, we have the limit

$$\lim_{L_0\to\infty}\left[\frac{\pi\,\mathrm{e}^{-\beta L_0'}}{2\beta^3}\int \mathrm{d}^3\mathbf{r}'\,\mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}'|}\right]=0. \tag{3.218}$$

Substitute (3.210), (3.213), (3.215) and (3.217) into the right-hand side of inequality (3.207), to obtain

$$\begin{aligned}
&-\int \mathrm{d}^3\mathbf{r}'\,\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}'|}\int \mathrm{d}^3\mathbf{r}\,\frac{\mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}'|}\,\mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|}\\
&\leqslant \frac{32\pi^2\,\mathrm{e}^{-2\beta L_0}}{2\beta}\frac{6}{\beta^4}-\frac{32\pi^2\,\mathrm{e}^{-3\beta L_0}}{2\beta}\left(\frac{6+6\beta L_0+3\beta^2L_0^2+\beta^3L_0^3}{\beta^4}\right)\\
&\quad+\mathrm{e}^{-2\beta L_0}\frac{16\pi^2}{2\beta^2}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right]\\
&\quad+\mathrm{e}^{-2\beta L_0}\left\{\frac{4\pi^2}{\beta^5}-\frac{4\pi^2\,\mathrm{e}^{-\beta L_0}\,(1+2\beta L_0)}{\beta^5}+\frac{4\pi^2\,\mathrm{e}^{-\beta L_0}\,(1+3\beta L_0)}{9\beta^5}\right\}\\
&\quad+\mathrm{e}^{-2\beta L_0}\frac{4\pi^2}{2\beta^3}\left[\frac{L_0^3}{2}+\frac{1}{\beta^3}+\frac{L_0}{2\beta^2}+\frac{L_0^2}{2\beta}\right].
\end{aligned} \tag{3.219}$$

For $L_0 \to \infty$, by using (3.219) or substituting (3.211), (3.214), (3.216) and

(3.218) into the right-hand side of inequality (3.207), we obtain

$$-\int \mathrm{d}^3\mathbf{r}'\, \mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}'|} \int \mathrm{d}^3\mathbf{r}\, \frac{\mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}'|}\, \mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|} \leqslant 0. \tag{3.220}$$

By referring (3.198), (3.203) and (3.220), we obtain the expectation value of electron-electron interaction for $L_0 \to \infty$:

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}'\, \mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}'|} \int \mathrm{d}^3\mathbf{r}\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|}\right] = 0, \tag{3.221a}$$

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}'\, \mathrm{e}^{-2\beta|\mathbf{r}'-\mathbf{L}|} \int \mathrm{d}^3\mathbf{r}\, \frac{\mathrm{e}^{-2\beta|\mathbf{r}-\mathbf{L}'|}}{|\mathbf{r}-\mathbf{r}'|}\right] = 0, \tag{3.221b}$$

$$\lim_{L_0\to\infty}\left[-\int \mathrm{d}^3\mathbf{r}'\, \mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}|}\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}'|} \int \mathrm{d}^3\mathbf{r}\, \frac{\mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}'|}\, \mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}|}}{|\mathbf{r}-\mathbf{r}'|}\right] = 0. \tag{3.221c}$$

By applying (3.221) on the right-hand side of (3.188), let $\mathbf{L}_1 = \mathbf{L}$, $\mathbf{L}_2 = \mathbf{L}'$, $\mathbf{r}_1 = \mathbf{r}$ and $\mathbf{r}_2 = \mathbf{r}'$, we obtain the expectation value of electron-electron interaction with $L_0 \to \infty$ for $k = 2$ hydrogen nuclei,

$$\langle\Psi| \sum_{i<j}^{2} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} |\Psi\rangle = \langle\Psi| \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} |\Psi\rangle \to 0. \tag{3.222}$$

From (3.222), we can imply the expectation value of electron-electron interaction when $L_0 \to \infty$ for k hydrogen nuclei in such a limit

$$\lim_{L_0\to\infty}\left[\langle\Psi| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} |\Psi\rangle\right] = 0. \tag{3.223}$$

To obtain the expectation value of nucleus-nucleus interaction for $k = 2$ hydrogen nuclei, let

$$\mathbf{R}_1 - \mathbf{R}_2 = \mathbf{L}_1 - \mathbf{L}_2 = \mathbf{L}_0 \tag{3.224}$$

then substitute into the fourth term on the right-hand side of (3.80), to obtain

$$\langle\Psi|\frac{Z_1Z_2e^2}{|\mathbf{R}_1-\mathbf{R}_2|}|\Psi\rangle = \frac{Z_1Z_2e^2}{|\mathbf{L}_0|}\langle\Psi|\Psi\rangle$$
$$= \frac{Z_1Z_2e^2}{L_0}. \tag{3.225}$$

From (3.224), for $k > 2$, we obtain

$$|\mathbf{R}_i-\mathbf{R}_j| \geqslant |\mathbf{L}_0|, \tag{3.226a}$$

$$\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|} \leqslant \frac{1}{|\mathbf{R}_1-\mathbf{R}_2|} \leqslant \frac{1}{|\mathbf{L}_0|}. \tag{3.226b}$$

By using (3.226), we obtain

$$\langle\Psi|\sum_{i<j}^{k}\frac{Z_jZ_je^2}{|\mathbf{R}_1-\mathbf{R}_2|}|\Psi\rangle \leqslant \frac{1}{|\mathbf{L}_0|}\sum_{i<j}^{k}Z_1Z_2e^2\langle\Psi|\Psi\rangle$$
$$= \frac{1}{L_0}\sum_{i<j}^{k}Z_iZ_je^2. \tag{3.227}$$

From (3.227), we obtain the bound of the expectation value of nucleus-nucleus interaction for k hydrogen nuclei

$$\langle\Psi|\sum_{i<j}^{k}\frac{Z_jZ_je^2}{|\mathbf{R}_i-\mathbf{R}_j|}|\Psi\rangle \leqslant \frac{1}{L_0}\sum_{i<j}^{k}Z_iZ_je^2. \tag{3.228}$$

From (3.228), for $L_0 \to \infty$, the bound of the expectation value of nucleus-nucleus interaction for k hydrogen nuclei in this a limit :

$$\lim_{L_0\to\infty}\langle\Psi|\sum_{i<j}^{k}\frac{Z_jZ_je^2}{|\mathbf{R}_i-\mathbf{R}_j|}|\Psi\rangle = 0. \tag{3.229}$$

By referring to (3.134), (3.186), (3.223), (3.229) and (3.62), we obtain

$$\begin{aligned}\langle\Psi| H |\Psi\rangle =& \langle\Psi| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} |\Psi\rangle - \langle\Psi| \sum_{i=1}^{N}\sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{r}_i - \mathbf{R}_j|} |\Psi\rangle \\ &+ \langle\Psi| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} |\Psi\rangle + \langle\Psi| \sum_{i<j}^{k} \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|} |\Psi\rangle \\ \leqslant& \frac{\hbar^2\beta^2}{2m} N - e^2\beta N + 0 + 0 \\ =& \frac{\hbar^2}{2m}\left(\frac{me^2}{\hbar^2}\right) N - e^2\left(\frac{me^2}{\hbar^2}\right) N \\ =& -\left(\frac{me^4}{2\hbar^2}\right) N. \end{aligned} \tag{3.230}$$

From (3.230), we obtain the following upper bound for the ground-state energy of hydrogen atom k nuclei following infinite separated $k = N$ clusters :

$$\langle\Psi| H |\Psi\rangle \leqslant -\left(\frac{me^4}{2\hbar^2}\right) N. \tag{3.231}$$

3.4 Upper Bound for the Exact Ground-State Energy of Matter II

In this section we derived the upper bound for the exact ground-state energy of matter by considering the following infinitely separated N clusters : k hydrogenic atoms, each in the ground-state with nuclear charges $Z_1|e|, \ldots, Z_k|e|$ having each one electron, and $(N-k)$ free electrons with vanishingly small kinetic energies. We introduce the following determinantal function in (3.1) with normalized wavefunction and normalized spin functions $\chi_j(\sigma)$ and $\mathbf{r}_i$ is vector from the origin to electron e_i. Set $\mathbf{L}$, $\mathbf{L}'$ are vector from the origin to nucleus $Z|e|$ and $Z'|e|$ localization, with normalized wavefunction, and let $|\mathbf{L}_i - \mathbf{L}_j| \to \infty$.

The wavefunctions of k bound electrons are

$$\psi_1(\mathbf{r},\sigma) = \psi\left(\mathbf{r}-\mathbf{L}_1\right)\chi_1(\sigma) = C\,\mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}_1|}\,\chi_1(\sigma)$$

$$\vdots$$

$$\psi_k(\mathbf{r},\sigma) = \psi\left(\mathbf{r}-\mathbf{L}_k\right)\chi_k(\sigma) = C\,\mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}_k|}\,\chi_k(\sigma) \tag{3.232}$$

and the following wavepackets of the $(N-k)$ free electrons

$$\psi_{k+1}(\mathbf{r},\sigma) = \phi_{k+1}(\mathbf{r},\sigma) = \phi\left(\mathbf{r}-\mathbf{L}_{k+1}\right)\chi_{k+1}(\sigma) = A\,\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}-\mathbf{L}_{k+1})}\,\mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L}_{k+1})^2}{4\sigma'^2}}\chi_{k+1}(\sigma)$$

$$\vdots$$

$$\psi_N(\mathbf{r},\sigma) = \phi_N(\mathbf{r},\sigma) = \phi\left(\mathbf{r}-\mathbf{L}_N\right)\chi_N(\sigma) = A\,\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}-\mathbf{L}_N)}\,\mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L}_N)^2}{4\sigma'^2}}\chi_N(\sigma) \tag{3.233}$$

where σ' is the standard derivation about the average positions and

$$C = \frac{\beta^{3/2}}{\sqrt{\pi}} \tag{3.234}$$

$$A = \frac{1}{\left(2\pi^{3/4}\right)\sigma'^{3/2}} \tag{3.235}$$

To obtain an upper bound of the ground-state energy of this system, we consider the Hamiltonian H

$$H = \sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m} + \sum_{i<j}^{N}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|} - \sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_j e^2}{|\mathbf{r}_i-\mathbf{R}_j|} + \sum_{i<j}^{k}\frac{Z_i Z_j e^2}{|\mathbf{R}_i-\mathbf{R}_j|}. \tag{3.236}$$

From (3.1), we obtain the expectation value of the Hamiltonian

$$\langle\Psi|\, H\,|\Psi\rangle = \langle\Psi| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m}\,|\Psi\rangle + \langle\Psi| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}\,|\Psi\rangle$$

$$- \langle\Psi| \sum_{i=1}^{N}\sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{r}_i - \mathbf{R}_j|}\,|\Psi\rangle + \langle\Psi| \sum_{i<j}^{k} \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|}\,|\Psi\rangle\,. \qquad (3.237)$$

To obtain an upper bound, we we start from the simple system, with $k = 1$ nucleus $(Z_1 = 2)$, one bound electron and one free electron, $N = 2$. By using the determinantal function (fermion wavefunction), the wave function of this simple system is

$$\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = \frac{1}{\sqrt{2}}\left[\psi_1(\mathbf{r}_1, \sigma_1)\,\phi_2(\mathbf{r}_2, \sigma_2) - \psi_1(\mathbf{r}_2, \sigma_2)\,\phi_2(\mathbf{r}_1, \sigma_1)\right] \qquad (3.238)$$

where

$$\psi_1(\mathbf{r}_1, \sigma_1) = C\,\exp -\beta\,|\mathbf{r}_1 - \mathbf{L}_1|\,\chi_1(\sigma_1), \qquad (3.239a)$$

$$\psi_1(\mathbf{r}_2, \sigma_2) = C\,\exp -\beta\,|\mathbf{r}_2 - \mathbf{L}_1|\,\chi_1(\sigma_2), \qquad (3.239b)$$

$$\phi_2(\mathbf{r}_1, \sigma_1) = A\,\exp \mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}_1 - \mathbf{L}_2)\,\exp -\frac{(\mathbf{r}_1 - \mathbf{L}_2)^2}{4\sigma'^2}\,\chi_2(\sigma_1), \qquad (3.239c)$$

$$\phi_2(\mathbf{r}_2, \sigma_2) = A\,\exp \mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}_2 - \mathbf{L}_2)\,\exp -\frac{(\mathbf{r}_2 - \mathbf{L}_2)^2}{4\sigma'^2}\,\chi_2(\sigma_2), \qquad (3.239d)$$

from (3.232) and (3.233), with normalized spin.

From (3.237) the expectation value of the Hamiltonian can be rewritten as

$$\langle\Psi|\, H\,|\Psi\rangle = \langle\Psi| \sum_{i=1}^{2} \frac{\mathbf{p}_i^2}{2m}\,|\Psi\rangle + \langle\Psi| \sum_{i<j}^{2} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}\,|\Psi\rangle$$

$$- \langle\Psi| \sum_{i=1}^{2}\sum_{j=1}^{1} \frac{Z_j e^2}{|\mathbf{r}_i - \mathbf{R}_j|}\,|\Psi\rangle\,. \qquad (3.240)$$

Substitute (3.239) into the first term on the right-hand side of (3.238), to obtain

$$\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2) = CA\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}_2-\mathbf{L}_2)}\,\mathrm{e}^{-\frac{(\mathbf{r}_2-\mathbf{L}_2)^2}{4\sigma'^2}}\,\chi_1(\sigma_1)\chi_2(\sigma_2) \tag{3.241}$$

and substitute (3.239) into the second term on the right-hand side of (3.238), to obtain

$$\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1) = CA\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\,\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}_1-\mathbf{L}_2)}\,\mathrm{e}^{-\frac{(\mathbf{r}_1-\mathbf{L}_2)^2}{4\sigma'^2}}\,\chi_1(\sigma_2)\chi_2(\sigma_1). \tag{3.242}$$

Then substitute (3.241) and (3.242) into the right-hand side of (3.238), to obtain for the anti-symmetric wavefunction with $k = 1$ nucleus with $(Z_1 = 2)$, one bound electron and one free electron, by denoting $\Psi = \Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$ we obtain

$$\begin{aligned}\Psi =& \frac{CA}{\sqrt{2}}\Big[\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}_2-\mathbf{L}_2)}\,\mathrm{e}^{-\frac{(\mathbf{r}_2-\mathbf{L}_2)^2}{4\sigma'^2}}\,\chi_1(\sigma_1)\chi_2(\sigma_2)\\ &\qquad - \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\,\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}_1-\mathbf{L}_2)}\,\mathrm{e}^{-\frac{(\mathbf{r}_1-\mathbf{L}_2)^2}{4\sigma'^2}}\,\chi_1(\sigma_2)\chi_2(\sigma_1)\Big]\\ =& \frac{CA}{\sqrt{2}}\Big[\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}_2-\mathbf{L}_2)}\,\mathrm{e}^{-\frac{(\mathbf{r}_2-\mathbf{L}_2)^2}{4\sigma'^2}}\,\chi_a\\ &\qquad - \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\,\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}_1-\mathbf{L}_2)}\,\mathrm{e}^{-\frac{(\mathbf{r}_1-\mathbf{L}_2)^2}{4\sigma'^2}}\,\chi_b\Big]. \end{aligned} \tag{3.243}$$

By using (3.243), as applied to the first term on the right-hand side of (3.240) for the expectation value of kinetic energy, we obtain

$$\langle\Psi|\sum_{i=1}^{2}\frac{\mathbf{p}_i^2}{2m}|\Psi\rangle = \langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle + \langle\Psi|\frac{\mathbf{p}_2^2}{2m}|\Psi\rangle \tag{3.244}$$

where

$$\langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle = \langle\Psi|\,T_1\,|\Psi\rangle = \frac{\hbar^2}{2m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\left[\nabla_1\Psi^*\right]\cdot\left[\nabla_1\Psi\right] \tag{3.245}$$

and

$$\langle\Psi|\,\frac{\mathbf{p}_2^2}{2m}\,|\Psi\rangle = \langle\Psi|\,T_2\,|\Psi\rangle = \frac{\hbar^2}{2m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\left[\nabla_2\Psi^*\right]\cdot\left[\nabla_2\Psi\right]. \tag{3.246}$$

Apply ∇ into (3.238), to obtain

$$\nabla_1\Psi(\mathbf{r}) = \frac{1}{\sqrt{2}}\left\{\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right] - \nabla_1\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]\right\} \tag{3.247}$$

and

$$\nabla_1\Psi^*(\mathbf{r}) = \frac{1}{\sqrt{2}}\left\{\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]^* - \nabla_1\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\right\}. \tag{3.248}$$

Substitute (3.247) and (3.248) into the right-hand side of (3.245), to obtain

$$\begin{aligned}\nabla_1\Psi^*(\mathbf{r})\cdot\nabla_1\Psi^*(\mathbf{r}) =& \frac{1}{2}\left\{\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\cdot\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]\right\}\\ &+\frac{1}{2}\left\{\nabla_1\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\cdot\nabla_1\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]\right\}\\ &-\frac{1}{2}\left\{\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\cdot\nabla_1\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]\right\}\\ &-\frac{1}{2}\left\{\nabla_1\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\cdot\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]\right\}\end{aligned} \tag{3.249}$$

and hence

$$\begin{aligned}\nabla_2\Psi^*(\mathbf{r})\cdot\nabla_2\Psi^*(\mathbf{r}) =& \frac{1}{2}\left\{\nabla_2\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\cdot\nabla_2\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]\right\}\\ &+\frac{1}{2}\left\{\nabla_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\cdot\nabla_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]\right\}\\ &-\frac{1}{2}\left\{\nabla_2\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\cdot\nabla_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]\right\}\end{aligned}$$

$$- \frac{1}{2} \left\{ \nabla_2 \left[\psi_1(\mathbf{r}_2, \sigma_2) \, \phi_2(\mathbf{r}_1, \sigma_1) \right]^* \cdot \nabla_2 \left[\psi_1(\mathbf{r}_1, \sigma_1) \, \phi_2(\mathbf{r}_2, \sigma_2) \right] \right\} . \tag{3.250}$$

Substitute (3.249) and (3.250) into (3.245), to obtain

$$\begin{aligned}
&\langle \Psi | \, \frac{\mathbf{p}_1^2}{2m} \, | \Psi \rangle \\
&\quad = \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \, \nabla_1 \left[\psi_1(\mathbf{r}_1, \sigma_1) \, \phi_2(\mathbf{r}_2, \sigma_2) \right]^* \cdot \nabla_1 \left[\psi_1(\mathbf{r}_1, \sigma_1) \, \phi_2(\mathbf{r}_2, \sigma_2) \right] \\
&\qquad + \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \, \nabla_1 \left[\psi_1(\mathbf{r}_2, \sigma_2) \, \phi_2(\mathbf{r}_1, \sigma_1) \right]^* \cdot \nabla_1 \left[\psi_1(\mathbf{r}_2, \sigma_2) \, \phi_2(\mathbf{r}_1, \sigma_1) \right] \\
&\qquad - \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \, \nabla_1 \left[\psi_1(\mathbf{r}_1, \sigma_1) \, \phi_2(\mathbf{r}_2, \sigma_2) \right]^* \cdot \nabla_1 \left[\psi_1(\mathbf{r}_2, \sigma_2) \, \phi_2(\mathbf{r}_1, \sigma_1) \right] \\
&\qquad - \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \, \nabla_1 \left[\psi_1(\mathbf{r}_2, \sigma_2) \, \phi_2(\mathbf{r}_1, \sigma_1) \right]^* \cdot \nabla_1 \left[\psi_1(\mathbf{r}_1, \sigma_1) \, \phi_2(\mathbf{r}_2, \sigma_2) \right]
\end{aligned} \tag{3.251}$$

and hence

$$\begin{aligned}
&\langle \Psi | \, \frac{\mathbf{p}_2^2}{2m} \, | \Psi \rangle \\
&\quad = \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \, \nabla_2 \left[\psi_1(\mathbf{r}_1, \sigma_1) \, \phi_2(\mathbf{r}_2, \sigma_2) \right]^* \cdot \nabla_2 \left[\psi_1(\mathbf{r}_1, \sigma_1) \, \phi_2(\mathbf{r}_2, \sigma_2) \right] \\
&\qquad + \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \, \nabla_2 \left[\psi_1(\mathbf{r}_2, \sigma_2) \, \phi_2(\mathbf{r}_1, \sigma_1) \right]^* \cdot \nabla_2 \left[\psi_1(\mathbf{r}_2, \sigma_2) \, \phi_2(\mathbf{r}_1, \sigma_1) \right] \\
&\qquad - \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \, \nabla_2 \left[\psi_1(\mathbf{r}_1, \sigma_1) \, \phi_2(\mathbf{r}_2, \sigma_2) \right]^* \cdot \nabla_2 \left[\psi_1(\mathbf{r}_2, \sigma_2) \, \phi_2(\mathbf{r}_1, \sigma_1) \right] \\
&\qquad - \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \mathrm{d}^3\mathbf{r}_2 \, \nabla_2 \left[\psi_1(\mathbf{r}_2, \sigma_2) \, \phi_2(\mathbf{r}_1, \sigma_1) \right]^* \cdot \nabla_2 \left[\psi_1(\mathbf{r}_1, \sigma_1) \, \phi_2(\mathbf{r}_2, \sigma_2) \right]
\end{aligned} \tag{3.252}$$

With the wavefunction normalization condition, the first term on the right-hand side of (3.251) can be rewritten as

$$\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\cdot\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\right]^*\cdot\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\right]$$

$$\times\qquad\int \mathrm{d}^3\mathbf{r}_2\,\left[\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\left[\phi_2(\mathbf{r}_2,\sigma_2)\right]$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\right]^*\cdot\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\right]\int \mathrm{d}^3\mathbf{r}_2\,\left|\phi_2(\mathbf{r}_2,\sigma_2)\right|^2$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\right]^*\cdot\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\right]. \qquad (3.253)$$

The second term on the right-hand side of (3.251) can be rewritten as

$$\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\nabla_1\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\cdot\nabla_1\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\;\nabla_1\left[\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\cdot\nabla_1\left[\phi_2(\mathbf{r}_1,\sigma_1)\right]$$

$$\times\int \mathrm{d}^3\mathbf{r}_2\;\left[\psi_1(\mathbf{r}_2,\sigma_2)\right]^*\;\left[\psi_1(\mathbf{r}_2,\sigma_2)\right]$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\;\nabla_1\left[\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\cdot\nabla_1\left[\phi_2(\mathbf{r}_1,\sigma_1)\right]\int \mathrm{d}^3\mathbf{r}_2\;\left|\psi_1(\mathbf{r}_2,\sigma_2)\right|^2$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\;\nabla_1\left[\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\cdot\nabla_1\left[\phi_2(\mathbf{r}_1,\sigma_1)\right]. \qquad (3.254)$$

The third term on the right-hand side of (3.251) and (3.252) can be rewritten as

$$\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\cdot\nabla_1\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\right]^*\cdot\nabla_1\left[\phi_2(\mathbf{r}_1,\sigma_1)\right]$$

$$\times \int \mathrm{d}^3\mathbf{r}_2 \; [\phi_2(\mathbf{r}_2,\sigma_2)]^* \; [\psi_1(\mathbf{r}_2,\sigma_2)] \tag{3.255}$$

and the fourth term on the right-hand side of (3.251) can be rewritten as

$$\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\nabla_1\,[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)]^*\cdot\nabla_1\,[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)]$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\nabla_1\,[\phi_2(\mathbf{r}_1,\sigma_1)]^*\cdot\nabla_1\,[\psi_1(\mathbf{r}_1,\sigma_1)\,]$$

$$\times \int \mathrm{d}^3\mathbf{r}_2\,[\psi_1(\mathbf{r}_2,\sigma_2)]^* \; [\phi_2(\mathbf{r}_2,\sigma_2)]\,. \tag{3.256}$$

In the same way, by referring to (3.253)–(3.256), the first term on the right-hand side of (3.252) can be rewritten as

$$\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\nabla_2\,[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)]^*\cdot\nabla_2\,[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)]$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_2\,\nabla_2\,[\,\phi_2(\mathbf{r}_2,\sigma_2)]^*\cdot\nabla_2\,[\phi_2(\mathbf{r}_2,\sigma_2)]$$

$$\times \int \mathrm{d}^3\mathbf{r}_1 \; [\psi_1(\mathbf{r}_1,\sigma_1)]^* \; [\psi_1(\mathbf{r}_1,\sigma_1)]$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_2\,\nabla_2\,[\,\phi_2(\mathbf{r}_2,\sigma_2)]^*\cdot\nabla_2\,[\phi_2(\mathbf{r}_2,\sigma_2)]\int \mathrm{d}^3\mathbf{r}_1\;|\psi_1(\mathbf{r}_1,\sigma_1)|^2$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_2\,\nabla_2\,[\,\phi_2(\mathbf{r}_2,\sigma_2)]^*\cdot\nabla_2\,[\phi_2(\mathbf{r}_2,\sigma_2)]\,. \tag{3.257}$$

The second term on the right-hand side of (3.252) can be rewritten as

$$\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\nabla_2\,[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)]^*\cdot\nabla_2\,[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)]$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_2\,\nabla_2\,[\psi_1(\mathbf{r}_2,\sigma_2)]^*\cdot\nabla_2\,[\psi_1(\mathbf{r}_2,\sigma_2)]$$

$$\int \mathrm{d}^3\mathbf{r}_1 \; [\phi_2(\mathbf{r}_1,\sigma_1)]^* \; [\phi_2(\mathbf{r}_1,\sigma_1)]$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_2\,\nabla_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\right]^*\cdot\nabla_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\right]\int \mathrm{d}^3\mathbf{r}_1\ \left|\phi_2(\mathbf{r}_1,\sigma_1)\right|^2$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_2\,\nabla_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\right]^*\cdot\nabla_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\right]. \tag{3.258}$$

The third term on the right-hand side of (3.252) can be rewritten as

$$\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\nabla_2\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\cdot\nabla_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]$$

$$=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_2\,\nabla_2\left[\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\cdot\nabla_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\right]$$

$$\times\int \mathrm{d}^3\mathbf{r}_1\ \left[\psi_1(\mathbf{r}_1,\sigma_1)\right]^*\ \left[\phi_2(\mathbf{r}_1,\sigma_1)\right]. \tag{3.259}$$

The fourth term on the right-hand side of (3.252) can be rewritten as

$$\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\nabla_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\cdot\nabla_2\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]$$

$$=\frac{\hbar^2}{4m}\mathrm{d}^3\mathbf{r}_2\,\nabla_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\right]^*\cdot\nabla_2\left[\phi_2(\mathbf{r}_2,\sigma_2)\right]$$

$$\times\int \mathrm{d}^3\mathbf{r}_1\ \left[\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\ \left[\psi_1(\mathbf{r}_1,\sigma_1)\right]. \tag{3.260}$$

By referring to (3.253)–(3.260), we can rewrite (3.251) and (3.252) as

$$\langle\Psi|\,\frac{\mathbf{p}_1^2}{2m}\,|\Psi\rangle=\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\right]^*\cdot\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\right]$$

$$+\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\ \nabla_1\left[\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\cdot\nabla_1\left[\phi_2(\mathbf{r}_1,\sigma_1)\right]$$

$$-\frac{\hbar^2}{4m}\int \mathrm{d}^3\mathbf{r}_1\,\nabla_1\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\right]^*\cdot\nabla_1\left[\phi_2(\mathbf{r}_1,\sigma_1)\right]$$

$$\times\int \mathrm{d}^3\mathbf{r}_2\ \left[\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\ \left[\psi_1(\mathbf{r}_2,\sigma_2)\right]$$

$$- \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \nabla_1 \left[\phi_2(\mathbf{r}_1, \sigma_1)\right]^* \cdot \nabla_1 \left[\psi_1(\mathbf{r}_1, \sigma_1)\right]$$

$$\times \int \mathrm{d}^3\mathbf{r}_2 \left[\psi_1(\mathbf{r}_2, \sigma_2)\right]^* \left[\phi_2(\mathbf{r}_2, \sigma_2)\right] \tag{3.261}$$

and

$$\begin{aligned}
\langle\Psi| \frac{\mathbf{p}_2^2}{2m} |\Psi\rangle = & \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_2 \, \nabla_2 \left[\phi_2(\mathbf{r}_2, \sigma_2)\right]^* \cdot \nabla_2 \left[\phi_2(\mathbf{r}_2, \sigma_2)\right] \\
& + \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_2 \, \nabla_2 \left[\psi_1(\mathbf{r}_2, \sigma_2)\right]^* \cdot \nabla_2 \left[\psi_1(\mathbf{r}_2, \sigma_2)\right] \\
& - \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_2 \, \nabla_2 \left[\phi_2(\mathbf{r}_2, \sigma_2)\right]^* \cdot \nabla_2 \left[\psi_1(\mathbf{r}_2, \sigma_2)\right] \\
& \times \int \mathrm{d}^3\mathbf{r}_1 \, \left[\psi_1(\mathbf{r}_1, \sigma_1)\right]^* \left[\phi_2(\mathbf{r}_1, \sigma_1)\right] \\
& - \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_2 \, \nabla_2 \left[\psi_1(\mathbf{r}_2, \sigma_2)\right]^* \cdot \nabla_2 \left[\phi_2(\mathbf{r}_2, \sigma_2)\right] \\
& \times \int \mathrm{d}^3\mathbf{r}_1 \, \left[\phi_2(\mathbf{r}_1, \sigma_1)\right]^* \left[\psi_1(\mathbf{r}_1, \sigma_1)\right].
\end{aligned} \tag{3.262}$$

We introduce the following functions

$$\phi\left(\mathbf{r}-\mathbf{L}\right) = A \, \exp \mathrm{i}\, \mathbf{k'} \cdot \left(\mathbf{r}-\mathbf{L}\right) \, \exp - \frac{\left(\mathbf{r}-\mathbf{L}\right)^2}{4\sigma'^2}, \tag{3.263a}$$

$$\phi^*\left(\mathbf{r}-\mathbf{L}\right) = A \, \exp -\mathrm{i}\, \mathbf{k'} \cdot \left(\mathbf{r}-\mathbf{L}\right) \, \exp - \frac{\left(\mathbf{r}-\mathbf{L}\right)^2}{4\sigma'^2}, \tag{3.263b}$$

$$\phi\left(\mathbf{r}-\mathbf{L}'\right) = A \, \exp \mathrm{i}\, \mathbf{k'} \cdot \left(\mathbf{r}-\mathbf{L}'\right) \, \exp - \frac{\left(\mathbf{r}-\mathbf{L}'\right)^2}{4\sigma'^2}, \tag{3.263c}$$

$$\phi^*\left(\mathbf{r}-\mathbf{L}'\right) = A \, \exp -\mathrm{i}\, \mathbf{k'} \cdot \left(\mathbf{r}-\mathbf{L}'\right) \, \exp - \frac{\left(\mathbf{r}-\mathbf{L}'\right)^2}{4\sigma'^2}. \tag{3.263d}$$

Apply ∇ to (3.263a), to obtain

$$\nabla\phi\left(\mathbf{r}-\mathbf{L}\right)=\nabla\left[A\ \exp\mathrm{i}\,\mathbf{k'}\cdot\left(\mathbf{r}-\mathbf{L}\right)\ \exp-\frac{\left(\mathbf{r}-\mathbf{L}\right)^{2}}{4\sigma'^{2}}\right]$$

$$=\left[\mathrm{i}\mathbf{k}'-\left(\frac{\mathbf{r}-\mathbf{L}}{2\sigma'^{2}}\right)\right]\phi\left(\mathbf{r}-\mathbf{L}\right) \tag{3.264}$$

and apply ∇ to (3.263d), we obtain

$$\nabla\phi\left(\mathbf{r}-\mathbf{L}'\right)^{*}=\nabla\left[A\ \exp-\mathrm{i}\,\mathbf{k}'\cdot\left(\mathbf{r}-\mathbf{L}'\right)\ \exp-\frac{\left(\mathbf{r}-\mathbf{L}\right)^{2}}{4\sigma'^{2}}\right]^{*}$$

$$=\left[-\mathrm{i}\mathbf{k}'-\left(\frac{\mathbf{r}-\mathbf{L}'}{2\sigma'^{2}}\right)\right]\phi^{*}\left(\mathbf{r}-\mathbf{L}'\right). \tag{3.265}$$

For $\mathbf{L}\neq\mathbf{L}'$, we obtain

$$\left|\int \mathrm{d}^{3}\mathbf{r}\,\nabla\phi\left(\mathbf{r}-\mathbf{L}'\right)^{*}\cdot\nabla\phi\left(\mathbf{r}-\mathbf{L}\right)\right|$$

$$=\left|\int \mathrm{d}^{3}\mathbf{r}\ \left[-\mathrm{i}\mathbf{k}'-\left(\frac{\mathbf{r}-\mathbf{L}'}{2\sigma'^{2}}\right)\right]\phi^{*}\left(\mathbf{r}-\mathbf{L}'\right)\cdot\left[\mathrm{i}\mathbf{k}'-\left(\frac{\mathbf{r}-\mathbf{L}}{2\sigma'^{2}}\right)\right]\phi\left(\mathbf{r}-\mathbf{L}\right)\right|$$

$$=\left|\int \mathrm{d}^{3}\mathbf{r}\ \left[-\mathrm{i}\mathbf{k}'-\left(\frac{\mathbf{r}-\mathbf{L}}{2\sigma'^{2}}\right)\right]\left[\mathrm{i}\mathbf{k}'-\left(\frac{\mathbf{r}-\mathbf{L}}{2\sigma'^{2}}\right)\right]\phi^{*}\left(\mathbf{r}-\mathbf{L}'\right)\phi\left(\mathbf{r}-\mathbf{L}\right)\right|$$

$$=\left|\int\left[\mathbf{k}'\cdot\mathbf{k}'+\frac{\mathrm{i}\mathbf{k}'\cdot\left(\mathbf{r}-\mathbf{L}\right)}{2\sigma'^{2}}-\frac{\mathrm{i}\mathbf{k}'\cdot\left(\mathbf{r}-\mathbf{L}'\right)}{2\sigma'^{2}}+\frac{\left(\mathbf{r}-\mathbf{L}'\right)\cdot\left(\mathbf{r}-\mathbf{L}\right)}{4\sigma'^{4}}\right]\right.$$

$$\left.\times\ \phi^{*}\left(\mathbf{r}-\mathbf{L}'\right)\phi\left(\mathbf{r}-\mathbf{L}\right)\ \mathrm{d}^{3}\mathbf{r}\right|. \tag{3.266}$$

Let $\mathbf{R}-\mathbf{r}-\mathbf{L}$, $\mathbf{L}_{0}=\mathbf{L}'-\mathbf{L}$ and $\mathbf{L}_{0}'=\mathbf{L}-\mathbf{L}'$. Substitute the latter into the right-hand side of (3.266), to obtain

$$\left|\int \mathrm{d}^{3}\mathbf{r}\,\nabla\phi\left(\mathbf{r}-\mathbf{L}'\right)^{*}\cdot\nabla\phi\left(\mathbf{r}-\mathbf{L}\right)\right|$$

$$\leqslant \int \left| \left[\mathbf{k}' \cdot \mathbf{k}' + \frac{\mathrm{i}\mathbf{k}' \cdot (\mathbf{r} - \mathbf{L})}{2\sigma'^2} - \frac{\mathrm{i}\mathbf{k}' \cdot (\mathbf{r} - \mathbf{L}')}{2\sigma'^2} + \frac{(\mathbf{r} - \mathbf{L}') \cdot (\mathbf{r} - \mathbf{L})}{4\sigma'^4} \right] \right.$$

$$\left. \times\ \phi^* (\mathbf{r} - \mathbf{L}')\, \phi (\mathbf{r} - \mathbf{L}) \right| \mathrm{d}^3\mathbf{r}$$

$$= \int \left| \left[\mathbf{k}' \cdot \mathbf{k}' + \frac{\mathrm{i}\mathbf{k}' \cdot \mathbf{R}}{2\sigma'^2} - \frac{\mathrm{i}\mathbf{k}' \cdot (\mathbf{R} - \mathbf{L}_0)}{2\sigma'^2} + \frac{(\mathbf{R} - \mathbf{L}_0) \cdot \mathbf{R}}{4\sigma'^4} \right] \right.$$

$$\left. \times\ \phi^* (\mathbf{R} - \mathbf{L}_0)\, \phi (\mathbf{R}) \right| \mathrm{d}^3\mathbf{R}$$

$$= \int \left| \left[\mathbf{k}' \cdot \mathbf{k}' + \frac{\mathrm{i}\mathbf{k}' \cdot \mathbf{R}}{2\sigma'^2} - \frac{\mathrm{i}\mathbf{k}' \cdot (\mathbf{R} - \mathbf{L}_0)}{2\sigma'^2} + \frac{(\mathbf{R} - \mathbf{L}_0) \cdot \mathbf{R}}{4\sigma'^4} \right] \right.$$

$$\times\ A \exp -\mathrm{i}\, \mathbf{k'} \cdot (\mathbf{R} - \mathbf{L}_0)\ \exp - \frac{(\mathbf{R} - \mathbf{L}_0)^2}{4\sigma'^2}$$

$$\left. \times\ A \exp \mathrm{i}\, \mathbf{k'} \cdot (\mathbf{R})\ \exp - \frac{(\mathbf{R})^2}{4\sigma'^2} \right| \mathrm{d}^3\mathbf{R}$$

$$\leqslant \int \left| \left[\mathbf{k}' \cdot \mathbf{k}' + \frac{\mathrm{i}\mathbf{k}' \cdot \mathbf{R}}{2\sigma'^2} - \frac{\mathrm{i}\mathbf{k}' \cdot (\mathbf{R} + \mathbf{L}_0)}{2\sigma'^2} + \frac{(\mathbf{R} + \mathbf{L}_0) \cdot \mathbf{R}}{4\sigma'^4} \right] \right.$$

$$\times\ A \exp -\mathrm{i}\, \mathbf{k'} \cdot (\mathbf{R} + \mathbf{L}'_0)\ \exp - \frac{(\mathbf{R} - \mathbf{L}_0)^2}{4\sigma'^2}$$

$$\left. \times\ A \exp \mathrm{i}\, \mathbf{k'} \cdot (\mathbf{R})\ \exp - \frac{(\mathbf{R})^2}{4\sigma'^2} \right| \mathrm{d}^3\mathbf{R}$$

$$\leqslant \int \left| \left[k'k' + \frac{\mathrm{i}\mathbf{k}' \cdot \mathbf{R}}{2\sigma'^2} - \frac{\mathrm{i}\mathbf{k}' \cdot (\mathbf{R} + \mathbf{L}_0)}{2\sigma'^2} + \frac{(\mathbf{R} + \mathbf{L}_0) \cdot \mathbf{R}}{4\sigma'^4} \right] \right.$$

$$\left. \times\ A^2\, \mathrm{e}^{-\mathrm{i}\, \mathbf{k'} \cdot \mathbf{L}'_0}\, \mathrm{e}^{-\frac{(\mathbf{R} - \mathbf{L}_0)^2}{4\sigma'^2}}\, \mathrm{e}^{-\frac{(\mathbf{R})^2}{4\sigma'^2}} \right| \mathrm{d}^3\mathbf{R}$$

$$\leqslant \int \left(k'k' + \frac{k'R}{2\sigma'^2} + \frac{k'(R + L_0)}{2\sigma'^2} + \frac{(R + L_0)R}{4\sigma'^4} \right)$$

$$\times \left| A^2\, \mathrm{e}^{-\mathrm{i}\, \mathbf{k'} \cdot \mathbf{L}'_0}\, \mathrm{e}^{-\frac{(\mathbf{R} - \mathbf{L}_0)^2}{4\sigma'^2}}\, \mathrm{e}^{-\frac{(\mathbf{R})^2}{4\sigma'^2}} \right| \mathrm{d}^3\mathbf{R}. \tag{3.267}$$

By using

$$\left| \mathrm{e}^{-\mathrm{i}\,\mathbf{k'}\cdot\mathbf{L}'_0} \right| \leqslant 1, \tag{3.268a}$$

$$\mathrm{e}^{-(\mathbf{R}-\mathbf{L}_0)^2} \leqslant \mathrm{e}^{-|\mathbf{R}-\mathbf{L}_0|^2} \leqslant \mathrm{e}^{-(R-L_0)^2}, \tag{3.268b}$$

$$\left| \mathrm{e}^{-\mathrm{i}\,\mathbf{k'}\cdot\mathbf{L}'_0}\, \mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}}\, \mathrm{e}^{-\frac{|\mathbf{R}|^2}{4\sigma'^2}} \right| \leqslant \mathrm{e}^{-\frac{(R-L_0)^2}{4\sigma'^2}}\, \mathrm{e}^{-\frac{R^2}{4\sigma'^2}}, \tag{3.268c}$$

as applied to the right-hand side of (3.267), to obtain

$$\begin{aligned}
&\left| \int \mathrm{d}^3\mathbf{r}\, \nabla\phi\left(\mathbf{r}-\mathbf{L}'\right)^* \cdot \nabla\phi\left(\mathbf{r}-\mathbf{L}\right) \right| \\
&\leqslant A^2 \int \mathrm{d}^3\mathbf{R}\, \left(k'^2 + \frac{k' R}{2\sigma'^2} + \frac{k'\left(R+L_0\right)}{2\sigma'^2} + \frac{(R+L_0)R}{4\sigma'^4} \right) \mathrm{e}^{-\frac{(R-L_0)^2}{4\sigma'^2}}\, \mathrm{e}^{-\frac{R^2}{4\sigma'^2}} \\
&\leqslant A^2 \int \mathrm{d}^3\mathbf{R} \left(k'^2 + \frac{k' R}{2\sigma'^2} + \frac{k'\left(R+L_0\right)}{2\sigma'^2} + \frac{(R+L_0)R}{4\sigma'^4} \right) \mathrm{e}^{-\frac{R(R-L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\
&= 4\pi A^2 \int_0^\infty \mathrm{d}R\, R^2 \left(k'^2 + \frac{k' R}{2\sigma'^2} + \frac{k'\left(R+L_0\right)}{2\sigma'^2} + \frac{(R+L_0)R}{4\sigma'^4} \right) \mathrm{e}^{-\frac{R(R-L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\
&\leqslant 4\pi A^2 \int_0^{L_0} \mathrm{d}R\, R^2 \left(k'^2 + \frac{k' L_0}{2\sigma'^2} + \frac{k'\left(L_0+L_0\right)}{2\sigma'^2} + \frac{(L_0+L_0)L_0}{4\sigma'^4} \right) \mathrm{e}^{\frac{R(L_0-R)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\
&\quad + 4\pi A^2 \int_{L_0}^\infty \mathrm{d}R\, R^2 \left(k'^2 + \frac{k' R}{2\sigma'^2} + \frac{k'\left(R+R\right)}{2\sigma'^2} + \frac{(R+R)R}{4\sigma'^4} \right) \mathrm{e}^{-\frac{R(R-L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}.
\end{aligned} \tag{3.269}$$

Consider the right-hand side of inequality (3.269), optimizing over by R, to obtain

$$\frac{\partial}{\partial R}\, R(L_0 - R) = L_0 - 2R = 0 \to R = \frac{L_0}{2} \tag{3.270}$$

and

$$\frac{\partial^2}{\partial R^2}\, R(L_0 - R) = -2. \tag{3.271}$$

By using (3.270) and (3.270) we obtain

$$\exp \frac{R\,(L_0 - R)}{2\sigma'^2} \quad \leqslant \exp \frac{L_0^2}{8\sigma'^2}. \tag{3.272}$$

Substitute (3.272) into the first term on the right-hand side of (3.269), to get

$$4\pi A^2 \int_0^{L_0} \mathrm{d}R\, R^2 \left(k'k' + \frac{k' L_0}{2\sigma'^2} + \frac{k'\,(L_0 + L_0)}{2\sigma'^2} + \frac{(L_0 + L_0)L_0}{4\sigma'^4} \right) \mathrm{e}^{\frac{R(L_0 - R)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$\leqslant 4\pi \int_0^{L_0} \mathrm{d}R\, R^2 \left(k'k' + \frac{3k' L_0}{2\sigma'^2} + \frac{L_0^2}{2\sigma'^4} \right) A^2 \mathrm{e}^{\frac{L_0^2}{8\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$= \frac{4\pi A^2 L_0^3}{3} \left(k'k' + \frac{3k' L_0}{2\sigma'^2} + \frac{L_0^2}{2\sigma'^4} \right) \exp - \frac{L_0^2}{8\sigma'^2}. \tag{3.273}$$

For the second term on the right hand side of inequality (3.269), let $X = R - L_0$, to obtain

$$4\pi A^2 \int_0^{\infty} \mathrm{d}R\, R^2 \left(k'k' + \frac{k' R}{2\sigma'^2} + \frac{k'\,(R + R)}{2\sigma'^2} + \frac{(R + R)R}{4\sigma'^4} \right) \mathrm{e}^{-\frac{R(R - L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$= 4\pi A^2 \int_{L_0}^{\infty} \mathrm{d}X\, (X + L_0)^2 \left(k'k' + \frac{3k'(X + L_0)}{2\sigma'^2} + \frac{(X + L_0)^2}{2\sigma'^4} \right)$$

$$\times\; \mathrm{e}^{-\frac{X(X + L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}. \tag{3.274}$$

by noting

$$\exp - \frac{L_0 X}{2\sigma'^2} \leqslant 1 \tag{3.275}$$

as applied to the right-hand side of inequality (3.269), to obtain

$$4\pi A^2 \int_{L_0}^{\infty} \mathrm{d}R\, R^2 \left(k'k' + \frac{k'R}{2\sigma'^2} + \frac{k'\,(R+R)}{2\sigma'^2} + \frac{(R+R)R}{4\sigma'^4}\right) \mathrm{e}^{-\frac{R(R-L_0)}{2\sigma'^2}}\,\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$\leqslant 4\pi A^2 \int_{L_0}^{\infty} \mathrm{d}X\,(X+L_0)^2 \left(k'k' + \frac{3k'(X+L_0)}{2\sigma'^2} + \frac{(X+L_0)^2}{2\sigma'^4}\right) \mathrm{e}^{-\frac{X^2}{2\sigma'^2}}\,\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$\leqslant 4\pi A^2 \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \int_{L_0}^{\infty} \mathrm{d}X\,(X+L_0)^2 \left(k'k' + \frac{3k'(X+L_0)}{2\sigma'^2} + \frac{(X+L_0)^2}{2\sigma'^4}\right) \mathrm{e}^{-\frac{X^2}{2\sigma'^2}}$$

$$\leqslant 4\pi A^2 \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \int_{0}^{\infty} \mathrm{d}X\, \left(k'k'(X+L_0)^2 + \frac{3k'(X+L_0)^3}{2\sigma'^2} + \frac{(X+L_0)^4}{2\sigma'^4}\right) \mathrm{e}^{-\frac{X^2}{2\sigma'^2}}$$

$$\leqslant 4\pi A^2\,|\mathrm{Polym}(L_0)|\,\exp -\frac{L_0^2}{8\sigma'^2}. \tag{3.276}$$

Substitute (3.273) and (3.276) into the right-hand side of inequality (3.269), to obtain the bound

$$\left|\int \mathrm{d}^3\mathbf{r}\,\nabla\phi\,(\mathbf{r}-\mathbf{L}')^* \cdot \nabla\phi\,(\mathbf{r}-\mathbf{L})\right|$$

$$\leqslant \frac{4\pi A^2 L_0^3}{3}\left(k'k' + \frac{3k'L_0}{2\sigma'^2} + \frac{L_0^2}{2\sigma'^4}\right)\exp -\frac{L_0^2}{8\sigma'^2} + 4\pi A^2\,|\mathrm{Polym}(L_0)|\,\exp -\frac{L_0^2}{8\sigma'^2}$$

$$= \exp -\frac{L_0^2}{8\sigma'^2}\left[\frac{4\pi A^2 L_0^3}{3}\left(k'k' + \frac{3k'L_0}{2\sigma'^2} + \frac{L_0^2}{2\sigma'^4}\right) + 4\pi A^2\,|\mathrm{Polym}(L_0)|\right] \tag{3.277}$$

which vanishes very rapidly for $L_0 \to \infty$.

Refer to (3.277), for $L_0 \to \infty$, when $\mathbf{L'} \neq \mathbf{L}$ to write as a limit

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\,\nabla\phi^*\,(\mathbf{r}-\mathbf{L}')\cdot\nabla\phi\,(\mathbf{r}-\mathbf{L})\right] = 0. \tag{3.278}$$

and for $\mathbf{L'} = \mathbf{L}, \to L_0 = 0$, Eq.(3.277) becomes the expectation value for free particle, with small kinetic energy we set $k' \to 0$, then Eq.(3.277) can be rewritten as a limit

$$\lim_{L_0,k'\to 0}\left[\int \mathrm{d}^3\mathbf{r}\,\nabla\phi^*\,(\mathbf{r}-\mathbf{L})\cdot\nabla\phi\,(\mathbf{r}-\mathbf{L})\right] = 0. \tag{3.279}$$

In the same way, we obtain a bound for the following integral

$$\int \mathrm{d}^3\mathbf{r}\, \nabla \left[\psi(\mathbf{r}-\mathbf{L})\right]^* \cdot \nabla \left[\phi(\mathbf{r}-\mathbf{L}')\right]. \tag{3.280}$$

From (3.102), let $\mathbf{R} = \mathbf{r} - \mathbf{L}$, we have

$$\begin{aligned} \nabla\psi^*(\mathbf{r}-\mathbf{L}) =& \nabla\psi^*(\mathbf{R}) \\ =& \nabla\, C\mathrm{e}^{-\beta|\mathbf{R}|} \\ =& -\beta\, C\mathrm{e}^{-\beta R}\, \hat{R} \end{aligned} \tag{3.281}$$

and from (3.264), we have

$$\begin{aligned} \nabla\phi\left(\mathbf{r}-\mathbf{L}'\right) =& \nabla\phi\left(\mathbf{R}+\mathbf{L}-\mathbf{L}'\right) \\ =& \nabla\left[A\, \exp \mathrm{i}\, \mathbf{k'}\cdot(\mathbf{R}+\mathbf{L}-\mathbf{L}')\, \exp - \frac{(\mathbf{R}+\mathbf{L}-\mathbf{L}')^2}{4\sigma'^2}\right] \\ =& \nabla\left[A\, \exp \mathrm{i}\, \mathbf{k'}\cdot(\mathbf{R}-\mathbf{L}_0)\, \exp - \frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}\right] \\ =& \left[\mathrm{i}\mathbf{k}' - \left(\frac{\mathbf{R}-\mathbf{L}_0}{2\sigma'^2}\right)\right]\phi\left(\mathbf{R}-\mathbf{L}_0\right) \qquad , \mathbf{L}_0 = \mathbf{L'} - \mathbf{L}. \end{aligned} \tag{3.282}$$

Substitute (3.281) and (3.282) into (3.280), to obtain

$$\begin{aligned} &\nabla\psi^*(\mathbf{r}-\mathbf{L})\cdot\nabla\phi\left(\mathbf{r}-\mathbf{L}'\right) \\ &= -\beta\, C\left[\hat{R}\cdot\mathrm{i}\mathbf{k}' - \frac{\hat{R}\cdot(\mathbf{R}-\mathbf{L}_0)}{2\sigma'^2}\right]\mathrm{e}^{-\beta R}\phi\left(\mathbf{R}-\mathbf{L}_0\right) \\ &= -\beta\, C\left[\hat{R}\cdot\mathrm{i}\mathbf{k}' - \frac{\mathbf{R}\cdot(\mathbf{R}-\mathbf{L}_0)}{2\sigma'^2|\mathbf{R}|}\right]\mathrm{e}^{-\beta R}\phi\left(\mathbf{R}-\mathbf{L}_0\right) \end{aligned}$$

$$= -\,\beta\, C \left[\hat{R}\cdot \mathrm{i}\mathbf{k}' - \frac{(R - L_0 \cos\theta)}{2\sigma'^2}\right] \mathrm{e}^{-\beta R} \phi\left(\mathbf{R} - \mathbf{L}_0\right). \tag{3.283}$$

By using (3.283), we obtain

$$\begin{aligned}
&\left|\int \mathrm{d}^3\mathbf{r} \nabla\psi^*(\mathbf{r} - \mathbf{L})\cdot\nabla\phi\left(\mathbf{r} - \mathbf{L}'\right)\right| \\
&\quad = \left|-\beta\, C \int \mathrm{d}^3\mathbf{R} \left[\hat{R}\cdot \mathrm{i}\mathbf{k}' - \frac{\hat{R}\cdot(\mathbf{R} - \mathbf{L}_0)}{2\sigma'^2}\right] \mathrm{e}^{-\beta R} \phi\left(\mathbf{R} - \mathbf{L}_0\right)\right| \\
&\quad = \left|-\beta\, C \int \mathrm{d}^3\mathbf{R} \left[\hat{R}\cdot \mathrm{i}\mathbf{k}' - \frac{(R - L_0 \cos\theta)}{2\sigma'^2}\right] \mathrm{e}^{-\beta R} \phi\left(\mathbf{R} - \mathbf{L}_0\right)\right| \\
&\quad = \left|-\beta\, C A \int \mathrm{d}^3\mathbf{R} \left[\hat{R}\cdot \mathrm{i}\mathbf{k}' - \frac{(R - L_0 \cos\theta)}{2\sigma'^2}\right] \mathrm{e}^{-\beta R}\, \mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{R} - \mathbf{L}_0)}\, \mathrm{e}^{-\frac{(\mathbf{R} - \mathbf{L}_0)^2}{4\sigma'^2}}\right|.
\end{aligned} \tag{3.284}$$

By using

$$\left|\mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{R} - \mathbf{L}_0)}\right| = 1 \tag{3.285}$$

and

$$\begin{aligned}
\mathrm{e}^{-(\mathbf{R} - \mathbf{L}_0)^2} &= \mathrm{e}^{-\left[R^2 + L_0^2 - 2RL_0 \cos\theta\right]} \\
&\leqslant \mathrm{e}^{-\left[R^2 + L_0^2 - 2RL_0\right]}
\end{aligned} \tag{3.286}$$

as applied to the right-hand side of (3.284), we obtain

$$\begin{aligned}
&\left|\int \mathrm{d}^3\mathbf{r}\, \nabla\psi^*(\mathbf{r} - \mathbf{L})\cdot\nabla\phi\left(\mathbf{r} - \mathbf{L}'\right)\right| \\
&\quad \leqslant \int \mathrm{d}^3\mathbf{R}\, \beta\, C A \left[k' + \frac{(R + L_0)}{2\sigma'^2}\right] \mathrm{e}^{-\beta R}\, \mathrm{e}^{-\frac{\left[R^2 + L_0^2 - 2RL_0\right]}{4\sigma'^2}}
\end{aligned}$$

$$= 4\pi\beta\, CA \int_0^\infty \mathrm{d}R\, R^2 \left[k' + \frac{(R+L_0)}{2\sigma'^2}\right] \mathrm{e}^{-\beta R}\, \mathrm{e}^{-\frac{\left[R^2+L_0^2-2RL_0\right]}{4\sigma'^2}}$$

$$= 4\pi\beta\, CA \int_0^\infty \mathrm{d}R\, R^2 \left[k' + \frac{(R+L_0)}{2\sigma'^2}\right] \mathrm{e}^{-\beta R}\, \mathrm{e}^{-\frac{R(R-L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\, CA \int_0^\infty \mathrm{d}R\, R^2 \left[k' + \frac{(R+L_0)}{2\sigma'^2}\right] \mathrm{e}^{-\frac{R(R-L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\, CA \int_0^{L_0} \mathrm{d}R\, L_0^2 \left[k' + \frac{(L_0+L_0)}{2\sigma'^2}\right] \mathrm{e}^{\frac{R(L_0-R)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$+ 4\pi\beta\, CA \int_{L_0}^\infty \mathrm{d}R\, R^2 \left[k' + \frac{(R+R)}{2\sigma'^2}\right] \mathrm{e}^{\frac{-R(R-L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}. \tag{3.287}$$

By using (3.270) and (3.272), the first term on the right-hand side of inequality (3.287), becomes

$$4\pi\beta\, CA \int_0^{L_0} \mathrm{d}R\, L_0^2 \left[k' + \frac{(L_0+L_0)}{2\sigma'^2}\right] \mathrm{e}^{\frac{R(L_0-R)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\, CA \int_0^{L_0} \mathrm{d}R\, L_0^2 \left[k' + \frac{L_0}{\sigma'^2}\right] \mathrm{e}^{\frac{L_0^2}{8\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$= 4\pi\beta\, CA\, L_0^3 \left[k' + \frac{L_0}{\sigma'^2}\right] \mathrm{e}^{-\frac{L_0^2}{8\sigma'^2}}. \tag{3.288}$$

Let $X = R - L_0$, and substitute the latter into the second term on the right-hand side of (3.287) to obtain

$$4\pi\beta\, CA \int_{L_0}^\infty \mathrm{d}R\, R^2 \left[k' + \frac{(R+R)}{2\sigma'^2}\right] \mathrm{e}^{\frac{-R(R-L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\, CA \int_0^\infty \mathrm{d}(X+L_0)\ (X+L_0)^2 \left[k' + \frac{X+L_0}{\sigma'^2}\right] \mathrm{e}^{\frac{-X(X+L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\, CA \int_0^\infty \mathrm{d}(X+L_0)\ (X+L_0)^2 \left[k' + \frac{X+L_0}{\sigma'^2}\right] \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$= 4\pi\beta\, CA \int_{L_0}^\infty \mathrm{d}u\ u^2 \left[k' + \frac{u}{\sigma'^2}\right] \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \quad , u = (X+L_0)$$

$$= 4\pi\beta\, CA\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \lim_{u\to\infty}\left[\frac{k'u^3}{3}+\frac{u^4}{4\sigma'^2}-\frac{k'L_0^3}{3}-\frac{L_0^4}{4\sigma'^2}\right]$$

$$\leqslant 4\pi\beta\, CA\mathrm{e}^{-\frac{L_0^2}{8\sigma'^2}} \lim_{u\to\infty}\left[\frac{k'u^3}{3}+\frac{u^4}{4\sigma'^2}-\frac{k'L_0^3}{3}-\frac{L_0^4}{4\sigma'^2}\right] \tag{3.289}$$

where

$$\mathrm{e}^{\frac{-X(X+L_0)}{2\sigma'^2}} \leqslant 1. \tag{3.290}$$

Substitute (3.288) and (3.289) into the right-hand side of inequality (3.285) to obtain

$$\left|\int \mathrm{d}^3\mathbf{r}\,\nabla\psi^*(\mathbf{r}-\mathbf{L})\cdot\nabla\phi\,(\mathbf{r}-\mathbf{L}')\right|$$

$$\leqslant 4\pi\beta\, CA\, L_0^3\left[k'+\frac{L_0}{\sigma'^2}\right]\mathrm{e}^{-\frac{L_0^2}{8\sigma'^2}}$$

$$+\,4\pi\beta\, CA\mathrm{e}^{-\frac{L_0^2}{8\sigma'^2}} \lim_{u\to\infty}\left[\frac{k'u^3}{3}+\frac{u^4}{4\sigma'^2}-\frac{k'L_0^3}{3}-\frac{L_0^4}{4\sigma'^2}\right] \tag{3.291}$$

which vanishes very rapidly for $L_0 \to \infty$.

Refer to (3.291), for $L_0 \to \infty$, to write as a limit

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\,\nabla\psi^*(\mathbf{r}-\mathbf{L})\cdot\nabla\phi\,(\mathbf{r}-\mathbf{L}')\right]=0. \tag{3.292}$$

In the same way, to obtain a bound for the following

$$\int \mathrm{d}^3\mathbf{r}\,\nabla\left[\phi(\mathbf{r}-\mathbf{L}')\right]^*\cdot\nabla\left[\psi(\mathbf{r}-\mathbf{L})\right]. \tag{3.293}$$

From (3.102), let $\mathbf{R}=\mathbf{r}-\mathbf{L}$, to obtain

$$\nabla\psi(\mathbf{r}-\mathbf{L}) = \nabla\psi(\mathbf{R})$$

$$= \nabla\, C\mathrm{e}^{-\beta|\mathbf{R}|}$$

$$= -\beta C e^{-\beta R} \hat{R} \tag{3.294}$$

and from (3.264), we have

$$\begin{aligned}
\nabla\phi^*(\mathbf{r}-\mathbf{L}') =& \nabla\phi^*(\mathbf{R}+\mathbf{L}-\mathbf{L}') \\
=& \nabla\left[A\,\exp -\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{R}+\mathbf{L}-\mathbf{L}')\,\exp -\frac{(\mathbf{R}+\mathbf{L}-\mathbf{L}')^2}{4\sigma'^2}\right] \\
=& \nabla\left[A\,\exp -\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{R}-\mathbf{L}_0)\,\exp -\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}\right] \\
=& \left[-\mathrm{i}\mathbf{k}' - \left(\frac{\mathbf{R}-\mathbf{L}_0}{2\sigma'^2}\right)\right]\phi(\mathbf{R}-\mathbf{L}_0)\,.
\end{aligned} \tag{3.295}$$

By using (3.294) and (3.295), we obtain

$$\begin{aligned}
&\nabla\phi^*(\mathbf{r}-\mathbf{L}')\cdot\nabla\psi(\mathbf{r}-\mathbf{L}) \\
&= -\beta C\left[-\hat{R}\cdot\mathrm{i}\mathbf{k}' - \frac{\hat{R}\cdot(\mathbf{R}-\mathbf{L}_0)}{2\sigma'^2}\right]\mathrm{e}^{-\beta R}\phi^*(\mathbf{R}-\mathbf{L}_0) \\
&= -\beta C\left[-\hat{R}\cdot\mathrm{i}\mathbf{k}' - \frac{\mathbf{R}\cdot(\mathbf{R}-\mathbf{L}_0)}{2\sigma'^2|\mathbf{R}|}\right]\mathrm{e}^{-\beta R}\phi^*(\mathbf{R}-\mathbf{L}_0) \\
&= -\beta C\left[-\hat{R}\cdot\mathrm{i}\mathbf{k}' - \frac{(R-L_0\cos\theta)}{2\sigma'^2}\right]\mathrm{e}^{-\beta R}\phi^*(\mathbf{R}-\mathbf{L}_0) \\
&= \beta C\left[\hat{R}\cdot\mathrm{i}\mathbf{k}' + \frac{(R-L_0\cos\theta)}{2\sigma'^2}\right]\mathrm{e}^{-\beta R}\phi^*(\mathbf{R}-\mathbf{L}_0)\,.
\end{aligned} \tag{3.296}$$

By using (3.296), we obtain

$$\begin{aligned}
&\left|\int \mathrm{d}^3\mathbf{r}\,\nabla\phi^*(\mathbf{r}-\mathbf{L}')\cdot\nabla\psi(\mathbf{r}-\mathbf{L})\right| \\
&= \left|\beta C\int \mathrm{d}^3\mathbf{R}\,\left[\hat{R}\cdot\mathrm{i}\mathbf{k}' + \frac{(R-L_0\cos\theta)}{2\sigma'^2}\right]\mathrm{e}^{-\beta R}\phi^*(\mathbf{R}-\mathbf{L}_0)\right|
\end{aligned}$$

$$= \left| \beta\, CA \int \mathrm{d}^3\mathbf{R}\ \left[\hat{R}\cdot \mathrm{i}\mathbf{k}' + \frac{(R - L_0\cos\theta)}{2\sigma'^2} \right] \mathrm{e}^{-\beta R}\, \mathrm{e}^{-\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{R}-\mathbf{L}_0)}\, \mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}} \right| . \tag{3.297}$$

By using (3.286) and

$$\left| \mathrm{e}^{-\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{R}-\mathbf{L}_0)} \right| = \left| \mathrm{e}^{-\mathrm{i}\,k' R\cos\theta + \mathrm{i}\,k' L_0 \cos\theta} \right| = 1, \tag{3.298a}$$

$$|\mathrm{i}k' \cos\theta| \leqslant |k'|, \tag{3.298b}$$

as applied to the right-hand side of (3.297), we obtain

$$\begin{aligned}
&\left| \int \mathrm{d}^3\mathbf{r}\, \nabla\phi^*(\mathbf{r}-\mathbf{L}')\cdot\nabla\psi(\mathbf{r}-\mathbf{L}) \right| \\
&\leqslant \beta\, CA \int \mathrm{d}^3\mathbf{R}\ \left[k' + \frac{(R+L_0)}{2\sigma'^2} \right] \mathrm{e}^{-\beta R}\, \mathrm{e}^{-\frac{\left[R^2 + L_0^2 - 2RL_0\right]}{4\sigma'^2}} \\
&= 4\pi\beta\, CA \int_0^\infty \mathrm{d}R\, R^2 \left[k' + \frac{(R+L_0)}{2\sigma'^2} \right] \mathrm{e}^{-\beta R}\, \mathrm{e}^{-\frac{\left[R^2 + L_0^2 - 2RL_0\right]}{4\sigma'^2}} \\
&= 4\pi\beta\, CA \int_0^\infty \mathrm{d}R\, R^2 \left[k' + \frac{(R+L_0)}{2\sigma'^2} \right] \mathrm{e}^{-\beta R}\, \mathrm{e}^{-\frac{R(R-L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\
&\leqslant 4\pi\beta\, CA \int_0^\infty \mathrm{d}R\, R^2 \left[k' + \frac{(R+L_0)}{2\sigma'^2} \right] \mathrm{e}^{-\frac{R(R-L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\
&\leqslant 4\pi\beta\, CA \int_0^{L_0} \mathrm{d}R\, L_0^2 \left[k' + \frac{(L_0+L_0)}{2\sigma'^2} \right] \mathrm{e}^{\frac{R(L_0-R)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\
&\quad + 4\pi\beta\, CA \int_{L_0}^\infty \mathrm{d}R\, R^2 \left[k' + \frac{(R+R)}{2\sigma'^2} \right] \mathrm{e}^{\frac{-R(R-L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} .
\end{aligned} \tag{3.299}$$

By using (3.270) and (3.272), the first term on the right-hand side of inequality (3.299) becomes

$$4\pi\beta\, CA \int_0^{L_0} \mathrm{d}R\, L_0^2 \left[k' + \frac{(L_0+L_0)}{2\sigma'^2} \right] \mathrm{e}^{\frac{R(L_0-R)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\, C A \int_0^{L_0} \mathrm{d}R\, L_0^2 \left[k' + \frac{L_0}{\sigma'^2}\right] \mathrm{e}^{\frac{L_0^2}{8\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$= 4\pi\beta\, C A\, L_0^3 \left[k' + \frac{L_0}{\sigma'^2}\right] \mathrm{e}^{-\frac{L_0^2}{8\sigma'^2}}. \tag{3.300}$$

Let $X = R - L_0$, then substitute into the second term on the right-hand side of (3.299) to get

$$4\pi\beta\, C A \int_{L_0}^{\infty} \mathrm{d}R\, R^2 \left[k' + \frac{(R+R)}{2\sigma'^2}\right] \mathrm{e}^{\frac{-R(R-L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\, C A \int_0^{\infty} \mathrm{d}(X+L_0)\ (X+L_0)^2 \left[k' + \frac{X+L_0}{\sigma'^2}\right] \mathrm{e}^{\frac{-X(X+L_0)}{2\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\, C A \int_0^{\infty} \mathrm{d}(X+L_0)\ (X+L_0)^2 \left[k' + \frac{X+L_0}{\sigma'^2}\right] \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$= 4\pi\beta\, C A \int_{L_0}^{\infty} \mathrm{d}u\ u^2 \left[k' + \frac{u}{\sigma'^2}\right] \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \quad , u = (X+L_0)$$

$$= 4\pi\beta\, C A \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \lim_{u\to\infty} \left[\frac{k'u^3}{3} + \frac{u^4}{4\sigma'^2} - \frac{k' L_0^3}{3} + \frac{L_0^4}{4\sigma'^2}\right]$$

$$\leqslant 4\pi\beta\, C A \mathrm{e}^{-\frac{L_0^2}{8\sigma'^2}} \lim_{u\to\infty} \left[\frac{k'u^3}{3} + \frac{u^4}{4\sigma'^2} - \frac{k' L_0^3}{3} + \frac{L_0^4}{4\sigma'^2}\right] \tag{3.301}$$

where

$$\mathrm{e}^{\frac{-X(X+L_0)}{2\sigma'^2}} \leqslant 1. \tag{3.302}$$

Substitute (3.300) and (3.301) into the right-hand side of inequality (3.299) to obtain

$$\left|\int \mathrm{d}^3\mathbf{r}\, \nabla\phi^*(\mathbf{r}-\mathbf{L}')\cdot\nabla\psi(\mathbf{r}-\mathbf{L})\right|$$

$$\leqslant 4\pi\beta\, C A\, L_0^3 \left[k' + \frac{L_0}{\sigma'^2}\right] \mathrm{e}^{-\frac{L_0^2}{8\sigma'^2}}$$

$$+ 4\pi\beta\, C A \mathrm{e}^{-\frac{L_0^2}{8\sigma'^2}} \lim_{u\to\infty} \left[\frac{k' u^3}{3} + \frac{u^4}{4\sigma'^2} - \frac{k' L_0^3}{3} + \frac{L_0^4}{4\sigma'^2} \right] \tag{3.303}$$

which vanishes very rapidly for $L_0 \to \infty$.

Refer to (3.303), for $L_0 \to \infty$, to write as a limit

$$\lim_{L_0\to\infty} \left[\int \mathrm{d}^3\mathbf{r}\, \nabla\phi^*(\mathbf{r} - \mathbf{L}') \cdot \nabla\psi(\mathbf{r} - \mathbf{L}) \right] = 0. \tag{3.304}$$

In the same way, we obtain a bound for the following

$$\int \mathrm{d}^3\mathbf{r}'\, \nabla' \left[\psi(\mathbf{r}' - \mathbf{L})\right]^* \cdot \nabla' \left[\phi(\mathbf{r}' - \mathbf{L}')\right]. \tag{3.305}$$

Let $\mathbf{R}' = \mathbf{r}' - \mathbf{L}'$, to obtain

$$\begin{aligned}
\nabla\psi^*(\mathbf{r}' - \mathbf{L}) =& \nabla'\psi^*(\mathbf{R}' + \mathbf{L}' - \mathbf{L}) \\
=& \nabla'\psi^*(\mathbf{R}' - \mathbf{L}_0') \qquad , \mathbf{L}_0' = \mathbf{L} - \mathbf{L}' \\
=& C\, \nabla' \mathrm{e}^{-\beta|\mathbf{R}' - \mathbf{L}_0'|} \\
=& \nabla' \mathrm{e}^{-\beta\sqrt{R'^2 - 2R'L_0'\cos\theta + L_0'^2}} \\
=& \left(\hat{R}' \frac{\partial}{\partial R'} + \hat{\theta} \frac{1}{R'} \frac{\partial}{\partial \theta} \right) \mathrm{e}^{\sqrt{R'^2 - 2R'L_0'\cos\theta + L_0'^2}} \\
=& -\beta \left[\frac{(R' - L_0'\cos\theta)\,\hat{R}'}{\sqrt{R'^2 + 2R'L_0\cos\theta + L_0'^2}} + \frac{L_0'\sin\theta\,\hat{\theta}}{\sqrt{R'^2 - 2R'L_0'\cos\theta + L_0'^2}} \right] \\
& \times \mathrm{e}^{-\beta|\mathbf{R}' - \mathbf{L}_0'|} \\
=& -\beta \left[\frac{(R' - L_0'\cos\theta)\,\hat{R}'}{|\mathbf{R}' - \mathbf{L}_0'|} + \frac{L_0'\sin\theta\,\hat{\theta}}{|\mathbf{R}' - \mathbf{L}_0'|} \right] \mathrm{e}^{-\beta|\mathbf{R}' - \mathbf{L}_0'|}
\end{aligned} \tag{3.306}$$

and by referring to (3.264), we have

$$\begin{aligned}\nabla\phi\left(\mathbf{r}'-\mathbf{L}'\right) =& \nabla\phi\left(\mathbf{R}'\right)\\ =& \nabla\left[A\,\exp\mathrm{i}\,\mathbf{k'}\cdot\mathbf{R}'\,\exp-\frac{\left(\mathbf{R}'\right)^2}{4\sigma'^2}\right]\\ =& \left[\mathrm{i}\mathbf{k}'-\left(\frac{\mathbf{R}'}{2\sigma'^2}\right)\right]\phi\left(\mathbf{R}'\right). \qquad (3.307)\end{aligned}$$

By using (3.306) and (3.307), we obtain

$$\begin{aligned}&\nabla\psi^*(\mathbf{r}'-\mathbf{L})\cdot\nabla\phi\left(\mathbf{r}'-\mathbf{L}'\right)\\ &=-\beta\,C\left[\frac{\left(R'-L_0'\cos\theta\right)\hat{R}'\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{L_0'\sin\theta\,\hat{\theta}\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}-\frac{\left(R'-L_0'\cos\theta\right)\hat{R}'}{|\mathbf{R}'-\mathbf{L}_0'|}\frac{\cdot\mathbf{R}'}{2\sigma'^2}\right.\\ &\qquad\left.-\frac{L_0\sin\theta\,\hat{\theta}}{|\mathbf{R}'-\mathbf{L}_0'|}\frac{\cdot\mathbf{R}'}{2\sigma'^2}\right]\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|}\phi\left(\mathbf{R}'\right)\\ &=-\beta\,C\left[\frac{\left(R'-L_0'\cos\theta\right)\hat{R}'\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{L_0'\sin\theta\,\hat{\theta}\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}-\frac{\left(R'-L_0'\cos\theta\right)R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}_0'|}\right]\\ &\qquad\times\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|}\phi\left(\mathbf{R}'\right). \qquad (3.308)\end{aligned}$$

By using (3.308), we obtain

$$\begin{aligned}&\left|\int\mathrm{d}^3\mathbf{r}'\,\nabla\psi^*(\mathbf{r}'-\mathbf{L})\cdot\nabla\phi\left(\mathbf{r}'-\mathbf{L}'\right)\right|\\ &=\left|-\beta\,C\int\left[\frac{\left(R'-L_0'\cos\theta\right)\hat{R}'\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{L_0'\sin\theta\,\hat{\theta}\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}-\frac{\left(R'-L_0'\cos\theta\right)R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}_0'|}\right]\right.\\ &\qquad\left.\times\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|}\phi\left(\mathbf{R}'\right)\,\mathrm{d}^3\mathbf{R}'\right|\end{aligned}$$

$$
\begin{aligned}
&\leqslant \left|\beta\, C \int \left[\frac{(R'+L'_0\cos\theta)\,\hat{R}'\cdot \mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}'_0|} + \frac{L'_0\sin\theta\,\hat{\theta}\cdot \mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}'_0|} + \frac{(R'+L'_0\cos\theta)\,R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}'_0|}\right]\right.\\
&\qquad\qquad \left.\times \mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}'_0|}\phi\left(\mathbf{R}'\right)\,\mathrm{d}^3\mathbf{R}'\right|\\
&\leqslant \left|\beta\, C \int \left[\frac{(R'+L'_0)\,\hat{R}'\cdot \mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}'_0|} + \frac{L'_0\,\hat{\theta}\cdot \mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}'_0|} + \frac{(R'+L'_0)\,R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}'_0|}\right]\right.\\
&\qquad\qquad \left.\times \mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}'_0|}\phi\left(\mathbf{R}'\right)\,\mathrm{d}^3\mathbf{R}'\right|\\
&\leqslant \beta\, C A \int \left[\frac{(R'+L'_0)\,k'}{|\mathbf{R}'-\mathbf{L}'_0|} + \frac{L'_0 k'}{|\mathbf{R}'-\mathbf{L}'_0|} + \frac{(R'+L'_0)\,R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}'_0|}\right]\\
&\qquad\qquad \times \left|\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}'_0|}\mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot\mathbf{R}'}\,\mathrm{e}^{-\frac{(\mathbf{R}')^2}{4\sigma'^2}}\right|\mathrm{d}^3\mathbf{R}'\\
&\leqslant \beta\, C A \int \left[\frac{(R'+2L'_0)\,k'}{|\mathbf{R}'-\mathbf{L}'_0|} + \frac{(R'+L'_0)\,R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}'_0|}\right]\left|\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}'_0|}\,\mathrm{e}^{-\frac{(\mathbf{R}')^2}{4\sigma'^2}}\right|\mathrm{d}^3\mathbf{R}'\\
&= \beta\, C A \int \mathrm{d}^3\mathbf{R}' \left[\frac{(R'+2L'_0)\,k'}{|\mathbf{R}'-\mathbf{L}'_0|} + \frac{(R'+L'_0)\,R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}'_0|}\right]\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}'_0|}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\\
&\leqslant 4\pi\beta\, C A \int_0^{\infty}\mathrm{d}R' \left[\frac{R'^2(R'+2L'_0)\,k'}{R_>} + \frac{(R'+L'_0)\,R'^3}{2\sigma'^2 R'_>}\right]\mathrm{e}^{-\beta\left|R'-L'_0\right|}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\\
&= 4\pi\beta\, C A \int_0^{L'_0}\mathrm{d}R' \left[\frac{R'^2(R'+2L'_0)\,k'}{L'_0} + \frac{(R'+L'_0)\,R'^3}{2\sigma'^2 L'_0}\right]\mathrm{e}^{-\beta\left(L'_0-R'\right)}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\\
&\quad + 4\pi\beta\, C A \int_{L'_0}^{\infty}\mathrm{d}R' \left[\frac{R'^2(R'+2L'_0)\,k'}{R'} + \frac{(R'+L'_0)\,R'^3}{2\sigma'^2 R'}\right]\mathrm{e}^{-\beta\left(R'-L'_0\right)}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}
\end{aligned}
\tag{3.309}
$$

where

$$
\int_0^{\pi}\int_0^{2\pi}\mathrm{d}\theta\,\mathrm{d}\varphi\,\frac{1}{|\mathbf{R}'-\mathbf{L}'_0|} = 4\pi\frac{1}{R'_>} \qquad , R_> = \max(R', L'_0). \tag{3.310}
$$

Consider the first term on the right-hand side of (3.309), to obtain

$$4\pi\beta\,CA\int_0^{L_0'}\mathrm{d}R'\left[\frac{R'^2(R'+2L_0')\,k'}{L_0'}+\frac{(R'+L_0')\,R'^3}{2\sigma'^2L_0'}\right]\mathrm{e}^{-\beta\left(L_0'-R'\right)}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\,CA\int_0^{L_0'}\mathrm{d}R'\left[\frac{R'^2(R'+2L_0')\,k'}{L_0'}+\frac{(R'+L_0')\,R'^3}{2\sigma'^2L_0'}\right]\mathrm{e}^{-\beta L_0'}$$

$$\leqslant 4\pi\beta\,CA\,\mathrm{e}^{-\beta L_0'}\ \times[\text{polynomian of degree } 4 \text{ in } (L_0')| \tag{3.311}$$

where

$$\mathrm{e}^{\beta R'}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}=\mathrm{e}^{-R'^2\left(\frac{1}{4\sigma'^2}-\frac{\beta}{R'}\right)}\leqslant\ 1. \tag{3.312}$$

Consider the second term on the right-hand side of (3.309), and let $X'=R'-L_0'$, to write

$$4\pi\beta\,CA\int_0^{\infty}\mathrm{d}R'\left[\frac{R'^2(R'+2L_0')\,k'}{R'}+\frac{(R'+L_0')\,R'^3}{2\sigma'^2R'}\right]\mathrm{e}^{-\beta\left(R'-L_0'\right)}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}$$

$$=4\pi\beta\,CA\int_0^{\infty}\mathrm{d}(X'+L_0')\,[(X'+L'_0)((X'+L_0')+2L_0')\,k'$$

$$+\frac{((X'+L_0')+L_0')\,(X'+L_0')^2}{2\sigma'^2}\Bigg]\,\mathrm{e}^{-\beta X}\,\mathrm{e}^{-\frac{(X'+L_0')^2}{4\sigma'^2}}$$

$$=4\pi\beta\,CA\int_{L_0'0}^{\infty}\mathrm{d}u\left[uk'(u+2L_0')+\frac{(u+L_0')\,u^2}{2\sigma'^2}\right]\mathrm{e}^{-\beta X}\,\mathrm{e}^{-\frac{X'^2+2X'L_0'+L'^2_0}{4\sigma'^2}}$$

$$=4\pi\beta\,CA\int_{L_0'}^{\infty}\mathrm{d}u\left[uk'(u+2L_0')+\frac{(u+L_0')\,u^2}{2\sigma'^2}\right]\mathrm{e}^{-\beta X}\,\mathrm{e}^{-\frac{X'^2+2X'L_0'+L'^2_0}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\,CA\int_0^{\infty}\mathrm{d}u\left[u^2k'+2uL_0'+\frac{(u^3+L_0'u^2)}{2\sigma'^2}\right]\,\mathrm{e}^{-\frac{L'^2_0}{4\sigma'^2}}$$

$$=4\pi\beta\,CA$$

$$\times \lim_{u\to\infty}\left[\frac{u^3k'}{3}+u^2L'_0+\frac{u^4}{8\sigma'^2}+\frac{L'{}_0u^3}{6\sigma'^2}-\frac{L'^3_0k'}{3}-L'^3_0-\frac{L'^4_0}{8\sigma'^2}-\frac{L'^3_0}{6\sigma'^2}\right]\mathrm{e}^{-\frac{L'^2_0}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\,CA\,\mathrm{e}^{-\frac{L'^2_0}{8\sigma'^2}}$$

$$\times \lim_{u\to\infty}\left[\frac{u^3k'}{3}+u^2L'_0+\frac{u^4}{8\sigma'^2}+\frac{L'{}_0u^3}{6\sigma'^2}-\frac{L'^3_0k'}{3}-L'^3_0-\frac{L'^4_0}{8\sigma'^2}-\frac{L'^3_0}{6\sigma'^2}\right] \tag{3.313}$$

where

$$\mathrm{e}^{-\beta X}\mathrm{e}^{-\frac{X'^2+2X'L'_0}{4\sigma'^2}}\leqslant 1. \tag{3.314}$$

Substitute (3.312) and (3.313) into the right-hand side of inequality (3.309), to obtain

$$\left|\int \mathrm{d}^3\mathbf{r}'\,\nabla\psi^*(\mathbf{r}'-\mathbf{L})\cdot\nabla\phi\,(\mathbf{r}'-\mathbf{L}')\right|$$

$$\leqslant 4\pi\beta\,CA\,\mathrm{e}^{-\beta L'_0}\ \times[\text{polynomian of degree } 4 \text{ in } (L'_0)]$$

$$+\,4\pi\beta\,CA\,\mathrm{e}^{-\frac{L'^2_0}{8\sigma'^2}}$$

$$\times \lim_{u\to\infty}\left[\frac{u^3k'}{3}+u^2L'_0+\frac{u^4}{8\sigma'^2}+\frac{L'{}_0u^3}{6\sigma'^2}-\frac{L'^3_0k'}{3}-L'^3_0-\frac{L'^4_0}{8\sigma'^2}-\frac{L'^3_0}{6\sigma'^2}\right] \tag{3.315}$$

which vanishes very rapidly for $L'_0\to\infty$.

Refer to (3.315), for $L'_0\to\infty$, have as a limit

$$\lim_{L'_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}'\,\nabla\psi^*(\mathbf{r}'-\mathbf{L})\cdot\nabla\phi\,(\mathbf{r}'-\mathbf{L}')\right]=0. \tag{3.316}$$

In the same way, we obtain a bound for the following

$$\int \mathrm{d}^3\mathbf{r}'\,\nabla'\left[\phi(\mathbf{r}'-\mathbf{L}')\right]^*\cdot\nabla'\left[\psi(\mathbf{r}'-\mathbf{L})\right]. \tag{3.317}$$

Let $\mathbf{R}' = \mathbf{r}' - \mathbf{L}'$ and $\mathbf{L}_0' = \mathbf{L} - \mathbf{L}'$, we have

$$
\begin{aligned}
\nabla\psi(\mathbf{r}' - \mathbf{L}) =& \nabla'\psi(\mathbf{R}' + \mathbf{L}' - \mathbf{L}) \\
=& \nabla'\psi(\mathbf{R}' - \mathbf{L}_0') \\
=& C\,\nabla' \mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|} \\
=& \nabla' \mathrm{e}^{-\beta\sqrt{R'^2 - 2R'L_0'\cos\theta + L'^2_0}} \\
=& \left(\hat{R}'\frac{\partial}{\partial R'} + \hat{\theta}\frac{1}{R'}\frac{\partial}{\partial\theta}\right)\mathrm{e}^{\sqrt{R'^2 - 2R'L_0'\cos\theta + L'^2_0}} \\
=& -\beta\left[\frac{(R' - L_0'\cos\theta)\,\hat{R}'}{\sqrt{R'^2 + 2R'L_0\cos\theta + L'^2_0}} + \frac{L_0'\sin\theta\,\hat{\theta}}{\sqrt{R'^2 - 2R'L_0'\cos\theta + L'^2_0}}\right] \\
& \times \mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|} \\
=& -\beta\left[\frac{(R' - L_0'\cos\theta)\,\hat{R}'}{|\mathbf{R}' - \mathbf{L}_0'|} + \frac{L_0'\sin\theta\,\hat{\theta}}{|\mathbf{R}' - \mathbf{L}_0'|}\right]\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|}
\end{aligned}
\tag{3.318}
$$

and by referring to (3.264), we have

$$
\begin{aligned}
\nabla\phi^*(\mathbf{r}' - \mathbf{L}') =& \nabla\phi^*(\mathbf{R}') \\
=& \nabla\left[A\,\exp -\mathrm{i}\,\mathbf{k'}\cdot\mathbf{R}'\,\exp -\frac{(\mathbf{R}')^2}{4\sigma'^2}\right] \\
=& \left[-\mathrm{i}\mathbf{k}' - \left(\frac{\mathbf{R}'}{2\sigma'^2}\right)\right]\phi^*(\mathbf{R}')\,.
\end{aligned}
\tag{3.319}
$$

By using (3.318) and (3.319), we obtain

$$
\nabla\phi^*(\mathbf{r}' - \mathbf{L}')\cdot\nabla\psi(\mathbf{r}' - \mathbf{L})
$$

$$= -\,\beta\, C\left[-\frac{(R'-L_0'\cos\theta)\,\hat{R}'\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}-\frac{L_0'\sin\theta\,\hat{\theta}\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}-\frac{(R'-L_0'\cos\theta)\,\hat{R}'}{|\mathbf{R}'-\mathbf{L}_0'|}\frac{\cdot\mathbf{R}'}{2\sigma'^2}\right.$$

$$\left.-\frac{L_0\sin\theta\,\hat{\theta}}{|\mathbf{R}'-\mathbf{L}_0'|}\frac{\cdot\mathbf{R}'}{2\sigma'^2}\right]\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|}\phi\left(\mathbf{R}'\right)$$

$$=\beta\, C\left[\frac{(R'-L_0'\cos\theta)\,\hat{R}'\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{L_0'\sin\theta\,\hat{\theta}\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{(R'-L_0'\cos\theta)\,R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}_0'|}\right]$$

$$\times\,\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|}\phi\left(\mathbf{R}'\right) \tag{3.320}$$

by using (3.320), we obtain

$$\left|\int \mathrm{d}^3\mathbf{r}'\,\nabla\phi^*\left(\mathbf{r}'-\mathbf{L}'\right)\cdot\nabla\psi(\mathbf{r}'-\mathbf{L})\right|$$

$$=\left|\beta\, C\int\left[\frac{(R'+L_0'\cos\theta)\,\hat{R}'\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{L_0'\sin\theta\,\hat{\theta}\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{(R'+L_0'\cos\theta)\,R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}_0'|}\right]\right.$$

$$\left.\times\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|}\phi\left(\mathbf{R}'\right)\,\mathrm{d}^3\mathbf{R}'\right|$$

$$\leqslant\left|\beta\, C\int\left[\frac{(R'+L_0')\,\hat{R}'\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{L_0'\,\hat{\theta}\cdot\mathrm{i}\mathbf{k}'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{(R'+L_0')\,R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}_0'|}\right]\right.$$

$$\left.\times\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|}\phi\left(\mathbf{R}'\right)\,\mathrm{d}^3\mathbf{R}'\right|$$

$$\leqslant\beta\, C A\int\left[\frac{(R'+L_0')\,k'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{L_0'k'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{(R'+L_0')\,R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}_0'|}\right]$$

$$\times\left|\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|}\mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot\mathbf{R}'}\,\mathrm{e}^{-\frac{(\mathbf{R}')^2}{4\sigma'^2}}\right|\mathrm{d}^3\mathbf{R}'$$

$$\leqslant\beta\, C A\int\left[\frac{(R'+2L_0')\,k'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{(R'+L_0')\,R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}_0'|}\right]\left|\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|}\,\mathrm{e}^{-\frac{(\mathbf{R}')^2}{4\sigma'^2}}\right|\mathrm{d}^3\mathbf{R}'$$

$$=\beta\, C A\int\mathrm{d}^3\mathbf{R}'\left[\frac{(R'+2L_0')\,k'}{|\mathbf{R}'-\mathbf{L}_0'|}+\frac{(R'+L_0')\,R'}{2\sigma'^2\,|\mathbf{R}'-\mathbf{L}_0'|}\right]\mathrm{e}^{-\beta|\mathbf{R}'-\mathbf{L}_0'|}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\, CA \int_0^\infty \mathrm{d}R' \left[\frac{R'^2(R'+2L_0')\,k'}{R_>} + \frac{(R'+L_0')\,R'^3}{2\sigma'^2 R_>'}\right] \mathrm{e}^{-\beta\left|R'-L_0'\right|}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}$$

$$= 4\pi\beta\, CA \int_0^{L_0'} \mathrm{d}R' \left[\frac{R'^2(R'+2L_0')\,k'}{L_0'} + \frac{(R'+L_0')\,R'^3}{2\sigma'^2 L_0'}\right] \mathrm{e}^{-\beta\left(L_0'-R'\right)}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}$$

$$+ 4\pi\beta\, CA \int_{L_0'}^\infty \mathrm{d}R' \left[\frac{R'^2(R'+2L_0')\,k'}{R'} + \frac{(R'+L_0')\,R'^3}{2\sigma'^2 R'}\right] \mathrm{e}^{-\beta\left(R'-L_0'\right)}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}} \tag{3.321}$$

where

$$\int_0^\pi \int_0^{2\pi} \mathrm{d}\theta\,\mathrm{d}\varphi\, \frac{1}{|\mathbf{R}'-\mathbf{L}_0'|} = 4\pi \frac{1}{R_>'} \qquad , R_> = \max(R', L_0'). \tag{3.322}$$

Consider the first term on the right-hand side of (3.321), to obtain

$$4\pi\beta\, CA \int_0^{L_0'} \mathrm{d}R' \left[\frac{R'^2(R'+2L_0')\,k'}{L_0'} + \frac{(R'+L_0')\,R'^3}{2\sigma'^2 L_0'}\right] \mathrm{e}^{-\beta\left(L_0'-R'\right)}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\, CA \int_0^{L_0'} \mathrm{d}R' \left[\frac{R'^2(R'+2L_0')\,k'}{L_0'} + \frac{(R'+L_0')\,R'^3}{2\sigma'^2 L_0'}\right] \mathrm{e}^{-\beta L_0'}$$

$$\leqslant 4\pi\beta\, CA\, \mathrm{e}^{-\beta L_0'} \times [\text{polynomial of degree } 4 \text{ in } (L_0')] \tag{3.323}$$

where

$$\mathrm{e}^{\beta R'}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}} = \mathrm{e}^{-R'^2\left(\frac{1}{4\sigma'^2}-\frac{\beta}{R'}\right)} \leqslant 1. \tag{3.324}$$

Consider the second term on the right-hand side of (3.321), and let $X' = R' - L_0'$, to write

$$4\pi\beta\, CA \int_0^\infty \mathrm{d}R' \left[\frac{R'^2(R'+2L_0')\,k'}{R'} + \frac{(R'+L_0')\,R'^3}{2\sigma'^2 R'}\right] \mathrm{e}^{-\beta\left(R'-L_0'\right)}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}$$

$$= 4\pi\beta\, CA \int_0^\infty \mathrm{d}(X'+L_0')\,[(X'+L'_0)((X'+L_0')+2L_0')\,k'$$

$$+\frac{((X'+L_0')+L_0')\,(X'+L_0')^2}{2\sigma'^2}\Bigg]\,\mathrm{e}^{-\beta X}\,\mathrm{e}^{-\frac{(X'+L_0')^2}{4\sigma'^2}}$$

$$=4\pi\beta\,CA\int_{L'_0}^{\infty}\mathrm{d}u\left[uk'(u+2L_0')+\frac{(u+L_0')\,u^2}{2\sigma'^2}\right]\mathrm{e}^{-\beta X}\,\mathrm{e}^{-\frac{X'^2+2X'L_0'+L'^2_0}{4\sigma'^2}}$$

$$=4\pi\beta\,CA\int_{L'_0}^{\infty}\mathrm{d}u\left[uk'(u+2L_0')+\frac{(u+L_0')\,u^2}{2\sigma'^2}\right]\mathrm{e}^{-\beta X}\,\mathrm{e}^{-\frac{X'^2+2X'L_0'+L'^2_0}{4\sigma'^2}}$$

$$\leqslant 4\pi\beta\,CA\,\mathrm{e}^{-\frac{L'^2_0}{4\sigma'^2}}\int_{L'_0}^{\infty}\mathrm{d}u\left[u^2k'+2uL_0'+\frac{(u^3+L_0'u^2)}{2\sigma'^2}\right]$$

$$=4\pi\beta\,CA\,\mathrm{e}^{-\frac{L'^2_0}{4\sigma'^2}}$$

$$\times\lim_{u\to\infty}\left[\frac{u^3k'}{3}+u^2L_0'+\frac{u^4}{8\sigma'^2}+\frac{L_0'u^3}{6\sigma'^2}-\frac{L'^3_0k'}{3}-L'^2_0-\frac{L'^4_0}{8\sigma'^2}-\frac{L'^4_0}{6\sigma'^2}\right]$$

$$\leqslant 4\pi\beta\,CA\,\mathrm{e}^{-\frac{L'^2_0}{8\sigma'^2}}$$

$$\times\lim_{u\to\infty}\left[\frac{u^3k'}{3}+u^2L_0'+\frac{u^4}{8\sigma'^2}+\frac{L_0'u^3}{6\sigma'^2}-\frac{L'^3_0k'}{3}-L'^2_0-\frac{L'^4_0}{8\sigma'^2}-\frac{L'^4_0}{6\sigma'^2}\right] \tag{3.325}$$

where

$$\mathrm{e}^{-\beta X}\mathrm{e}^{-\frac{X'^2+2X'L_0'}{4\sigma'^2}}\leqslant 1. \tag{3.326}$$

Substitute (3.324) and (3.325) into the right-hand side of inequality (3.321), to obtain

$$\left|\int \mathrm{d}^3\mathbf{r}'\,\nabla\phi^*\,(\mathbf{r}'-\mathbf{L}')\cdot\nabla\psi(\mathbf{r}'-\mathbf{L})\right|$$

$$\leqslant 4\pi\beta\,CA\,\mathrm{e}^{-\beta L_0'}\;\times[\text{polynomial of degree } 4 \text{ in } (L_0')]$$

$$+\,4\pi\beta\,CA\,\mathrm{e}^{-\frac{L'^2_0}{8\sigma'^2}}$$

$$\times\lim_{u\to\infty}\left[\frac{u^3k'}{3}+u^2L_0'+\frac{u^4}{8\sigma'^2}+\frac{L_0'u^3}{6\sigma'^2}-\frac{L'^3_0k'}{3}-L'^2_0-\frac{L'^4_0}{8\sigma'^2}-\frac{L'^4_0}{6\sigma'^2}\right] \tag{3.327}$$

which vanishes very rapidly for $L_0' \to \infty$.

Refer to (3.327), for $L_0' \to \infty$, to write as a limit

$$\lim_{L_0' \to \infty} \left[\int \mathrm{d}^3\mathbf{r}'\, \nabla\phi^*\left(\mathbf{r}' - \mathbf{L}'\right) \cdot \nabla\psi(\mathbf{r}' - \mathbf{L}) \right] = 0. \tag{3.328}$$

In the same way, we obtain a bound for the following integral. Let $\mathbf{R} = \mathbf{r} - \mathbf{L}$, to obtain

$$\begin{aligned}
\left| \int \mathrm{d}^3\mathbf{r}\, \left[\psi(\mathbf{r} - \mathbf{L})\right]^* \left[\phi(\mathbf{r} - \mathbf{L}')\right] \right| &= \left| CA \int \mathrm{d}^3\mathbf{r}\, \mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}|}\, \mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{r}-\mathbf{L}')}\, \mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L}')^2}{4\sigma'^2}} \right| \\
&= \left| CA \int \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-\beta|\mathbf{R}|}\, \mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{R}-\mathbf{L}_0)}\, \mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}} \right| \\
&\leqslant \int \mathrm{d}^3\mathbf{R} \left| CA\ \mathrm{e}^{-\beta|\mathbf{R}|}\ \mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}} \right| \\
&= \int \mathrm{d}^3\mathbf{R} \left| CA\ \mathrm{e}^{-\beta|\mathbf{R}|}\ \mathrm{e}^{-\frac{\left(\sqrt{R^2+L_0^2-2RL_0\cos\theta}\right)^2}{4\sigma'^2}} \right| \\
&\leqslant \int \mathrm{d}^3\mathbf{R} \left| CA\ \mathrm{e}^{-\beta|\mathbf{R}|}\ \mathrm{e}^{-\frac{\left(\sqrt{R^2+L_0^2-2RL_0}\right)^2}{4\sigma'^2}} \right| \\
&= \int \mathrm{d}^3\mathbf{R} \left| CA\ \mathrm{e}^{-\beta R}\, \mathrm{e}^{-\frac{(R-L_0)^2}{4\sigma'^2}} \right| \\
&\leqslant 4\pi CA \int_0^\infty \mathrm{d}R\ R^2\, \mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\
&\leqslant 4\pi CA \int_0^{L_0} \mathrm{d}R\ L_0^2\, \mathrm{e}^{-\frac{R(2L_0-R)}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\
&\quad + 4\pi CA \int_{L_0}^\infty \mathrm{d}R\ R^2\, \mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}.
\end{aligned} \tag{3.329}$$

Consider the right-hand side of inequality (3.329), optimize $R(L_0 - R)$ by R, to

obtain

$$\frac{\partial}{\partial R}\, R(2L_0 - R) = 2L_0 - 2R = 0 \rightarrow R = L_0 \tag{3.330}$$

and

$$\frac{\partial^2}{\partial R^2}\, R(2L_0 - R) = -2. \tag{3.331}$$

Substitute $R = L_0$ into the first term on the right-hand side of (3.329), to obtain

$$\begin{aligned} 4\pi CA \int_0^{L_0} \mathrm{d}R\; L_0^2\, \mathrm{e}^{-\frac{R(2L_0-R)}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} =& 4\pi CA \int_0^{L_0} \mathrm{d}R\; L_0^2\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\ =& 4\pi CA \int_0^{L_0} \mathrm{d}R\; L_0^2\, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \\ =& \frac{4\pi CA L_0^3}{3}\, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}}. \end{aligned} \tag{3.332}$$

Consider the second term on the right-hand side of inequality (3.329), let $X = R - 2L_0$, to obtain

$$\begin{aligned} & 4\pi CA \int_{L_0}^{\infty} \mathrm{d}R\; R^2\, \mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\ =& 4\pi CA \int_0^{\infty} \mathrm{d}(X+2L_0)\; (X+2L_0)^2\, \mathrm{e}^{-\frac{X(X+2L_0)}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\ \leqslant& 4\pi CA \int_0^{\infty} \mathrm{d}(X+2L_0)\; (X+2L_0)^2\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \qquad , \mathrm{e}^{-\frac{X(X+2L_0)}{4\sigma'^2}} \leqslant 1 \\ =& 4\pi CA \int_{2L_0}^{\infty} \mathrm{d}u\; u^2\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\ =& 4\pi CA\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \lim_{u\to\infty} \left[\frac{u^3}{3} - \frac{L_0^3}{3}\right]. \end{aligned} \tag{3.333}$$

Substitute (3.332) and (3.333) into the right-hand side of inequality (3.329), to obtain

$$\left|\int \mathrm{d}^3\mathbf{r}\ [\psi(\mathbf{r}-\mathbf{L})]^*\ [\phi(\mathbf{r}-\mathbf{L}')]\right| \leqslant \frac{4\pi C A L_0^3}{3}\,\mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} + 4\pi C A\,\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \lim_{u\to\infty}\left[\frac{u^3}{3}-\frac{L_0^3}{3}\right] \tag{3.334}$$

which vanishes very rapidly for $L_0 \to \infty$.

Refer to (3.334), for $L_0 \to \infty$, to write as a limit

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\ [\psi(\mathbf{r}-\mathbf{L})]^*\ [\phi(\mathbf{r}-\mathbf{L}')]\right] = 0. \tag{3.335}$$

In the same way, we obtain a bound for the following integral. Let $\mathbf{R} = \mathbf{r} - \mathbf{L}$, to obtain

$$\begin{aligned}
\left|\int \mathrm{d}^3\mathbf{r}\ [\phi(\mathbf{r}-\mathbf{L}')]^*\ [\psi(\mathbf{r}-\mathbf{L})]\right| &= \left|CA\int \mathrm{d}^3\mathbf{r}\,\mathrm{e}^{-\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{r}-\mathbf{L}')}\,\mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L}')^2}{4\sigma'^2}}\,\mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}|}\right| \\
&= \left|CA\int \mathrm{d}^3\mathbf{R}\,\mathrm{e}^{-\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{R}-\mathbf{L}_0)}\,\mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}}\,\mathrm{e}^{-\beta|\mathbf{R}|}\right| \\
&\leqslant \int \mathrm{d}^3\mathbf{R}\left|CA\ \mathrm{e}^{-\beta|\mathbf{R}|}\,\mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}}\right| \\
&= \int \mathrm{d}^3\mathbf{R}\left|CA\ \mathrm{e}^{-\beta|\mathbf{R}|}\,\mathrm{e}^{-\frac{\left(\sqrt{R^2+L_0^2-2RL_0\cos\theta}\right)^2}{4\sigma'^2}}\right| \\
&\leqslant \int \mathrm{d}^3\mathbf{R}\left|CA\ \mathrm{e}^{-\beta|\mathbf{R}|}\,\mathrm{e}^{-\frac{\left(\sqrt{R^2+L_0^2-2RL_0}\right)^2}{4\sigma'^2}}\right| \\
&= \int \mathrm{d}^3\mathbf{R}\left|CA\ \mathrm{e}^{-\beta R}\,\mathrm{e}^{-\frac{(R-L_0)^2}{4\sigma'^2}}\right| \\
&\leqslant 4\pi CA\int_0^\infty \mathrm{d}R\ R^2\,\mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}}\,\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}
\end{aligned}$$

$$\leqslant 4\pi CA \int_0^{L_0} \mathrm{d}R\ L_0^2\, \mathrm{e}^{-\frac{R(2L_0-R)}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$+ 4\pi CA \int_{L_0}^{\infty} \mathrm{d}R\ R^2\, \mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}. \quad (3.336)$$

Consider the right-hand side of inequality (3.336), optimize $R(2L_0 - R)$ over R, to obtain

$$\frac{\partial}{\partial R} R(2L_0 - R) = 2L_0 - 2R = 0. \quad (3.337)$$

From (3.337), we obtain

$$R = L_0. \quad (3.338)$$

Substitute $R = L_0$ into the first term on the right-hand side of (3.336), to obtain

$$\begin{aligned} 4\pi CA \int_0^{L_0} \mathrm{d}R\ L_0^2\, \mathrm{e}^{-\frac{R(2L_0-R)}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} =& 4\pi CA \int_0^{L_0} \mathrm{d}R\ L_0^2\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\ =& 4\pi CA \int_0^{L_0} \mathrm{d}R\ L_0^2\, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \\ =& \frac{4\pi CA L_0^3}{3}\, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}}. \end{aligned} \quad (3.339)$$

Consider the second term on the right-hand side of inequality (3.336), let $X = R - 2L_0$, to obtain

$$\begin{aligned} & 4\pi CA \int_{L_0}^{\infty} \mathrm{d}R\ R^2\, \mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\ =& 4\pi CA \int_0^{\infty} \mathrm{d}(X+2L_0)\ (X+2L_0)^2\, \mathrm{e}^{-\frac{X(X+2L_0)}{4\sigma'^2}}\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\ \leqslant& 4\pi CA \int_0^{\infty} \mathrm{d}(X+2L_0)\ (X+2L_0)^2\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \qquad , \mathrm{e}^{-\frac{X(X+2L_0)}{4\sigma'^2}} \leqslant 1 \end{aligned}$$

$$=4\pi CA\int_{2L_0}^{\infty}\mathrm{d}u\ u^2\,\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$

$$=4\pi CA\,\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\lim_{u\to\infty}\left[\frac{u^3}{3}-\frac{L_0^3}{3}\right]. \tag{3.340}$$

Substitute (3.339) and (3.340) into the right-hand side of inequality (3.336), to obtain

$$\left|\int \mathrm{d}^3\mathbf{r}\ [\phi(\mathbf{r}-\mathbf{L}')]^*\ [\psi(\mathbf{r}-\mathbf{L})]\right| \leqslant \frac{4\pi CAL_0^3}{3}\,\mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} + 4\pi CA\,\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\lim_{u\to\infty}\left[\frac{u^3}{3}-\frac{L_0^3}{3}\right] \tag{3.341}$$

which vanishes very rapidly for $L_0\to\infty$.

Refer to (3.341), for $L_0\to\infty$ to write as a limit

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\ [\phi(\mathbf{r}-\mathbf{L}')]^*\ [\psi(\mathbf{r}-\mathbf{L})]\right]=0. \tag{3.342}$$

In the same way, we obtain a bound for the following integral. Let $\mathbf{R}'=\mathbf{r}'-\mathbf{L}'$, to obtain

$$\begin{aligned}\left|\int \mathrm{d}^3\mathbf{r}'\ [\psi(\mathbf{r}'-\mathbf{L})]^*\ [\phi(\mathbf{r}'-\mathbf{L}')]\right| &= \left|CA\int \mathrm{d}^3\mathbf{r}'\,\mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{r}'-\mathbf{L}')}\,\mathrm{e}^{-\frac{(\mathbf{r}'-\mathbf{L}')^2}{4\sigma'^2}}\,\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}|}\right|\\ &= \left|CA\int \mathrm{d}^3\mathbf{R}'\,\mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot\mathbf{R}'}\,\mathrm{e}^{-\frac{\mathbf{R}'^2}{4\sigma'^2}}\,\mathrm{e}^{-\beta|\mathbf{R}+\mathbf{L}_0|}\right|\\ &\leqslant \int \mathrm{d}^3\mathbf{R}'\left|CA\ \mathrm{e}^{-\beta|\mathbf{R}'+\mathbf{L}_0|}\,\mathrm{e}^{-\frac{(\mathbf{R}')^2}{4\sigma'^2}}\right|\\ &\leqslant \int \mathrm{d}^3\mathbf{R}'\left|CA\ \mathrm{e}^{-\beta|R'-L_0|}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\right|\\ &\leqslant 4\pi CA\int_0^{\infty}\mathrm{d}R'\ R'^2\,\mathrm{e}^{-\beta|R'-L_0|}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\\ &\leqslant 4\pi CA\int_0^{\infty}\mathrm{d}R'\ R'^2\,\mathrm{e}^{-\beta|R'-L_0|}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\end{aligned}$$

$$=4\pi CA\int_0^{L_0} \mathrm{d}R'\ R'^2\ \mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\mathrm{e}^{-\beta(L_0-R')}$$
$$+\,4\pi CA\int_{L_0}^{\infty} \mathrm{d}R'\ R'^2\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\mathrm{e}^{-\beta(R'-L_0)}. \tag{3.343}$$

Consider the first term on right-hand side of inequality (3.343), to obtain

$$4\pi CA\int_0^{L_0} \mathrm{d}R'\ R'^2\ \mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\mathrm{e}^{-\beta(L_0-R')} \leqslant 4\pi CA\int_0^{L_0} \mathrm{d}R'\ R'^2\,\mathrm{e}^{-\beta L_0}$$
$$\leqslant \frac{4\pi CA\,L_0^3}{3}\,\mathrm{e}^{-\beta L_0} \tag{3.344}$$

where

$$\mathrm{e}^{\beta R'}\ \mathrm{e}^{-\frac{R'^2}{4\sigma'^2}} = \mathrm{e}^{-R'^2(\frac{1}{4\sigma'^2}-\frac{\beta}{R'})} \leqslant\ 1. \tag{3.345}$$

Consider the second term on right-hand side of inequality (3.343), let $X = R' - L_0$, to obtain

$$4\pi CA\int_{L_0}^{\infty} \mathrm{d}R'\ R'^2\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\mathrm{e}^{-\beta(R'-L_0)}$$
$$\leqslant 4\pi CA\int_0^{\infty} \mathrm{d}R'\ R'^2\,\mathrm{e}^{-\frac{(X+L_0)^2}{4\sigma'^2}}\mathrm{e}^{-\beta X}$$
$$=4\pi CA\int_0^{\infty} \mathrm{d}R'\ R'^2\,\mathrm{e}^{-\frac{X^2+L_0^2-2XL_0}{4\sigma'^2}}\mathrm{e}^{-\beta X}$$
$$\leqslant 4\pi CA\int_0^{\infty} \mathrm{d}R'\ R'^2\,\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}$$
$$=4\pi CA\,\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\ \lim_{R'\to\infty}\frac{R'^3}{3} \tag{3.346}$$

where

$$\mathrm{e}^{-\beta X}\mathrm{e}^{-\frac{X'^2+2X'L_0'}{4\sigma'^2}} \leqslant 1. \tag{3.347}$$

Substitute (3.345) and (3.346) into the right-hand side of inequality (3.343), to obtain

$$\left|\int \mathrm{d}^3\mathbf{r}'\ [\psi(\mathbf{r}'-\mathbf{L})]^*\ [\phi(\mathbf{r}'-\mathbf{L}')]\right| \leqslant \frac{4\pi CA\,L_0^3}{3}\,\mathrm{e}^{-\beta L_0} + 4\pi CA\,\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \lim_{R'\to\infty}\frac{R'^3}{3} \tag{3.348}$$

which vanishes very rapidly for $L_0 \to \infty$.

Refer to (3.348), for $L_0 \to \infty$ to write as a limit

$$\lim_{L_0'\to\infty}\left[\int \mathrm{d}^3\mathbf{r}'\ [\psi(\mathbf{r}'-\mathbf{L})]^*\ [\phi(\mathbf{r}'-\mathbf{L}')]\right] = 0. \tag{3.349}$$

In the same way, we obtain a bound for following integral. Let $\mathbf{R}' = \mathbf{r}' - \mathbf{L}'$, to obtain

$$\begin{aligned}
\left|\int \mathrm{d}^3\mathbf{r}'\ [\phi(\mathbf{r}'-\mathbf{L}')]^*\ [\psi(\mathbf{r}'-\mathbf{L})]\right| &= \left|CA\int \mathrm{d}^3\mathbf{r}'\,\mathrm{e}^{-\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{r}'-\mathbf{L}')}\,\mathrm{e}^{-\frac{(\mathbf{r}'-\mathbf{L}')^2}{4\sigma'^2}}\,\mathrm{e}^{-\beta|\mathbf{r}'-\mathbf{L}|}\right| \\
&= \left|CA\int \mathrm{d}^3\mathbf{R}'\,\mathrm{e}^{-\mathrm{i}\,\mathbf{k}'\cdot\mathbf{R}'}\,\mathrm{e}^{-\frac{\mathbf{R}'^2}{4\sigma'^2}}\,\mathrm{e}^{-\beta|\mathbf{R}+\mathbf{L}_0|}\right| \\
&\leqslant \int \mathrm{d}^3\mathbf{R}'\left|CA\ \mathrm{e}^{-\beta|\mathbf{R}'+\mathbf{L}_0|}\,\mathrm{e}^{-\frac{(\mathbf{R}')^2}{4\sigma'^2}}\right| \\
&\leqslant \int \mathrm{d}^3\mathbf{R}'\left|CA\ \mathrm{e}^{-\beta|R'-L_0|}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\right| \\
&\leqslant 4\pi CA\int_0^\infty \mathrm{d}R'\ R'^2\,\mathrm{e}^{-\beta|R'-L_0|}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}} \\
&\leqslant 4\pi CA\int_0^\infty \mathrm{d}R'\ R'^2\,\mathrm{e}^{-\beta|R'-L_0|}\,\mathrm{e}^{-\frac{R'^2}{4\sigma'^2}} \\
&= 4\pi CA\int_0^{L_0} \mathrm{d}R'\ R'^2\ \mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\,\mathrm{e}^{-\beta(L_0-R')}
\end{aligned}$$

$$+ 4\pi CA \int_{L_0}^{\infty} \mathrm{d}R'\ R'^2\, \mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\, \mathrm{e}^{-\beta(R'-L_0)}. \tag{3.350}$$

Consider the first term on right-hand side of inequality (3.350), to obtain

$$\begin{aligned} 4\pi CA \int_{0}^{L_0} \mathrm{d}R'\ R'^2\ \mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\, \mathrm{e}^{-\beta(L_0-R')} \leqslant& 4\pi CA \int_{0}^{L_0} \mathrm{d}R'\ R'^2\, \mathrm{e}^{-\beta L_0} \\ \leqslant& \frac{4\pi CA\, L_0^3}{3}\, \mathrm{e}^{-\beta L_0} \end{aligned} \tag{3.351}$$

where

$$\mathrm{e}^{\beta R'}\ \mathrm{e}^{-\frac{R'^2}{4\sigma'^2}} = \mathrm{e}^{-R'^2(\frac{1}{4\sigma'^2}-\frac{\beta}{R'})} \leqslant\ 1. \tag{3.352}$$

Consider the second term on right-hand side of inequality (3.350), let $X = R' - L_0$, to obtain

$$\begin{aligned} &4\pi CA \int_{L_0}^{\infty} \mathrm{d}R'\ R'^2\, \mathrm{e}^{-\frac{R'^2}{4\sigma'^2}}\, \mathrm{e}^{-\beta(R'-L_0)} \\ \leqslant& 4\pi CA \int_{0}^{\infty} \mathrm{d}R'\ R'^2\, \mathrm{e}^{-\frac{(X+L_0)^2}{4\sigma'^2}}\, \mathrm{e}^{-\beta X} \\ =& 4\pi CA \int_{0}^{\infty} \mathrm{d}R'\ R'^2\, \mathrm{e}^{-\frac{X^2+L_0^2-2XL_0}{4\sigma'^2}}\, \mathrm{e}^{-\beta X} \\ \leqslant& 4\pi CA \int_{0}^{\infty} \mathrm{d}R'\ R'^2\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \\ =& 4\pi CA\, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \lim_{R'\to\infty} \frac{R'^3}{3} \end{aligned} \tag{3.353}$$

where $\mathrm{e}^{-\beta X}\mathrm{e}^{-\frac{X'^2+2X'L_0'}{4\sigma'^2}} \leqslant 1$ is given by (3.347).

Substitute (3.352) and (3.353) into the right-hand side of inequality (3.350), to

obtain

$$\left|\int \mathrm{d}^3\mathbf{r}'\ [\phi(\mathbf{r}'-\mathbf{L}')]^*\ [\psi(\mathbf{r}'-\mathbf{L})]\right| \leqslant \frac{4\pi C A\, L_0^3}{3}\,\mathrm{e}^{-\beta L_0} + 4\pi C A\,\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\left[\lim_{R'\to\infty}\frac{R'^3}{3}\right] \tag{3.354}$$

which vanishes very rapidly for $L_0 \to \infty$.

Refer to (3.350), for $L_0 \to \infty$ to write as a limit

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}'\ [\phi(\mathbf{r}'-\mathbf{L}')]^*\ [\psi(\mathbf{r}'-\mathbf{L})]\right] = 0. \tag{3.355}$$

Refer to the integrations in (3.264)–(3.355), for $\mathbf{L} \neq \mathbf{L}'$ and $L_0, L_0' \to \infty$, to obtain the limit :

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\,\nabla\phi^*\left(\mathbf{r}-\mathbf{L}'\right)\cdot\nabla\phi\left(\mathbf{r}-\mathbf{L}\right)\right] = 0, \tag{3.356a}$$

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\,\nabla\psi^*(\mathbf{r}-\mathbf{L})\cdot\nabla\phi\left(\mathbf{r}-\mathbf{L}'\right)\right] = 0, \tag{3.356b}$$

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\,\nabla\phi^*(\mathbf{r}-\mathbf{L}')\cdot\nabla\psi(\mathbf{r}-\mathbf{L})\right] = 0, \tag{3.356c}$$

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}'\,\nabla\psi^*(\mathbf{r}'-\mathbf{L})\cdot\nabla\phi\left(\mathbf{r}'-\mathbf{L}'\right)\right] = 0, \tag{3.356d}$$

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}'\,\nabla\phi^*\left(\mathbf{r}'-\mathbf{L}'\right)\cdot\nabla\psi(\mathbf{r}'-\mathbf{L})\right] = 0, \tag{3.356e}$$

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\ [\psi(\mathbf{r}-\mathbf{L})]^*\ [\phi(\mathbf{r}-\mathbf{L}')]\right] = 0, \tag{3.356f}$$

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\ [\phi(\mathbf{r}-\mathbf{L}')]^*\ [\psi(\mathbf{r}-\mathbf{L})]\right] = 0, \tag{3.356g}$$

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}'\ [\psi(\mathbf{r}'-\mathbf{L})]^*\ [\phi(\mathbf{r}'-\mathbf{L}')]\right] = 0, \tag{3.356h}$$

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}'\ [\phi(\mathbf{r}'-\mathbf{L}')]^*\ [\psi(\mathbf{r}'-\mathbf{L})]\right]=0, \tag{3.356i}$$

and

$$\lim_{L_0\to\infty}\left[-\int \mathrm{d}^3\mathbf{r}\,\nabla\psi^*(\mathbf{r}-\mathbf{L})\cdot\nabla\phi\,(\mathbf{r}-\mathbf{L}')\int \mathrm{d}^3\mathbf{r}'\ [\phi(\mathbf{r}'-\mathbf{L}')]^*\ [\psi(\mathbf{r}'-\mathbf{L})]\right]=0, \tag{3.357a}$$

$$\lim_{L_0\to\infty}\left[-\int \mathrm{d}^3\mathbf{r}\,\nabla\phi^*(\mathbf{r}-\mathbf{L}')\cdot\nabla\psi(\mathbf{r}-\mathbf{L})\int \mathrm{d}^3\mathbf{r}'\ [\psi(\mathbf{r}'-\mathbf{L})]^*\ [\phi(\mathbf{r}'-\mathbf{L}')]\right]=0, \tag{3.357b}$$

$$\lim_{L_0\to\infty}\left[-\int \mathrm{d}^3\mathbf{r}'\,\nabla\phi^*\,(\mathbf{r}'-\mathbf{L}')\cdot\nabla\psi(\mathbf{r}'-\mathbf{L})\int \mathrm{d}^3\mathbf{r}\ [\psi(\mathbf{r}-\mathbf{L})]^*\ [\phi(\mathbf{r}-\mathbf{L}')]\right]=0, \tag{3.357c}$$

$$\lim_{L_0\to\infty}\left[-\int \mathrm{d}^3\mathbf{r}'\,\nabla\psi^*(\mathbf{r}'-\mathbf{L})\cdot\nabla\phi\,(\mathbf{r}'-\mathbf{L}')\int \mathrm{d}^3\mathbf{r}\ [\phi(\mathbf{r}-\mathbf{L}')]^*\ [\psi(\mathbf{r}-\mathbf{L})]\right]=0, \tag{3.357d}$$

from (3.279), with $\mathbf{L}'=\mathbf{L}$ for small kinetic energy $k'\to 0$, hence

$$\lim_{L_0,L_0',k'\to 0}\left[\int \mathrm{d}^3\mathbf{r}\,\nabla\phi\,(\mathbf{r}-\mathbf{L})^*\cdot\nabla\phi\,(\mathbf{r}-\mathbf{L})\right]=0 \tag{3.358}$$

as a limit, and by referring to (3.117)–(3.119), with $\mathbf{L}=\mathbf{L}'$, we obtain

$$\lim_{L_0\to 0}\left[\int \mathrm{d}^3\mathbf{r}\nabla\,[\psi(\mathbf{r}-\mathbf{L})\,]^*\cdot\nabla\,[\psi(\mathbf{r}-\mathbf{L})\,]\right]=\beta^2. \tag{3.359}$$

For $\mathbf{L}\neq\mathbf{L}'$, and $L_0\to\infty$ to write as a limit

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\nabla\,[\psi(\mathbf{r}-\mathbf{L})\,]^*\cdot\nabla\,[\psi(\mathbf{r}-\mathbf{L}')\,]\right]=0 \tag{3.360}$$

and hence, for $\mathbf{L} \neq \mathbf{L}'$, and $L_0 \to \infty$ to write as a limit

$$\lim_{L_0 \to \infty} \left[\int \mathrm{d}^3\mathbf{r} \, [\, \psi(\mathbf{r} - \mathbf{L})] \; [\, \psi(\mathbf{r} - \mathbf{L}')] \right] = 0. \tag{3.361}$$

By using (3.356)–(3.361), let $\mathbf{r}_1 = \mathbf{r}$, $\mathbf{r}_2 = \mathbf{r}'$, $\mathbf{L}_1 = \mathbf{L}$, $\mathbf{L}_2 = \mathbf{L}'$ $\mathbf{L}_0 = \mathbf{L}' - \mathbf{L}$ and $L_0 \to \infty$, as applied to the right-hand side of (3.261) with normalized spin, we can rewrite as

$$\begin{aligned}
\langle \Psi | \frac{\mathbf{p}_1^2}{2m} | \Psi \rangle =& \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \left(\nabla_1 \left[\psi(\mathbf{r}_1 - \mathbf{L}_1) \right]^* \cdot \nabla_1 \left[\psi(\mathbf{r}_1 - \mathbf{L}_1) \right] \right) (\chi_a^* \cdot \chi_a) \\
&+ \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \left(\nabla_1 \left[\phi(\mathbf{r}_1 - \mathbf{L}_2) \right]^* \cdot \nabla_1 \left[\phi(\mathbf{r}_1 - \mathbf{L}_2) \right] \right) (\chi_b^* \cdot \chi_b) \\
&- \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \nabla_1 \left[\psi(\mathbf{r}_1 - \mathbf{L}_1) \right]^* \cdot \nabla_1 \left[\phi(\mathbf{r}_1 - \mathbf{L}_2) \right] \\
&\quad \times \int \mathrm{d}^3\mathbf{r}_2 \, \left[\phi(\mathbf{r}_2 - \mathbf{L}_2) \right]^* \left[\psi(\mathbf{r}_2 - \mathbf{L}_1) \right] (\chi_a^* \cdot \chi_b) \\
&- \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \nabla_1 \left[\phi(\mathbf{r}_1, -\mathbf{L}_2) \right]^* \cdot \nabla_1 \left[\psi(\mathbf{r}_1 - \mathbf{L}_1) \right] \\
&\quad \times \int \mathrm{d}^3\mathbf{r}_2 \left[\psi(\mathbf{r}_2 - \mathbf{L}_1) \right]^* \left[\phi(\mathbf{r}_2 - \mathbf{L}_2) \right] (\chi_a^* \cdot \chi_b) \\
=& \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \left(\nabla_1 \left[\psi(\mathbf{r}_1 - \mathbf{L}_1) \right]^* \cdot \nabla_1 \left[\psi(\mathbf{r}_1 - \mathbf{L}_1) \right] \right) \delta_{aa} \\
&+ \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \left(\nabla_1 \left[\phi(\mathbf{r}_1 - \mathbf{L}_2) \right]^* \cdot \nabla_1 \left[\phi(\mathbf{r}_1 - \mathbf{L}_2) \right] \right) \delta_{bb} \\
&- \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \nabla_1 \left[\psi(\mathbf{r}_1 - \mathbf{L}_1) \right]^* \cdot \nabla_1 \left[\phi(\mathbf{r}_1 - \mathbf{L}_2) \right] \\
&\quad \times \int \mathrm{d}^3\mathbf{r}_2 \, \left[\phi(\mathbf{r}_2 - \mathbf{L}_2) \right]^* \left[\psi(\mathbf{r}_2 - \mathbf{L}_1) \right] \delta_{ab} \\
&- \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_1 \, \nabla_1 \left[\phi(\mathbf{r}_1, -\mathbf{L}_2) \right]^* \cdot \nabla_1 \left[\psi(\mathbf{r}_1 - \mathbf{L}_1) \right]
\end{aligned}$$

$$\times \int \mathrm{d}^3\mathbf{r}_2 \, [\psi(\mathbf{r}_2 - \mathbf{L}_1)]^* \; [\phi(\mathbf{r}_2 - \mathbf{L}_2)] \, \delta_{ab}$$

$$\leqslant \frac{\hbar^2 \beta^2}{4m} + 0 \tag{3.362}$$

and hence

$$\begin{aligned}
\langle \Psi | \frac{\mathbf{p}_2^2}{2m} | \Psi \rangle =& \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_2 \; (\nabla_2 [\phi(\mathbf{r}_2 - \mathbf{L}_2)]^* \cdot \nabla_2 [\phi(\mathbf{r}_2 - \mathbf{L}_2)]) \, \delta_{aa} \\
&+ \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_2 \; (\nabla_2 [\psi(\mathbf{r}_2 - \mathbf{L}_1)]^* \cdot \nabla_2 [\psi(\mathbf{r}_2 - \mathbf{L}_1)]) \, \delta_{aa} \\
&- \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_2 \, \nabla_2 [\phi(\mathbf{r}_2 - \mathbf{L}_2)]^* \cdot \nabla_2 [\psi(\mathbf{r}_2 - \mathbf{L}_1)] \\
&\times \int \mathrm{d}^3\mathbf{r}_1 \; [\psi(\mathbf{r}_1 - \mathbf{L}_1)]^* \; [\phi(\mathbf{r}_1 - \mathbf{L}_2)] \, \delta_{ab} \\
&- \frac{\hbar^2}{4m} \int \mathrm{d}^3\mathbf{r}_2 \, \nabla_2 [\psi(\mathbf{r}_2 - \mathbf{L}_1)]^* \cdot \nabla_2 [\phi(\mathbf{r}_2 - \mathbf{L}_2)] \\
&\times \int \mathrm{d}^3\mathbf{r}_1 \; [\phi(\mathbf{r}_1 - \mathbf{L}_2)]^* \; [\psi(\mathbf{r}_1 - \mathbf{L}_1)] \, \delta_{ab} \\
\leqslant& \frac{\hbar^2 \beta^2}{4m} + 0.
\end{aligned} \tag{3.363}$$

From (3.362) and (3.363), we obtain the expectation value of kinetic energy of the system which consists of one nucleus, one bound electron and one free electron :

$$\begin{aligned}
\langle \Psi | \sum_{i=1}^{2} \frac{\mathbf{p}_i^2}{2m} | \Psi \rangle &= \langle \Psi | \frac{\mathbf{p}_1^2}{2m} | \Psi \rangle + \langle \Psi | \frac{\mathbf{p}_2^2}{2m} | \Psi \rangle \\
&\leqslant \frac{\hbar^2 \beta^2}{2m}.
\end{aligned} \tag{3.364}$$

The expectation value of kinetic energy of of the system which consists of k nuclei, k bound electrons, and $(N-k)$ free electrons with the latter with vanishingly small kinetic energies :

$$\langle\Psi|\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}|\Psi\rangle=\langle\Psi|\frac{\mathbf{p}_1^2}{2m}|\Psi\rangle+\langle\Psi|\frac{\mathbf{p}_2^2}{2m}|\Psi\rangle+\ldots+\langle\Psi|\frac{\mathbf{p}_N^2}{2m}|\Psi\rangle$$

$$\leqslant\sum_{i=1}^{k}\frac{\hbar^2\beta^2}{2m}. \tag{3.365}$$

To obtain the bound of following integral function we let $\mathbf{R}=\mathbf{r}-\mathbf{L}$, to obtain

$$\begin{aligned}\int \mathrm{d}^3\mathbf{r}\,\phi^*(\mathbf{r}-\mathbf{L})\cdot\frac{\phi(\mathbf{r}-\mathbf{L})}{|\mathbf{r}-\mathbf{L}|} =& A^2\int \mathrm{d}^3\mathbf{r}\,\mathrm{e}^{-\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}-\mathbf{L})}\,\mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L})^2}{4\sigma'^2}}\cdot\frac{\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}-\mathbf{L})}\,\mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L})^2}{4\sigma'^2}}}{|\mathbf{r}-\mathbf{L}|}\\
=& A^2\int \mathrm{d}^3\mathbf{r}\,\frac{\mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L})^2}{2\sigma'^2}}}{|\mathbf{r}-\mathbf{L}|}\\
=& A^2\int \mathrm{d}^3\mathbf{R}\,\frac{\mathrm{e}^{-\frac{\mathbf{R}^2}{2\sigma'^2}}}{|\mathbf{R}|}\\
=& 4\pi A^2\int_0^\infty \mathrm{d}R\,R^2\,\frac{\mathrm{e}^{-\frac{R^2}{2\sigma'^2}}}{R}\\
=& 4\pi A^2\int_0^\infty \mathrm{d}R\,R\mathrm{e}^{-\frac{R^2}{2\sigma'^2}}\\
=& 4\pi A^2\left(-\frac{2\sigma'^2}{2}\,\mathrm{e}^{-\frac{R^2}{2\sigma'^2}}\Big|_0^\infty\right)\\
=& 4\pi A^2\sigma'^2\\
\geqslant& 0.\end{aligned} \tag{3.366}$$

This gives

$$-\int \mathrm{d}^3\mathbf{r}\,\phi^*(\mathbf{r}-\mathbf{L})\cdot\frac{\phi(\mathbf{r}-\mathbf{L})}{|\mathbf{r}-\mathbf{L}|}\leqslant 0. \tag{3.367}$$

Again, let $\mathbf{R} = \mathbf{r} - \mathbf{L}$, $\mathbf{L}_0 = \mathbf{L}' - \mathbf{L}$ and $\mathbf{L}_0' = \mathbf{L} - \mathbf{L}'$, to obtain

$$\begin{aligned}
&\left| \int \mathrm{d}^3\mathbf{r}\, \phi^* \left(\mathbf{r} - \mathbf{L}'\right) \cdot \frac{\phi\left(\mathbf{r} - \mathbf{L}'\right)}{|\mathbf{r} - \mathbf{L}|} \right| \\
&= A^2 \left| \int \mathrm{d}^3\mathbf{r}\, \mathrm{e}^{-\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}-\mathbf{L}')}\, \mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L}')^2}{4\sigma'^2}} \cdot \frac{\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}-\mathbf{L}')}\, \mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L}')^2}{4\sigma'^2}}}{|\mathbf{r} - \mathbf{L}|} \right| \\
&= A^2 \left| \int \mathrm{d}^3\mathbf{r} \frac{\mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L}')^2}{2\sigma'^2}}}{|\mathbf{r} - \mathbf{L}|} \right| \\
&= A^2 \left| \int \mathrm{d}^3\mathbf{R} \frac{\mathrm{e}^{-\frac{(\mathbf{R}+\mathbf{L}-\mathbf{L}')^2}{2\sigma'^2}}}{|\mathbf{R}|} \right| \\
&= A^2 \left| \int \mathrm{d}^3\mathbf{R} \frac{\mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0')^2}{2\sigma'^2}}}{|\mathbf{R}|} \right| \\
&= A^2 \left| \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int \mathrm{d}^3\mathbf{R} \frac{\mathrm{e}^{-\frac{R^2+2RL_0\cos\theta}{2\sigma'^2}}}{R} \right| \\
&\leqslant A^2 \left| \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int_0^\infty \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-\frac{R^2-2RL_0}{2\sigma'^2}} \right| \\
&= 4\pi A^2 \left| \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int_0^\infty \mathrm{d}R\, R\, \mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}} \right| \\
&\leqslant 4\pi A^2 \left| \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int_0^{L_0} \mathrm{d}R\, L_0\, \mathrm{e}^{\frac{R(2L_0-R)}{4\sigma'^2}} + \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int_0^{L_0} \mathrm{d}R\, L_0\, \mathrm{e}^{\frac{R(2L_0-R)}{4\sigma'^2}} \right| \\
&= 4\pi A^2 \left| \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int_0^\infty \mathrm{d}R\, R\, \mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}} \right| \\
&\leqslant 4\pi A^2 \left| \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int_0^{L_0} \mathrm{d}R\, L_0\, \mathrm{e}^{\frac{R(2L_0-R)}{4\sigma'^2}} + \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int_0^\infty \mathrm{d}R\, R\, \mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}} \right|. \qquad (3.368)
\end{aligned}$$

By optimizing $R(R+2L_0)$ over R, we obtain

$$\frac{\partial}{\partial R}R(2L_0-R)=2R-2L_0=0\rightarrow R=L_0 \tag{3.369}$$

substitute $R=L_0$ and $X=(R-2L_0)$ into the right-hand of inequality (3.368), to obtain

$$\begin{aligned}
&\left|\int \mathrm{d}^3\mathbf{r}\,\phi^*\left(\mathbf{r}-\mathbf{L}'\right)\cdot\frac{\phi\left(\mathbf{r}-\mathbf{L}'\right)}{|\mathbf{r}-\mathbf{L}|}\right| \\
&\leqslant 4\pi A^2\left|\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\int_0^{L_0}\mathrm{d}R\,L_0+\mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}}\int_0^{\infty}\mathrm{d}R\,R\,\mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}}\right| \\
&=4\pi A^2\left|\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\int_0^{L_0}\mathrm{d}R\,L_0+\mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}}\int_0^{\infty}\mathrm{d}(X+2L_0)\,(X+2L_0)\,\mathrm{e}^{-\frac{(X+2L_0)X}{4\sigma'^2}}\right| \\
&\leqslant 4\pi A^2\left|\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\int_0^{L_0}\mathrm{d}R\,L_0+\mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}}\int_{2L_0}^{\infty}\mathrm{d}u\,u\,\mathrm{e}^{-\frac{uX}{4\sigma'^2}}\right|\ ,\ u=(X+2L_0)
\end{aligned} \tag{3.370}$$

which vanishes very rapidly for $L_0\rightarrow\infty$.

From (3.370), for $L_0\rightarrow\infty$, to write as a limit

$$\lim_{L_0\rightarrow\infty}\left[\left|\int \mathrm{d}^3\mathbf{r}\,\phi^*\left(\mathbf{r}-\mathbf{L}'\right)\cdot\frac{\phi\left(\mathbf{r}-\mathbf{L}'\right)}{|\mathbf{r}-\mathbf{L}|}\right|\right]=0, \tag{3.371a}$$

$$\lim_{L_0\rightarrow\infty}\left[\int \mathrm{d}^3\mathbf{r}\,\phi^*\left(\mathbf{r}-\mathbf{L}'\right)\cdot\frac{\phi\left(\mathbf{r}-\mathbf{L}'\right)}{|\mathbf{r}-\mathbf{L}|}\right]=0, \tag{3.371b}$$

$$\lim_{L_0\rightarrow\infty}\left[-\int \mathrm{d}^3\mathbf{r}\,\phi^*\left(\mathbf{r}-\mathbf{L}'\right)\cdot\frac{\phi\left(\mathbf{r}-\mathbf{L}'\right)}{|\mathbf{r}-\mathbf{L}|}\right]=0. \tag{3.371c}$$

Let $\mathbf{R}=\mathbf{r}-\mathbf{L}$ and $\mathbf{L}_0=\mathbf{L}'-\mathbf{L}$, to obtain

$$\begin{aligned}
\int \mathrm{d}^3\mathbf{r}\,\psi^*\left(\mathbf{r}-\mathbf{L}\right)\cdot\frac{\phi\left(\mathbf{r}-\mathbf{L}'\right)}{|\mathbf{r}-\mathbf{L}|}=&CA\int \mathrm{d}^3\mathbf{r}\,\mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}|}\cdot\frac{\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{r}-\mathbf{L}')}\,\mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L}')^2}{4\sigma'^2}}}{|\mathbf{r}-\mathbf{L}|} \\
=&CA\int \mathrm{d}^3\mathbf{R}\,\mathrm{e}^{-\beta|\mathbf{R}|}\cdot\frac{\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{R}+\mathbf{L}-\mathbf{L}')}\,\mathrm{e}^{-\frac{(\mathbf{R}+\mathbf{L}-\mathbf{L}')^2}{4\sigma'^2}}}{|\mathbf{R}|}
\end{aligned}$$

$$=CA\int \mathrm{d}^3\mathbf{R}\,\mathrm{e}^{-\beta|\mathbf{R}|}\cdot\frac{\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{R}-\mathbf{L}_0)}\,\mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}}}{|\mathbf{R}|}. \tag{3.372}$$

From (3.372), we can rewrite

$$\begin{aligned}\left|\int \mathrm{d}^3\mathbf{r}\,\psi^*(\mathbf{r}-\mathbf{L})\cdot\frac{\phi(\mathbf{r}-\mathbf{L}')}{|\mathbf{r}-\mathbf{L}|}\right| &= \left|CA\int \mathrm{d}^3\mathbf{R}\,\mathrm{e}^{-\beta|\mathbf{R}|}\cdot\frac{\mathrm{e}^{\mathrm{i}\,\mathbf{k'}\cdot(\mathbf{R}-\mathbf{L}_0)}\,\mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}}}{|\mathbf{R}|}\right| \\
&= \left|CA\int \mathrm{d}^3\mathbf{R}\,\mathrm{e}^{-\beta|\mathbf{R}|}\cdot\frac{\mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}}}{|\mathbf{R}|}\right| \\
&= CA\left|\int \mathrm{d}^3\mathbf{R}\,\mathrm{e}^{-\beta|\mathbf{R}|}\frac{\mathrm{e}^{-\frac{\left(R^2+L_0^2-2RL_0\cos\theta\right)}{4\sigma'^2}}}{|\mathbf{R}|}\right| \\
&\leqslant CA\left|\int \mathrm{d}^3\mathbf{R}\frac{\mathrm{e}^{-\beta|\mathbf{R}|}}{|\mathbf{R}|}\,\mathrm{e}^{-\frac{R^2+L_0^2-RL_0}{4\sigma'^2}}\right| \\
&= CA\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\left|\int \mathrm{d}^3\mathbf{R}\frac{\mathrm{e}^{-\beta|\mathbf{R}|}}{|\mathbf{R}|}\,\mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}}\right| \\
&= 4\pi CA\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\left|\int_0^\infty \mathrm{d}R\,R^2\frac{\mathrm{e}^{-\beta R}}{R}\,\mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}}\right| \\
&\leqslant 4\pi CA\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\left|\int_0^\infty \mathrm{d}R\,R\,\mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}}\right| \\
&\leqslant 4\pi CA\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\left|\int_0^{L_0} \mathrm{d}R\,L_0\,\mathrm{e}^{\frac{R(2L_0-R)}{4\sigma'^2}}\right. \\
&\qquad\left.+\int_{L_0}^\infty \mathrm{d}R\,R\,\mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}}\right|.\end{aligned} \tag{3.373}$$

Consider the right-hand side of inequality (3.373), optimize $R(2L_0-R)$ over R, to obtain

$$\frac{\partial}{\partial R}R(2L_0-R) = 2L_0-2R = 0 \rightarrow R = L_0 \tag{3.374}$$

and

$$\frac{\partial^2}{\partial R^2} R(2L_0 - R) = -2 \quad , \qquad \mathrm{e}^{\frac{L_0^2}{4\sigma'^2}} \leqslant \mathrm{e}^{\frac{L_0^2}{8\sigma'^2}} . \tag{3.375}$$

Substitute $R = L_0$ into the first term on the right-hand side of inequality (3.373), to obtain

$$\begin{aligned} 4\pi C A \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \int_0^{L_0} \mathrm{d}R \, L_0 \, \mathrm{e}^{\frac{R(2L_0-R)}{4\sigma'^2}} \leqslant & 4\pi C A \, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \mathrm{e}^{\frac{L_0^2}{8\sigma'^2}} \int_0^{L_0} \mathrm{d}R \; L_0^2 \\ = & 4\pi C A \, \mathrm{e}^{-\frac{L_0^2}{8\sigma'^2}} \int_0^{L_0} \mathrm{d}R \; L_0 \\ = & \frac{4\pi C A L_0^2}{2} \, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} . \end{aligned} \tag{3.376}$$

Consider the second term on the right-hand side of inequality (3.373), let $X = R - 2L_0$, to obtain

$$\begin{aligned} & 4\pi C A \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \int_{L_0}^{\infty} \mathrm{d}R \; R \, \mathrm{e}^{-\frac{R(R-2L_0)}{4\sigma'^2}} \\ & \leqslant 4\pi C A \, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \int_0^{\infty} \mathrm{d}(X + 2L_0) \; (X + 2L_0) \, \mathrm{e}^{-\frac{X(X+2L_0)}{4\sigma'^2}} \\ & \leqslant 4\pi C A \int_0^{\infty} \mathrm{d}(X + 2L_0) \; (X + 2L_0) \, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \, \mathrm{e}^{-\frac{uX}{4\sigma'^2}} \\ & = 4\pi C A \, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \int_{2L_0}^{\infty} \mathrm{d}u \, u \, \mathrm{e}^{-\frac{uX}{4\sigma'^2}} . \end{aligned} \tag{3.377}$$

Substitute (3.376) and (3.378) into the right-hand side of inequality (3.373), to obtain

$$\begin{aligned} \left| \int \mathrm{d}^3\mathbf{r} \, \psi^* \left(\mathbf{r} - \mathbf{L} \right) \cdot \frac{\phi \left(\mathbf{r} - \mathbf{L}' \right)}{|\mathbf{r} - \mathbf{L}|} \right| \leqslant & \left| \frac{4\pi C A L_0^2}{2} \, \mathrm{e}^{-\frac{L_0^2}{8\sigma'^2}} \right. \\ & \left. + \, 4\pi C A \, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \int_{2L_0}^{\infty} \mathrm{d}u \, u \, \mathrm{e}^{-\frac{uX}{4\sigma'^2}} \right| \end{aligned} \tag{3.378}$$

which vanishes very rapidly for $L_0 \to \infty$.

Refer to (3.378), for $L_0 \to \infty$, to write as a limit

$$\lim_{L_0 \to \infty} \left[\int \mathrm{d}^3\mathbf{r}\, \psi^* \left(\mathbf{r} - \mathbf{L}\right) \cdot \frac{\phi\left(\mathbf{r} - \mathbf{L}'\right)}{|\mathbf{r} - \mathbf{L}|} \right] = 0 \tag{3.379}$$

and hence

$$\lim_{L_0 \to \infty} \left[\int \mathrm{d}^3\mathbf{r}\, \phi^* \left(\mathbf{r} - \mathbf{L}'\right) \cdot \frac{\psi\left(\mathbf{r} - \mathbf{L}\right)}{|\mathbf{r} - \mathbf{L}|} \right]. = 0 \tag{3.380}$$

To obtain a bound for the following integral function we let $\mathbf{x} = \mathbf{r} - \mathbf{L}'$, to get

$$\begin{aligned}
&\left| \int \mathrm{d}^3\mathbf{r}\, \phi^* \left(\mathbf{r} - \mathbf{L}\right) \cdot \frac{\phi\left(\mathbf{r} - \mathbf{L}\right)}{|\mathbf{r} - \mathbf{L}'|} \right| \\
&= \left| A^2 \int \mathrm{d}^3\mathbf{r}\, \mathrm{e}^{-\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{r}-\mathbf{L}')}\, \mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L})^2}{4\sigma'^2}} \cdot \frac{\mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{r}-\mathbf{L})}\, \mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L})^2}{4\sigma'^2}}}{|\mathbf{r} - \mathbf{L}'|} \right| \\
&= \left| A^2 \int \mathrm{d}^3\mathbf{r} \frac{\mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L})^2}{2\sigma'^2}}}{|\mathbf{r} - \mathbf{L}|} \right| \\
&= \left| A^2 \int \mathrm{d}^3\mathbf{x} \frac{\mathrm{e}^{-\frac{(\mathbf{x}+\mathbf{L}'-\mathbf{L})^2}{2\sigma'^2}}}{|\mathbf{x}|} \right| \\
&= \left| A^2 \int \mathrm{d}^3\mathbf{x} \frac{\mathrm{e}^{-\frac{(\mathbf{x}-\mathbf{L}'_0)^2}{2\sigma'^2}}}{|\mathbf{x}|} \right| \\
&= A^2\, \mathrm{e}^{-\frac{L_0'^2}{2\sigma'^2}} \left| \int_0^\infty \mathrm{d}^3\mathbf{x} \frac{\mathrm{e}^{-\frac{x^2 - 2xL'_0 \cos\theta}{2\sigma'^2}}}{x} \right| \\
&\leqslant A^2\, \mathrm{e}^{-\frac{L_0'^2}{2\sigma'^2}} \left| \int_0^\infty \mathrm{d}^3\mathbf{x}\, \mathrm{e}^{-\frac{x^2 - 2xL'_0}{2\sigma'^2}} \right| \\
&= 4\pi A^2\, \mathrm{e}^{-\frac{L_0'^2}{2\sigma'^2}} \left| \int_0^\infty \mathrm{d}x\, x\, \mathrm{e}^{-\frac{x(x-2L'_0)}{2\sigma'^2}} \right|
\end{aligned}$$

$$\leqslant 4\pi A^2\, e^{-\frac{L'^2_0}{2\sigma'^2}} \left| \int_0^{L'_0} dx\, L'_0\, e^{-\frac{x(x-2L'_0)}{2\sigma'^2}} + \int_{L'_0}^{\infty} dx\, x\, e^{-\frac{x(x-2L'_0)}{2\sigma'^2}} \right|$$

$$\leqslant 4\pi A^2 \left| e^{-\frac{L'^2_0}{4\sigma'^2}} \int_0^{L'_0} dx\, L'_0 + e^{-\frac{L'^2_0}{2\sigma'^2}} \int_{L'_0}^{\infty} dx\, x\, e^{-\frac{x(x-2L'_0)}{2\sigma'^2}} \right| \ , e^{-\frac{x(x-2L'_0)}{2\sigma'^2}} \leqslant e^{\frac{L'^2_0}{4\sigma'^2}}$$

$$= 4\pi A^2\, e^{-\frac{L'^2_0}{4\sigma'^2}} \left| \frac{L'^2_0}{2} + 4\pi A^2\, e^{-\frac{L'^2_0}{2\sigma'^2}} \int_{L'_0}^{\infty} dx\, x\, e^{-\frac{x(x-2L'_0)}{2\sigma'^2}} \right| \ , X = (x - 2L'_0)$$

$$= 4\pi A^2 \left| e^{-\frac{L'^2_0}{4\sigma'^2}} \frac{L'^2_0}{2} + e^{-\frac{L'^2_0}{2\sigma'^2}} \int_0^{\infty} d(X + 2L_0)\, (X + 2L'_0)\, e^{-\frac{(X+2L'_0)X}{2\sigma'^2}} \right|$$

$$= 4\pi A^2 \left| e^{-\frac{L'^2_0}{4\sigma'^2}} \frac{L'^2_0}{2} + e^{-\frac{L'^2_0}{2\sigma'^2}} \int_{2L_0}^{\infty} du\, u\, e^{-\frac{uX}{2\sigma'^2}} \right| \ , u = (X + 2L'_0) \qquad (3.381)$$

which vanishes very rapidly for $L'_0 \to \infty$.

From (3.381), for $L'_0 \to \infty$ to write as a limit

$$\lim_{L_0 \to \infty} \left[\left| \int d^3\mathbf{r}\, \phi^*(\mathbf{r} - \mathbf{L}) \cdot \frac{\phi(\mathbf{r} - \mathbf{L})}{|\mathbf{r} - \mathbf{L}'|} \right| \right] = 0 \qquad (3.382)$$

and hence

$$\lim_{L_0 \to \infty} \left[\int d^3\mathbf{r}\, \phi^*(\mathbf{r} - \mathbf{L}) \cdot \frac{\phi(\mathbf{r} - \mathbf{L})}{|\mathbf{r} - \mathbf{L}'|} \right] = 0. \qquad (3.383)$$

Again, let $\mathbf{x}' = \mathbf{r}' - \mathbf{L}$, and $\mathbf{L}'_0 = \mathbf{L} - \mathbf{L}'$, to get

$$\left| \int d^3\mathbf{r}'\, \phi^*(\mathbf{r}' - \mathbf{L}') \cdot \frac{\phi(\mathbf{r}' - \mathbf{L}')}{|\mathbf{r}' - \mathbf{L}|} \right|$$

$$= A^2 \left| \int d^3\mathbf{r}'\, e^{-i\,\mathbf{k}'\cdot(\mathbf{r}'-\mathbf{L}')}\, e^{-\frac{(\mathbf{r}'-\mathbf{L}')^2}{4\sigma'^2}} \cdot \frac{e^{i\,\mathbf{k}'\cdot(\mathbf{r}'-\mathbf{L}')}\, e^{-\frac{(\mathbf{r}'-\mathbf{L}')^2}{4\sigma'^2}}}{|\mathbf{r} - \mathbf{L}|} \right|$$

$$= A^2 \left| \int d^3\mathbf{r}'\, \frac{e^{-\frac{(\mathbf{r}'-\mathbf{L}')^2}{2\sigma'^2}}}{|\mathbf{r}' - \mathbf{L}|} \right|$$

$$= A^2 \left| \int \mathrm{d}^3\mathbf{x}' \, \frac{\mathrm{e}^{-\frac{(\mathbf{x}'+\mathbf{L}-\mathbf{L}')^2}{2\sigma'^2}}}{|\mathbf{x}'|} \right|$$

$$= A^2 \left| \int \mathrm{d}^3\mathbf{x}' \, \frac{\mathrm{e}^{-\frac{(\mathbf{x}'-\mathbf{L}_0')^2}{2\sigma'^2}}}{|\mathbf{x}'|} \right|$$

$$= A^2 \, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \left| \int_0^\infty \mathrm{d}^3\mathbf{x}' \, \frac{\mathrm{e}^{-\frac{x'^2-2x'L_0\cos\theta}{2\sigma'^2}}}{x'} \right|$$

$$\leqslant A^2 \, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \left| \int_0^\infty \mathrm{d}^3\mathbf{x}' \, \mathrm{e}^{-\frac{x'^2-2x'L_0}{2\sigma'^2}} \right|$$

$$= 4\pi A^2 \, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \left| \int_0^\infty \mathrm{d}x' \, x' \, \mathrm{e}^{-\frac{x'(x'-2L_0)}{2\sigma'^2}} \right|$$

$$\leqslant 4\pi A^2 \, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \left| \int_0^{L_0} \mathrm{d}x \, L_0 \, \mathrm{e}^{-\frac{x'(x'-2L_0)}{2\sigma'^2}} + \int_{L_0}^\infty \mathrm{d}x' \, x' \, \mathrm{e}^{-\frac{x'(x'-2L_0)}{2\sigma'^2}} \right|$$

$$\leqslant 4\pi A^2 \left| \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \int_0^{L_0} \mathrm{d}x' \, L_0 + \, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int_{L_0}^\infty \mathrm{d}x' \, x' \, \mathrm{e}^{-\frac{x'(x'-2L_0)}{2\sigma'^2}} \right| \; , \mathrm{e}^{-\frac{x'(x'-2L_0)}{2\sigma'^2}} \leqslant \mathrm{e}^{\frac{L_0^2}{4\sigma'^2}}$$

$$= 4\pi A^2 \, \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \left| \frac{L_0^2}{2} + 4\pi A^2 \, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int_{L_0}^\infty \mathrm{d}x' \, x' \, \mathrm{e}^{-\frac{x'(x'-2L_0)}{2\sigma'^2}} \right| \; , X = (x' - 2L_0)$$

$$= 4\pi A^2 \left| \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \frac{L_0^2}{2} + \, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int_0^\infty \mathrm{d}(X + 2L_0) \, (X + 2L_0') \, \mathrm{e}^{-\frac{(X+2L_0)X}{2\sigma'^2}} \right|$$

$$= 4\pi A^2 \left| \mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}} \frac{L_0^2}{2} + \, \mathrm{e}^{-\frac{L_0^2}{2\sigma'^2}} \int_{2L_0}^\infty \mathrm{d}u \, u \, \mathrm{e}^{-\frac{uX}{2\sigma'^2}} \right| \; , u = (X + 2L_0) \tag{3.384}$$

which vanishes very rapidly for $L_0 \to \infty$. We note that

$$\frac{\partial}{\partial x'} \, x'(2L_0 - x') = 2L_0 - 2x' = 0 \to x' = L_0 \tag{3.385}$$

and (3.384), for $L_0 \to \infty$, we get

$$\left| \int \mathrm{d}^3\mathbf{r}' \, \phi^* \left(\mathbf{r}' - \mathbf{L}'\right) \cdot \frac{\phi\left(\mathbf{r}' - \mathbf{L}'\right)}{|\mathbf{r}' - \mathbf{L}|} \right| \leqslant 4\pi A^2 \sigma'^2 \mathrm{e}^{-\frac{L_0'^2}{2\sigma'^2}} \tag{3.386}$$

the right-hand side of inequality (3.386) is positive, so that we can rewrite (3.386) for $L_0, L_0' \to \infty$ as a limit

$$\lim_{L_0, L_0' \to \infty} \left[\int \mathrm{d}^3\mathbf{r}'\, \phi^*\left(\mathbf{r}' - \mathbf{L}'\right) \cdot \frac{\phi\left(\mathbf{r}' - \mathbf{L}'\right)}{\left|\mathbf{r}' - \mathbf{L}\right|} \right] = 0. \tag{3.387}$$

Let $\mathbf{R} = \mathbf{r} - \mathbf{L}$ and $\mathbf{L}_0 = \mathbf{L}' - \mathbf{L}$ to obtain

$$\begin{aligned}
\int \mathrm{d}^3\mathbf{r}\, \psi^*\left(\mathbf{r} - \mathbf{L}\right) \cdot \frac{\phi\left(\mathbf{r} - \mathbf{L}'\right)}{\left|\mathbf{r} - \mathbf{L}'\right|} &= CA \int \mathrm{d}^3\mathbf{r}\, \mathrm{e}^{-\beta|\mathbf{r}-\mathbf{L}|} \cdot \frac{\mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{r}-\mathbf{L}')}\, \mathrm{e}^{-\frac{(\mathbf{r}-\mathbf{L}')^2}{4\sigma'^2}}}{\left|\mathbf{r} - \mathbf{L}'\right|} \\
&= CA \int \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-\beta|\mathbf{R}|} \cdot \frac{\mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{R}+\mathbf{L}-\mathbf{L}')}\, \mathrm{e}^{-\frac{(\mathbf{R}+\mathbf{L}-\mathbf{L}')^2}{4\sigma'^2}}}{\left|\mathbf{R} + \mathbf{L} - \mathbf{L}'\right|} \\
&= CA \int \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-\beta|\mathbf{R}|} \cdot \frac{\mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{R}-\mathbf{L}_0)}\, \mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}}}{\left|\mathbf{R} - \mathbf{L_0}\right|}.
\end{aligned} \tag{3.388}$$

From (3.388), we can write

$$\begin{aligned}
\left| \int \mathrm{d}^3\mathbf{r}\, \psi^*\left(\mathbf{r} - \mathbf{L}\right) \cdot \frac{\phi\left(\mathbf{r} - \mathbf{L}'\right)}{\left|\mathbf{r} - \mathbf{L}\right|} \right| &= \left| CA \int \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-\beta|\mathbf{R}|} \cdot \frac{\mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{R}-\mathbf{L}_0)}\, \mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}}}{\left|\mathbf{R} - \mathbf{L_0}\right|} \right| \\
&= \left| CA \int \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-\beta|\mathbf{R}|} \cdot \frac{\mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}}}{\left|\mathbf{R} - \mathbf{L_0}\right|} \right| \\
&= CA \left| \int \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-\beta|\mathbf{R}|} \frac{\mathrm{e}^{-\frac{\left(R^2+L_0^2-2RL_0\cos\theta\right)}{4\sigma'^2}}}{\left|\mathbf{R} - \mathbf{L_0}\right|} \right| \\
&\leqslant CA \left| \int \mathrm{d}^3\mathbf{R} \frac{\mathrm{e}^{-\beta|\mathbf{R}|}}{\left|\mathbf{R} - \mathbf{L_0}\right|}\, \mathrm{e}^{-\frac{R^2+L_0^2-RL_0}{4\sigma'^2}} \right| \\
&= CA \int \mathrm{d}^3\mathbf{R} \frac{\mathrm{e}^{-\beta|\mathbf{R}|}}{\left|\mathbf{R} - \mathbf{L_o}\right|}\, \mathrm{e}^{-\frac{(R-L_0)^2}{4\sigma'^2}} \\
&\leqslant CA \int \mathrm{d}^3\mathbf{R} \frac{\mathrm{e}^{-\beta|\mathbf{R}|}}{\left|\mathbf{R} - \mathbf{L_o}\right|} \quad , \mathrm{e}^{-\frac{(R-L_0)^2}{4\sigma'^2}} \leqslant 1
\end{aligned}$$

$$
\begin{aligned}
=&4\pi CA \int_0^\infty \mathrm{d}R\, \frac{R^2}{R_>} \mathrm{e}^{-\beta R} \quad , R_> = \max(L_0, R) \\
=&\frac{4\pi CA}{L_0} \int_0^{L_0} \mathrm{d}R\, R^2\, \mathrm{e}^{-\beta R} + 4\pi CA \int_{L_0}^\infty \mathrm{d}R\, R\, \mathrm{e}^{-\beta R} \\
=&\frac{4\pi CA}{L_0} \left[-\frac{\mathrm{e}^{-\beta R}(2 + 2R\beta + R^2\beta^2)}{\beta^3} \right]_0^{L_0} \\
&+ 4\pi CA \left[-\frac{\mathrm{e}^{-\beta R}(1 + 2R\beta)}{\beta^2} \right]_{L_0}^\infty \\
=&\frac{8\pi CA}{L_0 \beta^2} + \frac{4\pi CA}{L_0}\, \mathrm{e}^{-\beta L_0} \left[\frac{(-2 + 2L_0\beta - L_0^2\beta^2)}{\beta^3} \right] \\
&+ 4\pi CA\, \mathrm{e}^{-\beta L_0} \frac{(1 + 2\beta L_0)}{\beta^2}
\end{aligned} \tag{3.389}
$$

which vanishes very rapidly for $L_0 \to \infty$.

Refer to (3.389), for $L_0 \to \infty$, to note that as a limit

$$
\lim_{L_0 \to \infty} \left[\int \mathrm{d}^3\mathbf{r}\, \psi^* (\mathbf{r} - \mathbf{L}) \cdot \frac{\phi(\mathbf{r} - \mathbf{L}')}{|\mathbf{r} - \mathbf{L}'|} \right] = 0 \tag{3.390}
$$

and hence

$$
\lim_{L_0 \to \infty} \left[\int \mathrm{d}^3\mathbf{r}\, \phi^* (\mathbf{r} - \mathbf{L}') \cdot \frac{\psi(\mathbf{r} - \mathbf{L})}{|\mathbf{r} - \mathbf{L}'|} \right] = 0. \tag{3.391}
$$

Refer to the integrations in (3.366)–(3.391), for $\mathbf{L} \neq \mathbf{L}'$ and $L_0, L_0' \to \infty$, to obtain the limit :

$$
\lim_{L_0 \to \infty} \left[\int \mathrm{d}^3\mathbf{r}\, \psi^* (\mathbf{r} - \mathbf{L}) \cdot \frac{\phi(\mathbf{r} - \mathbf{L}')}{|\mathbf{r} - \mathbf{L}|} \right] = 0, \tag{3.392a}
$$

$$
\lim_{L_0 \to \infty} \left[\int \mathrm{d}^3\mathbf{r}\, \phi^* (\mathbf{r} - \mathbf{L}') \cdot \frac{\psi(\mathbf{r} - \mathbf{L})}{|\mathbf{r} - \mathbf{L}|} \right] = 0, \tag{3.392b}
$$

$$
\lim_{L_0 \to \infty} \left[\int \mathrm{d}^3\mathbf{r}'\, \phi^* (\mathbf{r}' - \mathbf{L}') \cdot \frac{\phi(\mathbf{r}' - \mathbf{L}')}{|\mathbf{r}' - \mathbf{L}|} \right] = 0, \tag{3.392c}
$$

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\,\psi^*\left(\mathbf{r}-\mathbf{L}\right)\cdot\frac{\phi\left(\mathbf{r}-\mathbf{L}'\right)}{\left|\mathbf{r}-\mathbf{L}'\right|}\right]=0, \tag{3.392d}$$

$$\lim_{L_0\to\infty}\left[\int \mathrm{d}^3\mathbf{r}\,\phi^*\left(\mathbf{r}-\mathbf{L}'\right)\cdot\frac{\psi\left(\mathbf{r}-\mathbf{L}\right)}{\left|\mathbf{r}-\mathbf{L}'\right|}\right]=0, \tag{3.392e}$$

and from (3.145)

$$-\int \mathrm{d}^3\mathbf{r}\,\frac{\psi^*(\mathbf{r}-\mathbf{L})\cdot\psi(\mathbf{r}-\mathbf{L})}{|\mathbf{r}-\mathbf{L}|}=-\,\beta, \tag{3.393a}$$

$$-\int \mathrm{d}^3\mathbf{r}'\,\frac{\psi^*(\mathbf{r}'-\mathbf{L})\cdot\psi(\mathbf{r}'-\mathbf{L})}{|\mathbf{r}'-\mathbf{L}|}=-\,\beta. \tag{3.393b}$$

The expectation value of the nucleus-electron interaction for system consists of one nucleus, one bound electron and one free electron, ($N=2$, $k=1$ $Z_1=2$), let $\mathbf{R}_j=\mathbf{L}_j$, we have

$$-\left\langle\Psi\right|\sum_{i=1}^{2}\sum_{j=1}^{1}\frac{Z_je^2}{|\mathbf{r}_i-\mathbf{R}_j|}\left|\Psi\right\rangle=-\left\langle\Psi\right|\frac{Z_1e^2}{|\mathbf{r}_1-\mathbf{L}_1|}\left|\Psi\right\rangle-\left\langle\Psi\right|\frac{Z_1e^2}{|\mathbf{r}_2-\mathbf{L}_1|}\left|\Psi\right\rangle. \tag{3.394}$$

Consider the first term on the right-hand side of (3.394) , by using (3.238), to obtain

$$\begin{aligned}
&-\left\langle\Psi\right|\frac{Z_1e^2}{|\mathbf{r}_1-\mathbf{L}_1|}\left|\Psi\right\rangle\\
&\quad=-\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\cdot\frac{1}{|\mathbf{r}_1-\mathbf{L}_1|}\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]\right\}\\
&\quad-\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\cdot\frac{1}{|\mathbf{r}_1-\mathbf{L}_1|}\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]\right\}\\
&\quad+\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]^*\cdot\frac{1}{|\mathbf{r}_1-\mathbf{L}_1|}\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]\right\}\\
&\quad+\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\left[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)\right]^*\cdot\frac{1}{|\mathbf{r}_1-\mathbf{L}_1|}\left[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)\right]\right\}
\end{aligned}$$

$$= -\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1 \frac{|\psi_1(\mathbf{r}_1,\sigma_1)|^2}{|\mathbf{r}_1-\mathbf{L}_1|}\int \mathrm{d}^3\mathbf{r}_2\ |\phi_2(\mathbf{r}_2,\sigma_2)|^2\right\}$$

$$-\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1 \frac{|\phi_2(\mathbf{r}_1,\sigma_1)|^2}{|\mathbf{r}_1-\mathbf{L}_1|}\int \mathrm{d}^3\mathbf{r}_2\,|\psi_1(\mathbf{r}_2,\sigma_2)|^2\right\}$$

$$+\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\ \frac{\psi_1^*(\mathbf{r}_1,\sigma_1)\cdot\phi_2(\mathbf{r}_1,\sigma_1)}{|\mathbf{r}_1-\mathbf{L}_1|}\int \mathrm{d}^3\mathbf{r}_2\,\phi_2^*(\mathbf{r}_2,\sigma_2)\,\psi_1(\mathbf{r}_2,\sigma_2)\right\}$$

$$+\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1 \frac{\phi_2^*(\mathbf{r}_1,\sigma_1)\cdot\psi_1(\mathbf{r}_1,\sigma_1)}{|\mathbf{r}_1-\mathbf{L}_1|}\int \mathrm{d}^3\mathbf{r}_2\,\psi_1^*(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_2,\sigma_2)\right\}. \quad (3.395)$$

Refer to (3.232)–(3.235), with normalized wavefunction to rewrite (3.395) as

$$-\langle\Psi|\,\frac{Z_1 e^2}{|\mathbf{r}_1-\mathbf{L}_1|}\,|\Psi\rangle$$

$$= -\frac{Z_1 e^2}{2}\int \mathrm{d}^3\mathbf{r}_1 \frac{|\psi_1(\mathbf{r}_1,\sigma_1)|^2}{|\mathbf{r}_1-\mathbf{L}_1|} - \frac{Z_1 e^2}{2}\int \mathrm{d}^3\mathbf{r}_1 \frac{|\phi_2(\mathbf{r}_1,\sigma_1)|^2}{|\mathbf{r}_1-\mathbf{L}_1|}$$

$$+\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\ \frac{\psi_1^*(\mathbf{r}_1,\sigma_1)\cdot\phi_2(\mathbf{r}_1,\sigma_1)}{|\mathbf{r}_1-\mathbf{L}_1|}\int \mathrm{d}^3\mathbf{r}_2\,\phi_2^*(\mathbf{r}_2,\sigma_2)\,\psi_1(\mathbf{r}_2,\sigma_2)\right\}$$

$$+\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1 \frac{\phi_2^*(\mathbf{r}_1,\sigma_1)\cdot\psi_1(\mathbf{r}_1,\sigma_1)}{|\mathbf{r}_1-\mathbf{L}_1|}\int \mathrm{d}^3\mathbf{r}_2\,\psi_1^*(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_2,\sigma_2)\right\}$$

$$= -\frac{Z_1 e^2}{2}\int \mathrm{d}^3\mathbf{r}_1 \frac{|\psi(\mathbf{r}_1-\mathbf{L}_1)|^2}{|\mathbf{r}_1-\mathbf{L}_1|}\delta_{aa} - \frac{Z_1 e^2}{2}\int \mathrm{d}^3\mathbf{r}_1 \frac{|\phi(\mathbf{r}_1-\mathbf{L}_2)|^2}{|\mathbf{r}_1-\mathbf{L}_1|}\delta_{bb}$$

$$+\,\delta_{ab}\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\ \frac{\psi^*(\mathbf{r}_1-\mathbf{L}_1)\cdot\phi(\mathbf{r}_1-\mathbf{L}_2)}{|\mathbf{r}_1-\mathbf{L}_1|}\int \mathrm{d}^3\mathbf{r}_2\,\phi^*(\mathbf{r}_2-\mathbf{L}_2)\,\psi(\mathbf{r}_2-\mathbf{L}_1)\right\}$$

$$+\,\delta_{ab}\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1 \frac{\phi^*(\mathbf{r}_1-\mathbf{L}_2)\cdot\psi(\mathbf{r}_1-\mathbf{L}_1)}{|\mathbf{r}_1-\mathbf{L}_1|}\int \mathrm{d}^3\mathbf{r}_2\,\psi^*(\mathbf{r}_2-\mathbf{L}_1)\,\phi(\mathbf{r}_2-\mathbf{L}_2)\right\}. \quad (3.396)$$

Consider the second term on the right-hand side of (3.394), by using (3.238), to

obtain

$$
\begin{aligned}
&-\langle\Psi|\,\frac{Z_1e^2}{|\mathbf{r}_2-\mathbf{L}_1|}\,|\Psi\rangle \\
&\quad=-\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)]^*\cdot\frac{1}{|\mathbf{r}_2-\mathbf{L}_1|}\,[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)]\right\} \\
&\qquad-\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)]^*\cdot\frac{1}{|\mathbf{r}_2-\mathbf{L}_1|}\,[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)]\right\} \\
&\qquad+\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)]^*\cdot\frac{1}{|\mathbf{r}_2-\mathbf{L}_1|}\,[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)]\right\} \\
&\qquad+\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)]^*\cdot\frac{1}{|\mathbf{r}_2-\mathbf{L}_1|}\,[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)]\right\} \\
&\quad=-\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,|\psi_1(\mathbf{r}_1,\sigma_1)|^2\int \mathrm{d}^3\mathbf{r}_2\,\frac{|\phi_2(\mathbf{r}_2,\sigma_2)|^2}{|\mathbf{r}_2-\mathbf{L}_1|}\right\} \\
&\qquad-\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\;|\phi_2(\mathbf{r}_1,\sigma_1)|^2\int \mathrm{d}^3\mathbf{r}_2\frac{|\psi_1(\mathbf{r}_2,\sigma_2)|^2}{|\mathbf{r}_2-\mathbf{L}_1|}\right\} \\
&\qquad+\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\psi_1^*(\mathbf{r}_1,\sigma_1)\phi_2(\mathbf{r}_1,\sigma_1)\int \mathrm{d}^3\mathbf{r}_2\,\frac{\phi_2^*(\mathbf{r}_2,\sigma_2)\cdot\psi_1(\mathbf{r}_2,\sigma_2)}{|\mathbf{r}_2-\mathbf{L}_1|}\right\} \\
&\qquad+\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\phi_2^*(\mathbf{r}_1,\sigma_1)\psi_1(\mathbf{r}_1,\sigma_1)\int \mathrm{d}^3\mathbf{r}_2\,\frac{\psi_1^*(\mathbf{r}_2,\sigma_2)\cdot\phi_2(\mathbf{r}_2,\sigma_2)}{|\mathbf{r}_2-\mathbf{L}_1|}\right\}. \qquad (3.397)
\end{aligned}
$$

Refer to (3.232)–(3.235), with normalized wavefunction to rewrite (3.397) as

$$
\begin{aligned}
&-\langle\Psi|\,\frac{Z_1e^2}{|\mathbf{r}_2-\mathbf{L}_1|}\,|\Psi\rangle \\
&\quad=-\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_2\,\frac{|\phi_2(\mathbf{r}_2,\sigma_2)|^2}{|\mathbf{r}_2-\mathbf{L}_1|}\right\}-\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_2\frac{|\psi_1(\mathbf{r}_2,\sigma_2)|^2}{|\mathbf{r}_2-\mathbf{L}_1|}\right\} \\
&\qquad+\frac{Z_1e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\psi_1^*(\mathbf{r}_1,\sigma_1)\phi_2(\mathbf{r}_1,\sigma_1)\int \mathrm{d}^3\mathbf{r}_2\,\frac{\phi_2^*(\mathbf{r}_2,\sigma_2)\cdot\psi_1(\mathbf{r}_2,\sigma_2)}{|\mathbf{r}_2-\mathbf{L}_1|}\right\}
\end{aligned}
$$

$$+\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\, \phi_2^*(\mathbf{r}_1,\sigma_1)\psi_1(\mathbf{r}_1,\sigma_1)\int \mathrm{d}^3\mathbf{r}_2\, \frac{\psi_1^*(\mathbf{r}_2,\sigma_2)\cdot\phi_2(\mathbf{r}_2,\sigma_2)}{|\mathbf{r}_2-\mathbf{L}_1|}\right\}$$

$$=-\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_2\, \frac{|\phi(\mathbf{r}_2-\mathbf{L}_2)|^2}{|\mathbf{r}_2-\mathbf{L}_1|}\delta_{aa}\right\}-\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_2\frac{|\psi(\mathbf{r}_2-\mathbf{L}_1)|^2}{|\mathbf{r}_2-\mathbf{L}_1|}\delta_{bb}\right\}$$

$$+\delta_{ab}\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\, \psi^*(\mathbf{r}_1-\mathbf{L}_1)\phi(\mathbf{r}_1-\mathbf{L}_2)\int \mathrm{d}^3\mathbf{r}_2\, \frac{\phi^*(\mathbf{r}_2-\mathbf{L}_2)\cdot\psi(\mathbf{r}_2-\mathbf{L}_1)}{|\mathbf{r}_2-\mathbf{L}_1|}\right\}$$

$$+\delta_{ab}\frac{Z_1 e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\, \phi^*(\mathbf{r}_1-\mathbf{L}_2)\psi(\mathbf{r}_1-\mathbf{L}_1)\int \mathrm{d}^3\mathbf{r}_2\, \frac{\psi^*(\mathbf{r}_2-\mathbf{L}_1)\cdot\phi(\mathbf{r}_2-\mathbf{L}_2)}{|\mathbf{r}_2-\mathbf{L}_1|}\right\}. \tag{3.398}$$

Using (3.392)–(3.393), let $\mathbf{r}_1=\mathbf{r}$, $\mathbf{r}_2=\mathbf{r}'$, $\mathbf{L}_1=\mathbf{L}$ and $\mathbf{L}_2=\mathbf{L}'$, as $L_0\to\infty$, substituted into the right-hand side of (3.396) and (3.398), we obtain

$$\langle\Psi|\,\frac{Z_1 e^2}{|\mathbf{r}_1-\mathbf{L}_1|}\,|\Psi\rangle=-\frac{Z_1 e^2}{2}\beta \tag{3.399}$$

and hence

$$\langle\Psi|\,\frac{Z_1 e^2}{|\mathbf{r}_2-\mathbf{L}_1|}\,|\Psi\rangle=-\frac{Z_1 e^2}{2}\beta. \tag{3.400}$$

Substitute (3.399) and (3.400) into the right-hand side of (3.394), we obtain for the expectation value of the nucleus-electron interaction for a system which consists of one nucleus, one bound electron and one free electron, ($N=2$, $k=1$ $Z_1=2$)

$$\begin{aligned}-\langle\Psi|\sum_{i=1}^{2}\sum_{j=1}^{1}\frac{Z_j e^2}{|\mathbf{r}_i-\mathbf{R}_j|}\,|\Psi\rangle &= -\langle\Psi|\,\frac{Z_1 e^2}{|\mathbf{r}_1-\mathbf{L}_1|}\,|\Psi\rangle-\langle\Psi|\,\frac{Z_1 e^2}{|\mathbf{r}_2-\mathbf{L}_1|}\,|\Psi\rangle\\ &\leqslant -\frac{Z_1 e^2}{2}\beta-\frac{Z_1 e^2}{2}\beta\\ &= -Z_1 e^2\beta\end{aligned}$$

$$\therefore\quad -\langle\Psi|\sum_{i=1}^{2}\sum_{j=1}^{1}\frac{Z_j e^2}{|\mathbf{r}_i-\mathbf{R}_j|}\,|\Psi\rangle\leqslant-\sum_{j=1}^{1}Z_j e^2\beta. \tag{3.401}$$

From (3.401), we have for the expectation value of the nucleus-electron interaction for a system which consists of k nuclei, k bound electrons and $(N-k)$ free electrons, $(\sum_{j=1}^{k} Z_j = N)$:

$$-\langle\Psi|\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_j e^2}{|\mathbf{r}_i-\mathbf{R}_j|}|\Psi\rangle \leqslant -\sum_{j=1}^{k} Z_j e^2\beta. \tag{3.402}$$

By using (3.237), the expectation value of the electron-electron interaction for a system with consists of one nucleus, one bound electron and one free electron, ($N=2$, $k=1$ $Z_1=2$)

$$\langle\Psi|\sum_{i<j}^{2}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}|\Psi\rangle$$

$$=\langle\Psi|\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}|\Psi\rangle$$

$$=\frac{e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\frac{[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)]^*\cdot[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)]}{|\mathbf{r}_1-\mathbf{r}_2|}\right\}$$

$$+\frac{e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\frac{[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)]^*\cdot[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)]}{|\mathbf{r}_1-\mathbf{r}_2|}\right\}$$

$$-\frac{e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\frac{[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)]^*\cdot[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)]}{|\mathbf{r}_1-\mathbf{r}_2|}\right\}$$

$$-\frac{e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\frac{[\psi_1(\mathbf{r}_2,\sigma_2)\,\phi_2(\mathbf{r}_1,\sigma_1)]^*\cdot[\psi_1(\mathbf{r}_1,\sigma_1)\,\phi_2(\mathbf{r}_2,\sigma_2)]}{|\mathbf{r}_1-\mathbf{r}_2|}\right\}$$

$$=\frac{e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{|\psi_1(\mathbf{r}_1,\sigma_1)|^2\,|\phi_2(\mathbf{r}_2,\sigma_2)|^2}{|\mathbf{r}_1-\mathbf{r}_2|}\right\}$$

$$+\frac{e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\frac{|\phi_2(\mathbf{r}_1,\sigma_1)|^2\,|\psi_1(\mathbf{r}_2,\sigma_2)|^2}{|\mathbf{r}_1-\mathbf{r}_2|}\right\}$$

$$-\frac{e^2}{2}\left\{\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\psi_1^*(\mathbf{r}_1,\sigma_1)\,\phi_2^*(\mathbf{r}_2,\sigma_2)\cdot\phi_2(\mathbf{r}_1,\sigma_1)\,\psi_1(\mathbf{r}_2,\sigma_2)}{|\mathbf{r}_1-\mathbf{r}_2|}\right\}$$

$$- \frac{e^2}{2} \left\{ \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\phi_2^*(\mathbf{r}_1,\sigma_1)\, \psi_1^*(\mathbf{r}_2,\sigma_2) \cdot \psi_1(\mathbf{r}_1,\sigma_1)\, \phi_2(\mathbf{r}_2,\sigma_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} \right\}. \tag{3.403}$$

With normalized spin, we can rewrite (3.403) as

$$\begin{aligned}
&\langle \Psi |\, \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}\, |\Psi\rangle \\
&= \frac{e^2}{2} \left\{ \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{|\psi(\mathbf{r}_1 - \mathbf{L}_1)|^2\, |\phi(\mathbf{r}_2 - \mathbf{L}_2)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \delta_{aa} \right\} \\
&+ \frac{e^2}{2} \left\{ \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2 \frac{|\phi(\mathbf{r}_1 - \mathbf{L}_2)|^2\, |\psi(\mathbf{r}_2 - \mathbf{L}_1)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \delta_{bb} \right\} \\
&- \frac{e^2}{2} \left\{ \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\psi^*(\mathbf{r}_1 - \mathbf{L}_1)\, \phi^*(\mathbf{r}_2 - \mathbf{L}_2) \cdot \phi_2(\mathbf{r}_1 - \mathbf{L}_2)\, \psi(\mathbf{r}_2 - \mathbf{L}_1)}{|\mathbf{r}_1 - \mathbf{r}_2|} \delta_{ab} \right\} \\
&- \frac{e^2}{2} \left\{ \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{\phi^*(\mathbf{r}_1 - \mathbf{L}_2)\, \psi^*(\mathbf{r}_2 - \mathbf{L}_1) \cdot \psi(\mathbf{r}_1 - \mathbf{L}_1)\, \phi(\mathbf{r}_2 - \mathbf{L}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} \delta_{ab} \right\}.
\end{aligned} \tag{3.404}$$

Consider the first term on the right-hand side of (3.403), by using (3.239). Let $\mathbf{R} = \mathbf{r}_1 - \mathbf{L}_1$, $\mathbf{R}' = \mathbf{r}_2 - \mathbf{L}_2$ and $\mathbf{L}_0 = \mathbf{L}_2 - \mathbf{L}_1$, to obtain

$$\begin{aligned}
&\frac{e^2}{2} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{|\psi(\mathbf{r}_1 - \mathbf{L}_1)|^2\, |\phi(\mathbf{r}_2 - \mathbf{L}_2)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \\
&\qquad = \frac{e^2}{2} C^2 A^2 \int \mathrm{d}^3\mathbf{R}'\, \mathrm{e}^{-\frac{\mathbf{R'}^2}{2\sigma'^2}} \int \mathrm{d}^3\mathbf{R} \frac{\mathrm{e}^{-2\beta|\mathbf{R}|}}{|\mathbf{R} + \mathbf{L}_1 - \mathbf{R'} - \mathbf{L}_2|} \\
&\qquad = \frac{e^2}{2} C^2 A^2 \int \mathrm{d}^3\mathbf{R}'\, \mathrm{e}^{-\frac{\mathbf{R'}^2}{2\sigma'^2}} \int \mathrm{d}^3\mathbf{R} \frac{\mathrm{e}^{-2\beta|\mathbf{R}|}}{|\mathbf{R} - (\mathbf{R'} + \mathbf{L}_0)|}.
\end{aligned} \tag{3.405}$$

Consider the integral

$$\int \mathrm{d}^3\mathbf{R}\, \frac{\mathrm{e}^{-2\beta|\mathbf{R}|}}{|\mathbf{R} - (\mathbf{R}' + \mathbf{L}_0)|} = \int \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-2\beta|\mathbf{R}|} \sum_{\ell=0}^{\infty} \left(\frac{R_<}{R_>} \right)^{\ell} \frac{1}{R_>}\, P_\ell(\cos\theta)$$

$$
\begin{aligned}
&= \int_0^\infty \mathrm{d}R \, \frac{R^2}{R_>} \, \mathrm{e}^{-2\beta|\mathbf{R}|} \int \mathrm{d}\Omega \sum_{\ell=0}^{\infty} \left(\frac{R_<}{R_>}\right)^\ell P_\ell(\cos\theta) \\
&=4\pi \int_0^\infty \mathrm{d}R \, \frac{R^2}{R_>} \, \mathrm{e}^{-2\beta|\mathbf{R}|} \\
&=4\pi \int_0^{R'+L_0} \mathrm{d}R \, \frac{R^2}{R'+L_0} \, \mathrm{e}^{-2\beta R} + 4\pi \int_{R'+L_0}^\infty \mathrm{d}R \, \frac{R^2}{R} \, \mathrm{e}^{-2\beta R} \\
&=\frac{4\pi}{R'+L_0} \int_0^{R'+L_0} \mathrm{d}R \, R^2 \, \mathrm{e}^{-2\beta R} + 4\pi \int_{R'+L_0}^\infty \mathrm{d}R \, R \, \mathrm{e}^{-2\beta R} \\
&=\frac{4\pi}{R'+L_0} \frac{\partial^2}{\partial u^2} \int_0^{R'+L_0} \mathrm{d}R \, \mathrm{e}^{-uR} \\
&\quad + 4\pi \int_{R'+L_0}^\infty \mathrm{d}R \, R \, \mathrm{e}^{-uR} \ , u = 2\beta
\end{aligned}
\tag{3.406}
$$

where

$$
\frac{1}{|\mathbf{R}_i - (\mathbf{R}' + \mathbf{L}_0)|} = \sum_{\ell=0}^{\infty} \left(\frac{R_{i<}}{R_{i>}}\right)^\ell \frac{1}{R_{i>}} P_\ell(\cos\theta), \tag{3.407a}
$$

$$
R_> = \max(R, R' + L_0), \tag{3.407b}
$$

$$
\int \mathrm{d}\Omega \, P_\ell(\cos\theta) = 4\pi\delta_{\ell 0}. \tag{3.407c}
$$

Consider the first term on the right-hand side of (3.406), to obtain

$$
\begin{aligned}
\frac{\partial^2}{\partial u^2} \int_0^{R'+L_0} \mathrm{d}R \, \mathrm{e}^{-uR} &= \frac{\partial^2}{\partial u^2} \left[-\frac{\mathrm{e}^{-uR}}{u} \bigg|_0^{R'+L_0} \right] \\
&= -\frac{\partial^2}{\partial u^2} \left[\frac{\mathrm{e}^{-u(R'+L_0)}}{u} - \frac{1}{u} \right].
\end{aligned}
\tag{3.408}
$$

Since, for $L_0 \to 0$ we can rewrite (3.408) as

$$
\frac{\partial^2}{\partial u^2} \int_0^{R'+L_0} \mathrm{d}R \, \mathrm{e}^{-uR} = \frac{2}{u} = \frac{1}{\beta} \tag{3.409}
$$

the second term on the right-hand side of (3.406) becomes

$$\int_{R'+L_0}^{\infty} \mathrm{d}R\, R\, \mathrm{e}^{-2\beta R} = \left(-\frac{\mathrm{e}^{-2\beta R}}{2\beta}\left[R + \frac{1}{2\beta}\right]\right)\Bigg|_{R'+L_0}^{\infty}$$

$$= 0 - \left(-\frac{\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta}\left[(R'+L_0) + \frac{1}{2\beta}\right]\right)$$

$$= \frac{\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta}\left[(R'+L_0) + \frac{1}{2\beta}\right]$$

$$= \frac{(R'+L_0)\,\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta} + \frac{\mathrm{e}^{-2\beta(R'+L_0)}}{4\beta^2}. \tag{3.410}$$

Substitute (3.408) and (3.409) into the right-hand side of (3.406), for $L_0 \to \infty$, to obtain

$$\int \mathrm{d}^3\mathbf{R}\, \frac{\mathrm{e}^{-2\beta|\mathbf{R}|}}{|\mathbf{R} - (\mathbf{R}' + \mathbf{L}_0)|} = \frac{4\pi}{R'+L_0}\frac{\partial^2}{\partial u^2}\int_0^{R'+L_0} \mathrm{d}R\, \mathrm{e}^{-uR} + 4\pi \int_{R'+L_0}^{\infty} \mathrm{d}R\, R\, \mathrm{e}^{-2\beta R}$$

$$= \frac{4\pi}{\beta}\frac{1}{R'+L_0} + 4\pi\left[\frac{(R'+L_0)\,\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta}\right.$$

$$\left. + \frac{\mathrm{e}^{-2\beta(R'+L_0)}}{4\beta^2}\right]. \tag{3.411}$$

By using (3.411), the right-hand side of (3.405) becomes

$$\frac{e^2}{2}\int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{|\psi(\mathbf{r}_1 - \mathbf{L}_1)|^2\, |\phi(\mathbf{r}_2 - \mathbf{L}_2)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

$$= \frac{e^2}{2}C^2A^2 \int \mathrm{d}^3\mathbf{R}'\, \mathrm{e}^{-\frac{\mathbf{R}'^2}{2\sigma'^2}} \int \mathrm{d}^3\mathbf{R} \frac{\mathrm{e}^{-2\beta|\mathbf{R}|}}{|\mathbf{R} - (\mathbf{R}' + \mathbf{L}_0)|}$$

$$= \frac{e^2}{2}C^2A^2 4\pi \int \mathrm{d}^3\mathbf{R}'\, \mathrm{e}^{-\frac{\mathbf{R}'^2}{2\sigma'^2}} \left[\frac{1}{\beta(R'+L_0)} + \frac{(R'+L_0)\,\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta} + \frac{\mathrm{e}^{-2\beta(R'+L_0)}}{4\beta^2}\right]$$

$$= \frac{e^2}{2}C^2A^2 16\pi^2 \int_0^{\infty} \mathrm{d}R'\, R'^2\, \mathrm{e}^{-\frac{\mathbf{R}'^2}{2\sigma'^2}} \left[\frac{1}{\beta(R'+L_0)} + \frac{(R'+L_0)\,\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta}\right.$$

$$\left. + \frac{\mathrm{e}^{-2\beta(R'+L_0)}}{4\beta^2}\right]$$

$$\leqslant \frac{e^2}{2} C^2 A^2 16\pi^2 \int_0^\infty \mathrm{d}R'\, R'^2 \left[\frac{1}{\beta(R'+L_0)} + \frac{(R'+L_0)\,\mathrm{e}^{-2\beta(R'+L_0)}}{2\beta} + \frac{\mathrm{e}^{-2\beta(R'+L_0)}}{4\beta^2} \right]. \tag{3.412}$$

For $L_0 \to \infty$, we can rewrite (3.412) as a limit

$$\lim_{L_0\to\infty} \left[\frac{e^2}{2} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2\, \frac{|\psi(\mathbf{r}_1-\mathbf{L}_1)|^2\, |\phi(\mathbf{r}_2-\mathbf{L}_2)|^2}{|\mathbf{r}_1-\mathbf{r}_2|} \right] = 0. \tag{3.413}$$

Consider the second term on the right-hand side of (3.404), let $\mathbf{R'} = \mathbf{r}_2 - \mathbf{L}_1$, $\mathbf{R} = \mathbf{r}_1 - \mathbf{L}_2$ and $\mathbf{A} = (\mathbf{r_1} - \mathbf{L_1})$ to obtain

$$\begin{aligned}
&\frac{e^2}{2} \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{d}^3\mathbf{r}_2 \frac{|\phi(\mathbf{r}_1-\mathbf{L}_2)|^2\, |\psi(\mathbf{r}_2-\mathbf{L}_1)|^2}{|\mathbf{r}_1-\mathbf{r}_2|} \\
&\qquad = \frac{e^2}{2} C^2 A^2 \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{e}^{-\frac{(\mathbf{r_1}-\mathbf{L_2})^2}{2\sigma'^2}} \int \mathrm{d}^3\mathbf{r}_2 \frac{\mathrm{e}^{-2\beta|\mathbf{r}_2-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{r}_2|} \\
&\qquad = \frac{e^2}{2} C^2 A^2 \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{e}^{-\frac{(\mathbf{r_1}-\mathbf{L_2})^2}{2\sigma'^2}} \int \mathrm{d}^3\mathbf{R'} \frac{\mathrm{e}^{-2\beta|\mathbf{R'}|}}{|(\mathbf{r_1}-\mathbf{L_1})-\mathbf{R'}|} \\
&\qquad = \frac{e^2}{2} C^2 A^2 \int \mathrm{d}^3\mathbf{r}_1\, \mathrm{e}^{-\frac{(\mathbf{r_1}-\mathbf{L_2})^2}{2\sigma'^2}} \int \mathrm{d}^3\mathbf{R'} \frac{\mathrm{e}^{-2\beta|\mathbf{R'}|}}{|\mathbf{R'}-\mathbf{A}|}.
\end{aligned} \tag{3.414}$$

Consider integral

$$\begin{aligned}
\int \mathrm{d}^3\mathbf{R'} \frac{\mathrm{e}^{-2\beta|\mathbf{R'}|}}{|\mathbf{R'}-\mathbf{A}|} &= \int_0^\infty \mathrm{d}R'\, R'^2 \mathrm{e}^{-2\beta R'} \int \mathrm{d}\Omega \sum_{\ell=0}^{\infty} \left(\frac{R'_<}{R'_>}\right)^\ell \frac{1}{R'_>} P_\ell(\cos\theta) \\
&= 4\pi \int_0^\infty \mathrm{d}R'\, \mathrm{e}^{-2\beta R'} \frac{R'^2}{R'_>} \\
&= \frac{4\pi}{A} \int_0^A \mathrm{d}R'\, R'^2 \mathrm{e}^{-2\beta R'} + 4\pi \int_A^\infty \mathrm{d}R'\, R' \mathrm{e}^{-2\beta R'} \\
&= \frac{4\pi}{A} \frac{\partial^2}{\partial u^2} \int_0^A \mathrm{d}R'\, \mathrm{e}^{uR'} + 4\pi \frac{\partial}{\partial u} \int_A^\infty \mathrm{d}R'\, \mathrm{e}^{uR'} \quad , u = -2\beta
\end{aligned}$$

$$
\begin{aligned}
=&\frac{4\pi}{A}\ \frac{\mathrm{e}^{uR'}}{u}\left(R'^2-\frac{2R'}{u}+\frac{2}{u^2}\right)\Bigg|_0^A+4\pi\ \frac{\mathrm{e}^{uR'}}{u}\left(R'-\frac{1}{u^2}\right)\Bigg|_A^\infty \\
=&\frac{4\pi}{A}\left[\frac{\mathrm{e}^{uA}}{u}\left(A^2-\frac{2A}{u}+\frac{2}{u^2}\right)-\frac{2}{u^3}\right] \\
&+4\pi\left[0-\frac{\mathrm{e}^{uA}}{u}\left(A-\frac{1}{u^2}\right)\right] \\
=&\frac{4\pi}{A}\left[\frac{\mathrm{e}^{uA}}{u}\left(A^2-\frac{2A}{u}+\frac{2}{u^2}\right)-\frac{2}{u^3}\right] \\
&-4\pi\frac{\mathrm{e}^{uA}}{u}\left(A-\frac{1}{u^2}\right) \\
=&\frac{4\pi}{A}\frac{2}{8\beta^3}-\frac{4\pi}{A}\left[\frac{\mathrm{e}^{-2\beta A}}{2\beta}\left(A^2+\frac{2A}{2\beta}+\frac{2}{4\beta^2}\right)\right] \\
&+4\pi\frac{\mathrm{e}^{-2\beta A}}{2\beta}\left(A+\frac{1}{4\beta^2}\right) \\
=&\frac{4\pi}{A}\frac{2}{8\beta^3}-\frac{4\pi\mathrm{e}^{-2\beta A}}{2\beta}\left[\frac{1}{A}\left(A^2+\frac{A}{\beta}+\frac{2}{4\beta^2}\right)\right] \\
&+\frac{4\pi\mathrm{e}^{-2\beta A}}{2\beta}\left(A+\frac{1}{4\beta^2}\right) \\
=&\frac{4\pi}{A}\frac{2}{8\beta^3}-\frac{4\pi\mathrm{e}^{-2\beta A}}{2\beta}\left\{\left(A+\frac{1}{\beta}+\frac{1}{2A\beta^2}\right)+\left(A+\frac{1}{4\beta^2}\right)\right\} \\
\leqslant&\frac{\pi}{\beta^3}\frac{1}{A}.
\end{aligned}
\tag{3.415}
$$

Substitute $A = |\mathbf{r}_1 - \mathbf{L}_1|$ into the right-hand side of inequality (3.415), to obtain the inequality

$$
\int \mathrm{d}^3\mathbf{R}'\frac{\mathrm{e}^{-2\beta|\mathbf{R}'|}}{|\mathbf{R}'-(\mathbf{r}-\mathbf{L})|}\leqslant\frac{\pi}{\beta^3}\frac{1}{|\mathbf{r}-\mathbf{L}|}. \tag{3.416}
$$

Substitute (3.416) into the right-hand side of (3.414), and let $\mathbf{R} = \mathbf{r}_1 - \mathbf{L}_1$, to obtain

$$\frac{e^2}{2}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\frac{|\phi(\mathbf{r}_1-\mathbf{L}_2)|^2\,|\psi(\mathbf{r}_2-\mathbf{L}_1)|^2}{|\mathbf{r}_1-\mathbf{r}_2|}$$

$$=\frac{e^2}{2}C^2A^2\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{e}^{-\frac{(\mathbf{r}_1-\mathbf{L}_2)^2}{2\sigma'^2}}\int \mathrm{d}^3\mathbf{R}'\frac{\mathrm{e}^{-2\beta|\mathbf{R}'|}}{|\mathbf{R}'-\mathbf{A}|}$$

$$\leqslant\frac{e^2}{2}\frac{\pi}{\beta^3}C^2A^2\int \mathrm{d}^3\mathbf{r}_1\,\frac{\mathrm{e}^{-\frac{(\mathbf{R}+\mathbf{L}_1-\mathbf{L}_2)^2}{2\sigma'^2}}}{|\mathbf{r}_1-\mathbf{L}_1|}. \tag{3.417}$$

Substitute (3.392c) into the right-hand side of inequality (3.417), for $L_0 \to \infty$, we obtain as a limit

$$\lim_{L_0\to\infty}\left[\frac{e^2}{2}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\frac{|\phi(\mathbf{r}_1-\mathbf{L}_2)|^2\,|\psi(\mathbf{r}_2-\mathbf{L}_1)|^2}{|\mathbf{r}_1-\mathbf{r}_2|}\right]=0. \tag{3.418}$$

Consider the third term on the right-hand side of (3.404), and let $\mathbf{R} = \mathbf{r}_1 - \mathbf{L}_1$, $\mathbf{R}' = \mathbf{r}_2 - \mathbf{L}_2$, $\mathbf{L}_0 = \mathbf{L}_2 - \mathbf{L}_1$ and $\mathbf{L}'_0 = \mathbf{L}_1 - \mathbf{L}_2$, to obtain

$$\left|\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\psi^*(\mathbf{r}_1-\mathbf{L}_1)\,\phi^*(\mathbf{r}_2-\mathbf{L}_2)\cdot\phi_2(\mathbf{r}_1-\mathbf{L}_2)\,\psi(\mathbf{r}_2-\mathbf{L}_1)}{|\mathbf{r}_1-\mathbf{r}_2|}\right|$$

$$=C^2A^2\left|\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\mathrm{e}^{-\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{r}_2-\mathbf{L}_2)}\,\mathrm{e}^{-\frac{(\mathbf{r}_2-\mathbf{L}_2)^2}{4\sigma'^2}}\right.$$

$$\left.\times\;\frac{\cdot\,\mathrm{e}^{\mathrm{i}\,\mathbf{k}'\cdot(\mathbf{r}_1-\mathbf{L}_2)}\,\mathrm{e}^{-\frac{(\mathbf{r}_1-\mathbf{L}_2)^2}{4\sigma'^2}}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{r}_2|}\right|$$

$$\leqslant C^2A^2\left|\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\mathrm{e}^{-\frac{(\mathbf{r}_2-\mathbf{L}_2)^2}{4\sigma'^2}}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\frac{(\mathbf{r}_1-\mathbf{L}_2)^2}{4\sigma'^2}}}{|\mathbf{r}_1-\mathbf{r}_2|}\right|$$

$$\leqslant C^2A^2\left|\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\mathrm{e}^{-\frac{(\mathbf{r}_2-\mathbf{L}_2)^2}{4\sigma'^2}}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\,\frac{\mathrm{e}^{-\beta|\mathbf{R}|}\,\mathrm{e}^{-\frac{(\mathbf{R}+\mathbf{L}_1-\mathbf{L}_2)^2}{4\sigma'^2}}}{|\mathbf{R}+\mathbf{L}_1-\mathbf{r}_2|}\right|$$

$$=C^2A^2\left|\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\mathrm{e}^{-\frac{(\mathbf{r}_2-\mathbf{L}_2)^2}{4\sigma'^2}}\,\mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|}\,\frac{\mathrm{e}^{-\beta|\mathbf{R}|}\,\mathrm{e}^{-\frac{(\mathbf{R}+\mathbf{L}'_0)^2}{4\sigma'^2}}}{|\mathbf{R}-(\mathbf{r}_2-\mathbf{L}_1)|}\right|$$

$$\leqslant C^2 A^2 \left| \int \mathrm{d}^3\mathbf{r}_2\, \mathrm{e}^{-\frac{(\mathbf{r}_2-\mathbf{L}_2)^2}{4\sigma'^2}}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \int \mathrm{d}^3\mathbf{R} \frac{\mathrm{e}^{-\beta|\mathbf{R}|}}{|\mathbf{R}-(\mathbf{r}_2-\mathbf{L}_1)|} \right|$$

$$\leqslant C^2 A^2 \left| \int \mathrm{d}^3\mathbf{r}_2\, \mathrm{e}^{-\frac{(\mathbf{r}_2-\mathbf{L}_2)^2}{4\sigma'^2}}\, \mathrm{e}^{-\beta|\mathbf{r}_2-\mathbf{L}_1|} \right| \left| \int \mathrm{d}^3\mathbf{R} \frac{\mathrm{e}^{-\beta|\mathbf{R}|}}{|\mathbf{R}-\mathbf{B}|} \right|, \quad \mathbf{B} = (\mathbf{r}_2 - \mathbf{L}_1)$$

(3.419)

where

$$0 \leqslant \mathrm{e}^{-\frac{(\mathbf{R}+\mathbf{L}_0')^2}{4\sigma'^2}} \leqslant 1 \tag{3.420}$$

Consider the integral

$$\left| \int \mathrm{d}^3\mathbf{R'} \frac{\mathrm{e}^{-\beta R'}}{|\mathbf{R'}-\mathbf{B}|} \right| = \left| \int_0^\infty \mathrm{d}R' \int \mathrm{d}\Omega\, R'^2\, \mathrm{e}^{-\beta R'} \sum_{\ell=0}^{\infty} \left(\frac{R'_<}{R'_>}\right)^\ell \frac{1}{R'_>} P_\ell(\cos\theta) \right|$$

$$= 4\pi \left| \int_0^\infty \mathrm{d}R' \frac{R'^2}{R'_>} \mathrm{e}^{-\beta R'} \right| \qquad , R'_> = \max(B, R')$$

$$= \frac{4\pi}{B} \left| \int_0^B \mathrm{d}R'\, R'^2\, \mathrm{e}^{-\beta R'} + 4\pi \int_B^\infty \mathrm{d}R'\, R'\, \mathrm{e}^{-\beta R'} \right| \; , u = -\beta$$

$$= \frac{4\pi}{B} \left| \frac{\mathrm{e}^{uR}}{u} \left[R^2 - \frac{2R}{u} + \frac{2}{u^2} \right]_0^B + 4\pi \frac{\mathrm{e}^{uR}}{u} \left[R - \frac{1}{u^2} \right]_B^\infty \right|$$

$$= \frac{4\pi}{B} \left| \frac{\mathrm{e}^{uB}}{u} \left(B^2 - \frac{2B}{u} + \frac{2}{u^2} \right) - \frac{2}{u^3} - 4\pi \frac{\mathrm{e}^{uB}}{u} \left(B - \frac{1}{u^2} \right) \right|$$

$$= \left| \frac{4\pi B\, \mathrm{e}^{uB}}{u} - \frac{8\pi \mathrm{e}^{uB}}{u^2} + \frac{8\pi}{B} \frac{\mathrm{e}^{uB}}{u^3} - \frac{8\pi}{Bu^3} - \frac{4B\pi\, \mathrm{e}^{uB}}{u} + 4\pi \frac{\mathrm{e}^{uB}}{u^3} \right|$$

$$= \left| -\frac{8\pi \mathrm{e}^{-\beta B}}{\beta^2} - \frac{8\pi\, \mathrm{e}^{-\beta B}}{\beta^2 B} + \frac{8\pi}{\beta^3 B} - 4\pi \frac{\mathrm{e}^{-\beta B}}{\beta^3} \right|$$

$$\leqslant \left| \frac{8\pi \mathrm{e}^{-\beta B}}{\beta^2} + \frac{8\pi\, \mathrm{e}^{-\beta B}}{\beta^2 B} + \frac{8\pi}{\beta^3 B} + 4\pi \frac{\mathrm{e}^{-\beta B}}{\beta^3} \right|. \tag{3.421}$$

Substitute (3.421) and $B = |\mathbf{r}_1 - \mathbf{L}_2|$ into the right-hand side of (3.419), to obtain

$$\begin{aligned}
&\left|\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\psi^*(\mathbf{r}_1-\mathbf{L}_1)\,\phi^*(\mathbf{r}_2-\mathbf{L}_2)\cdot\phi_2(\mathbf{r}_1-\mathbf{L}_2)\,\psi(\mathbf{r}_2-\mathbf{L}_1)}{|\mathbf{r}_1-\mathbf{r}_2|}\right| \\
\leqslant & C^2A^2\left|\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\frac{(\mathbf{r}_1-\mathbf{L}_2)^2}{4\sigma'^2}}\right|\left|\int \mathrm{d}^3\mathbf{R'}\,\frac{\mathrm{e}^{-\beta R'}}{|\mathbf{R'}-\mathbf{B}|}\right| \\
= & C^2A^2\left|\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\frac{(\mathbf{r}_1-\mathbf{L}_2)^2}{4\sigma'^2}}\right|\left|\frac{8\pi\mathrm{e}^{-\beta B}}{\beta^2}+\frac{8\pi\,\mathrm{e}^{-\beta B}}{\beta^2 B}+\frac{8\pi}{\beta^3 B}+4\pi\,\frac{\mathrm{e}^{-\beta B}}{\beta^3}\right| \\
= & C^2A^2\left|\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\frac{(\mathbf{r}_1-\mathbf{L}_2)^2}{4\sigma'^2}}\left[\frac{8\pi\mathrm{e}^{-\beta B}}{\beta^2}+\frac{8\pi\,\mathrm{e}^{-\beta B}}{\beta^2 B}+\frac{8\pi}{\beta^3 B}+4\pi\,\frac{\mathrm{e}^{-\beta B}}{\beta^3}\right]\right| \\
= & C^2A^2\left|\int \mathrm{d}^3\mathbf{R}\,\mathrm{e}^{-\beta|\mathbf{R}|}\,\mathrm{e}^{-\frac{(\mathbf{R}+\mathbf{L}_1-\mathbf{L}_2)^2}{4\sigma'^2}}\left[\frac{8\pi\mathrm{e}^{-\beta B}}{\beta^2}+\frac{8\pi\,\mathrm{e}^{-\beta B}}{\beta^2 B}+\frac{8\pi}{\beta^3 B}+4\pi\,\frac{\mathrm{e}^{-\beta B}}{\beta^3}\right]\right| \\
= & C^2A^2\left|\int \mathrm{d}^3\mathbf{R}\,\mathrm{e}^{-\beta|\mathbf{R}|}\,\mathrm{e}^{-\frac{(\mathbf{R}-\mathbf{L}_0)^2}{4\sigma'^2}}\left[\frac{8\pi\mathrm{e}^{-\beta B}}{\beta^2}+\frac{8\pi\,\mathrm{e}^{-\beta B}}{\beta^2 B}+\frac{8\pi}{\beta^3 B}+4\pi\,\frac{\mathrm{e}^{-\beta B}}{\beta^3}\right]\right| \\
\leqslant & C^2A^2\mathrm{e}^{-\frac{L_0^2}{4\sigma'^2}}\int \mathrm{d}^3\mathbf{r}_1\,\Bigg|\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\,\mathrm{e}^{-\frac{R(R-2RL_0)}{4\sigma'^2}} \\
&\times\left\{\frac{8\pi\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}}{\beta^2}+\frac{8\pi\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}}{\beta^2|\mathbf{r}_1-\mathbf{L}_2|}+\frac{8\pi}{\beta^3|\mathbf{r}_1-\mathbf{L}_2|}+\frac{4\pi\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}}{\beta^3}\right\}\Bigg| \\
= & C^2A^2\mathrm{e}^{-\frac{L_0'^2}{4\sigma'^2}}\left\{\frac{8\pi}{\beta^2}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}+\frac{8\pi}{\beta^3}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right. \\
&\left.+\frac{8\pi}{\beta^3}\int \mathrm{d}^3\mathbf{r}_1\,\frac{\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}}{|\mathbf{r}_1-\mathbf{L}_2|}+\frac{4\pi}{\beta^3}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_1|}\mathrm{e}^{-\beta|\mathbf{r}_1-\mathbf{L}_2|}\right\}.
\end{aligned} \tag{3.422}$$

By referring to (3.392) and (3.393) for $L_0 \to \infty$, we obtain as a limit

$$\lim_{L_0\to\infty}\left[-\frac{e^2}{2}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\psi^*(\mathbf{r}_1-\mathbf{L}_1)\,\phi^*(\mathbf{r}_2-\mathbf{L}_2)\cdot\phi_2(\mathbf{r}_1-\mathbf{L}_2)\,\psi(\mathbf{r}_2-\mathbf{L}_1)}{|\mathbf{r}_1-\mathbf{r}_2|}\right]=0 \tag{3.423}$$

and by referring (3.403)–(3.423), we have for the fourth term on the right-hand side of

(3.404), for $L_0 \to \infty$, as a limit

$$\lim_{L_0\to\infty}\left[-\frac{e^2}{2}\int \mathrm{d}^3\mathbf{r}_1\,\mathrm{d}^3\mathbf{r}_2\,\frac{\phi^*(\mathbf{r}_1-\mathbf{L}_2)\,\psi^*(\mathbf{r}_2-\mathbf{L}_1)\cdot\psi(\mathbf{r}_1-\mathbf{L}_1)\,\phi(\mathbf{r}_2-\mathbf{L}_2)}{|\mathbf{r}_1-\mathbf{r}_2|}\right]=0. \tag{3.424}$$

By substituting (3.413), (3.418), (3.423) and (3.424) into the right-hand side of (3.404), we obtain a bound for the expectation value of electron-electron interaction for a system which consists of one nucleus, one bound electron and one free electron, ($N = 2$, $k = 1$ $Z_1 = 2$), for $L_0 \to \infty$ as a limit

$$\lim_{L_0\to\infty}\langle\Psi|\,\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\,|\Psi\rangle = 0. \tag{3.425}$$

From (3.425), we have for the expectation value of electron-electron interaction for a system with consists of k nuclei, k bound electron and $N-k$ free electron with vanishingly small kinetic energies, for $L_0 \to \infty$, as a limit

$$\lim_{L_0\to\infty}\langle\Psi|\sum_{i<j}^{N}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}\,|\Psi\rangle = 0. \tag{3.426}$$

Using (3.237), the expectation value of the nucleus-nucleus interaction for a system which consists of two nuclei, k bound electrons and $N-k$ free electrons, $((\sum_{j=1}^{k} Z_j = N)$, and letting $\mathbf{R}_1 - \mathbf{R}_2 = \mathbf{L}_1 - \mathbf{L}_2 = \mathbf{L}_0$, we obtain

$$\begin{aligned}\langle\Psi|\,\frac{Z_1Z_2e^2}{|\mathbf{R}_1-\mathbf{R}_2|}\,|\Psi\rangle =&\frac{Z_1Z_2e^2}{|\mathbf{L}_0|}\,\langle\Psi|\Psi\rangle\\ =&\frac{Z_1Z_2e^2}{L_0}\end{aligned} \tag{3.427}$$

for $k > 2$, we have

$$|\mathbf{R}_i - \mathbf{R}_j| \geqslant |\mathbf{L}_0|, \tag{3.428a}$$

$$\frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} \leqslant \frac{1}{|\mathbf{L}_0|}. \tag{3.428b}$$

By using (3.428), we obtain

$$\langle\Psi|\sum_{i<j}^{k}\frac{Z_jZ_je^2}{|\mathbf{R}_1-\mathbf{R}_2|}|\Psi\rangle \leqslant \frac{1}{|\mathbf{L}_0|}\sum_{i<j}^{k}Z_1Z_2e^2\langle\Psi|\Psi\rangle$$

$$= \frac{1}{L_0}\sum_{i<j}^{k}Z_iZ_je^2. \tag{3.429}$$

From (3.429), we obtain a bound for the expectation value for nucleus-nucleus interaction for k hydrogen nuclei

$$\langle\Psi|\sum_{i<j}^{k}\frac{Z_jZ_je^2}{|\mathbf{R}_i-\mathbf{R}_j|}|\Psi\rangle \leqslant \frac{1}{L_0}\sum_{i<j}^{k}Z_iZ_je^2. \tag{3.430}$$

From (3.430), for $L_0 \to \infty$, a bound for the expectation value of nucleus-nucleus interaction for k hydrogen nuclei as a limit

$$\lim_{L_0\to\infty}\langle\Psi|\sum_{i<j}^{k}\frac{Z_jZ_je^2}{|\mathbf{R}_i-\mathbf{R}_j|}|\Psi\rangle = 0. \tag{3.431}$$

By referring (3.240), (3.365), (3.401) and (3.426), we obtain

$$\langle\Psi|H|\Psi\rangle = \langle\Psi|\sum_{i=1}^{2}\frac{\mathbf{p}_i^2}{2m}|\Psi\rangle + \langle\Psi|\sum_{i<j}^{2}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}|\Psi\rangle$$

$$-\langle\Psi|\sum_{i=1}^{2}\sum_{j=1}^{1}\frac{Z_je^2}{|\mathbf{r}_i-\mathbf{R}_j|}|\Psi\rangle$$

$$\therefore \quad \langle\Psi|H|\Psi\rangle \leqslant \frac{\hbar^2\beta^2}{2m} - Z_1e^2\beta. \tag{3.432}$$

Optimize (3.432) over β, we obtain

$$0 = \frac{\hbar^2\beta}{m} - Z_1e^2$$

$$\beta = \frac{Z_1 m e^2}{\hbar^2}. \tag{3.433}$$

Substitute β into the right-hand side of (3.432), to obtain an upper bound of the ground-state energy of the following infinity separated 2 clusters : one nucleus, one bound electron, and one free electron with vanishingly small kinetic, where $Z_1 = 2$

$$\begin{aligned}
\langle\Psi| H |\Psi\rangle \leqslant & \frac{\hbar^2\beta^2}{2m}\left(\frac{Z_1^2 m^2 e^4}{\hbar^2}\right) - Z_1 e^2 \left(\frac{Z_1 m e^2}{\hbar^2}\right) \\
= & -\frac{Z_1^2 m e^4}{2\hbar^2} \\
\leqslant & -\frac{Z_1 m e^4}{2\hbar^2} \\
= & -2\frac{m e^4}{2\hbar^2}
\end{aligned}$$

$$\langle\Psi| H |\Psi\rangle \leqslant -2\left(\frac{m e^4}{2\hbar^2}\right). \tag{3.434}$$

By referring to (3.237), (3.365), (3.402), (3.426) and (3.431), we obtain an upper bound for the ground-state energy of the following infinitely separated clusters : k nuclei, k bound electrons, and $(N-k)$ free electrons with vanishingly small kinetic, where $\sum_{j=1}^{k} Z_j = N$ and $-\sum_{j=1}^{k} Z_j^2 \leqslant -\sum_{j=1}^{k} Z_j$:

$$\begin{aligned}
\langle\Psi| H |\Psi\rangle = & \langle\Psi| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} |\Psi\rangle + \langle\Psi| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} |\Psi\rangle \\
& - \langle\Psi| \sum_{i=1}^{N}\sum_{j=1}^{k} \frac{Z_j e^2}{|\mathbf{r}_i - \mathbf{R}_j|} |\Psi\rangle + \langle\Psi| \sum_{i<j}^{k} \frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|} |\Psi\rangle \\
\leqslant & \sum_{j=1}^{k} \frac{\hbar^2\beta^2}{2m} - \sum_{j=1}^{k} Z_j e^2 \beta.
\end{aligned} \tag{3.435}$$

Optimize (3.435) over β, to obtain

$$0 = \frac{\hbar^2 \beta}{m} - Z_j e^2$$

$$\beta = \frac{Z_j m e^2}{\hbar^2}. \tag{3.436}$$

Substitute β into the right-hand side of (3.435), to obtain

$$\begin{aligned}
\langle\Psi| H |\Psi\rangle &\leqslant \sum_{j=1}^{k} \frac{\hbar^2 \beta^2}{2m} - \sum_{j=1}^{k} Z_j e^2 \beta \\
&= \sum_{j=1}^{k} \frac{\hbar^2}{2m} \left(\frac{Z_j^2 m^2 e^4}{\hbar^4} \right) - \sum_{j=1}^{k} Z_j e^2 \left(\frac{Z_j m e^2}{\hbar^2} \right) \\
&= - \sum_{j=1}^{k} \left(\frac{Z_j^2 m e^4}{2\hbar^2} \right) \\
&\leqslant - \sum_{j=1}^{k} Z_j \left(\frac{m e^4}{2\hbar^2} \right).
\end{aligned} \tag{3.437}$$

From (3.437), the upper bound of the ground-state energy of the following infinitely separated N clusters : k nuclei , k bound electrons, and $(N-k)$ free electrons with the latter vanishingly small kinetic energies is given by

$$E_N \leqslant - \left(\frac{m e^4}{2\hbar^2} \right) N \quad , \sum_{j=1}^{k} Z_j = N \tag{3.438}$$

thus increasing the coefficient .0450 to one.

CHAPTER IV

INFLATION OF MATTER

4.1 Introduction

The purpose of this chapter is to establish the following key result concerning the stability of matter. We prove rigorously that for a non-vanishing probability of having the electrons in matter within a sphere of radius R, the latter, *necessarily*, grows not any slower than $N^{1/3}$ for large N. No wonder why matter occupies so large a volume! Here it is worth repeating some of the words addressed by Ehrenfest to Pauli in 1931 on the occasion of the Lorentz medal (Dyson, 1967) to this effect : *"We take a piece of metal, or a stone. When we think about it, we are astonished that this quantity of matter should occupy so large a volume"*. He went on by stating that the Pauli exclusion principle is the reason : *"Answer : only the Pauli principle, no two electrons in the same state"*. On the other hand for "bosonic matter" if deflation occurs upon collapse as more and more such matter is put together, then, we show in Appendix B of the thesis, for a non-vanishing probability of having the negatively charged particles within a sphere of radius R, the latter *necessarily* cannot decrease faster than $N^{-1/3}$ for negatively charged particles. This is in clear distinction with matter (i.e., matter with the exclusion principle) which inflates and R necessarily increases as proved below and is the subject matter of the present chapter.

To carry out this analysis we first derive in Sect. 4.2 an upper bound for the integral $\int \mathrm{d}^3\mathbf{x}\, \rho^{5/3}(\mathbf{x})$ involving the particle density $\rho(\mathbf{x})$ (see (4.22)). This upper bound is then used to obtain the major result of this thesis, that is, of the inflation of matter, stated above, in Sect. 4.3. The final section (Sect. 4.4) is devoted to deriving a non-zero lower bound for a measure of the extension of matter which relies on the analysis carried out in Sect. 4.3 on the inflation of matter.

4.2 Upper Bound for $\int \mathrm{d}^3\mathbf{x}\,\rho^{5/3}(\mathbf{x})$

The Hamiltonian under consideration is taken to be the N-electron one in (1.1). Also, as before, we consider neutral matter $\sum\limits_{i=1}^{k} Z_i = N$.

We first derive an upper bound to the expectation value of the kinetic energy of the electrons. Let $|\Psi(m)\rangle$ denote a normalized state giving a strictly negative expectation value for the Hamiltonian, i.e.,

$$-\mathcal{E}_N\,[m] \leqslant \langle\Psi(m)|\, H\, |\Psi(m)\rangle < 0 \tag{4.1}$$

where $-\mathcal{E}_N[m] = E_N < 0$ is the ground-state energy. The negative spectrum of H is not empty easily follows by noting that $-\mathcal{E}_N[m]$ is bounded above by $-\left(me^4/2\hbar^2\right)\sum\limits_{i=1}^{k} Z_i^2$, and we have emphasized its dependence on the mass m of the electron. Here we note, in general, that a part of a negative spectrum does not necessarily coincide with bound states. By definition of the ground-state energy, the state $|\Psi(m/2)\rangle$ cannot lead for $\langle\Psi(m/2)|\, H\, |\Psi(m/2)\rangle$ a numerical value lower than $-\mathcal{E}_N[m]$. That is

$$-\mathcal{E}_N\,[m] \leqslant \langle\Psi(m/2)|\, H\, |\Psi(m/2)\rangle \tag{4.2}$$

we note that the interaction part V of the Hamiltonian H in (1.1) is not explicitly dependent on m :

$$V = -\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_j e^2}{|\mathbf{x}_i - \mathbf{R}_j|} + \sum_{i<j}^{N}\frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} + \sum_{i<j}^{k}\frac{Z_i Z_j e^2}{|\mathbf{R}_i - \mathbf{R}_j|}. \tag{4.3}$$

Substituting (4.3) into the right-hand side of (1.1), we can rewrite (4.1) as

$$-\mathcal{E}_N\,[m] \leqslant \langle\Psi(m/2)|\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m} + V\,|\Psi(m/2)\rangle\,. \tag{4.4}$$

By using (4.4), replace m by $2m$, we obtain

$$-\mathcal{E}_N\left[2m\right] \leqslant \langle\Psi(m)| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{4m} + V\left|\Psi(m)\right\rangle . \tag{4.5}$$

From (1.1) and (4.3), we may also rewrite the Hamiltonian as

$$\begin{aligned} H &= \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + V \\ &= \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{4m} + \left(\sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{4m} + V \right) . \end{aligned} \tag{4.6}$$

The extreme right-hand side of the inequality (4.1) then leads to

$$\langle\Psi(m)| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{4m} \left|\Psi(m)\right\rangle < -\left\langle\Psi(m)\right| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{4m} + V\left|\Psi(m)\right\rangle \leqslant \mathcal{E}_N[2m]. \tag{4.7}$$

Multiply both sides of (4.7) by 2, to obtain

$$T \equiv \langle\Psi(m)| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \left|\Psi(m)\right\rangle < 2\,\mathcal{E}_N[2m] \tag{4.8}$$

This inequality may be equivalently obtained in the following manner. If we define the energy functional $\langle\phi|\, H\, |\phi\rangle = E_\phi$ for any normalized state $|\phi\rangle$ such that $E_\phi < 0$, then by using (4.6) we may write $E_\phi = (1/2)\, T_\phi + E'_\phi$, where $E'_\phi = \langle\phi|\, H'\, |\phi\rangle$ and H' denotes the second term in (4.6) within the brackets defining a Hamiltonian with mass $2m$. This immediately gives $T_\phi < 2\left|E'_\phi\right|$ and from the definition of the ground-state energy $-\mathcal{E}_N[2m]$ as the infimum of the spectrum in a theory with the mass m replaced by $2m$ leads to the inequality in (4.8).

The explicit lower bound for the ground-state energy of matter with the mass of the electron multiplied by 2, together from (2.19) and (2.49), leads to the following the lower bound for the kinetic energy

$$T \geqslant \frac{3}{\underline{q}^{1/3}} \left(\frac{\pi}{2}\right)^{2/3} \left(\frac{\hbar^2}{2m}\right) \left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^{2/3}. \tag{4.9}$$

We now use Hölder's inequality :

$$\left|\int \mathrm{d}^\nu\mathbf{x}\, f^*(\mathbf{x})\, g(\mathbf{x})\right| \leqslant \left(\int \mathrm{d}^\nu\mathbf{x}\ |f(\mathbf{x})|^p\right)^{1/p} \left(\int \mathrm{d}^\nu\mathbf{x}\ |g(\mathbf{x})|^q\right)^{1/q} \tag{4.10}$$

where p, $q > 1$, such that

$$\frac{1}{p} + \frac{1}{q} = 1. \tag{4.11}$$

From this inequality with $p = 3/2$ and $q = 3$, we obtain

$$\begin{aligned}
\int \mathrm{d}^3\mathbf{x}\, \rho^{5/3}(\mathbf{x}) &= \int \mathrm{d}^3\mathbf{x}\, \rho^{4/3}(\mathbf{x})\, \rho^{1/3}(\mathbf{x}) \\
&\leqslant \left(\int \mathrm{d}^3\mathbf{x}\ \left|\rho^{4/3}(\mathbf{x})\right|^{3/2}\right)^{2/3} \left(\int \mathrm{d}^3\mathbf{x}\ \left|\rho^{1/3}(\mathbf{x})\right|^{3}\right)^{1/3} \\
&= \left(\int \mathrm{d}^3\mathbf{x}\ \left|\rho^{2}(\mathbf{x})\right|\right)^{2/3} \left(\int \mathrm{d}^3\mathbf{x}\ |\rho(\mathbf{x})|\right)^{1/3} \\
&= \left(\int \mathrm{d}^3\mathbf{x}\, \rho^{2}(\mathbf{x})\right)^{2/3} \left(\int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\right)^{1/3} \\
&= \left(\int \mathrm{d}^3\mathbf{x}\, \rho^{2}(\mathbf{x})\right)^{2/3} N^{1/3}
\end{aligned}$$

$$\int \mathrm{d}^3\mathbf{x}\, \rho^{5/3}(\mathbf{x}) \leqslant N^{1/3} \left(\int \mathrm{d}^3\mathbf{x}\, \rho^{2}(\mathbf{x})\right)^{2/3} \tag{4.12}$$

where, from the normalization condition

$$\int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) = N \tag{4.13}$$

and from (4.12), we can rewrite as

$$\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3} \geqslant \frac{1}{N^{1/3}} \int \mathrm{d}^3\mathbf{x}\,\rho^{5/3}(\mathbf{x}). \tag{4.14}$$

Substitute (4.14) into the right-hand side of inequality (4.9), to obtain

$$T \geqslant \frac{3}{\underline{q}^{1/3}} \left(\frac{\pi}{2}\right)^{2/3} \left(\frac{\hbar^2}{2m}\right) \frac{1}{N^{1/3}} \int \mathrm{d}^3\mathbf{x}\,\rho^{5/3}(\mathbf{x}). \tag{4.15}$$

From (2.149), we obtain the lower for the ground-state energy of N fermions :

$$\langle\Psi|H|\Psi\rangle = -\mathcal{E}_N[m] > -\,1.89\,\underline{q}^{1/3} \left(\frac{me^4}{2\hbar^2}\right) \left(N + \sum_{i=1}^{k} Z_i^2\right)^{4/3}. \tag{4.16}$$

Replace m by $2m$, to obtain

$$\mathcal{E}_N[2m] > 1.89\,\underline{q}^{1/3} \left(\frac{me^4}{\hbar^2}\right) \left(N + \sum_{i=1}^{k} Z_i^2\right)^{4/3} \tag{4.17}$$

when we recall that $\underline{q} = 2s + 1 = 2$ for electrons.

For $\sum_{i=1}^{k} Z_i^2$, we can write

$$\begin{aligned} \sum_{i=1}^{k} Z_i^2 &\leqslant \sum_{i=1}^{k} Z_i\, Z_{\max} \\ &= N Z_{\max} \end{aligned} \tag{4.18}$$

where $Z_{\max}$ corresponds to the nucleus of having the charge. Therefore

$$\sum_{i=1}^{k} Z_i^2 \leqslant N Z_{\max}. \tag{4.19}$$

Substitute (4.19) into the right-hand side of inequality (4.17), to obtain

$$\begin{aligned}\mathcal{E}_N[2m] >& 1.89\,\underline{q}^{1/3}\left(\frac{me^4}{\hbar^2}\right)(N+NZ_{\max})^{4/3}\\ =& 1.89\,\underline{q}^{1/3}\left(\frac{me^4}{\hbar^2}\right)N^{4/3}(1+Z_{\max})^{4/3}\\ \therefore\quad \mathcal{E}_N[2m] >& 1.89\,\underline{q}^{1/3}\left(\frac{me^4}{\hbar^2}\right)N^{4/3}(1+Z_{\max})^{4/3}\,. \end{aligned} \tag{4.20}$$

Also substituting (4.15) and (4.20) into (4.8), we obtain

$$\frac{3}{\underline{q}^{1/3}N^{1/3}}\left(\frac{\pi}{2}\right)^{2/3}\left(\frac{\hbar^2}{2m}\right)\int \mathrm{d}^3\mathbf{x}\,\rho^{5/3}(\mathbf{x}) \leqslant T < 1.89\,\underline{q}^{1/3}\left(\frac{me^4}{\hbar^2}\right)N^{4/3}(1+Z_{\max})^{4/3} \tag{4.21}$$

where $\rho(\mathbf{x})$ is the particle density

$$\rho(\mathbf{x}) = N\sum_{\sigma_1,\ldots,\sigma_N}\int \mathrm{d}^3\mathbf{x}_2\ldots\mathrm{d}^3\mathbf{x}_N\,|\Psi(\mathbf{x}\sigma_1,\mathbf{x}_2\sigma_2,\ldots,\mathbf{x}_N\sigma_N)|^2 \tag{4.22}$$

and $\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x}) = N$, with a sum in (4.22) over spin indices σ_i.

4.3 Inflation of Matter and the Ehrenfest-Pauli Debate

Let $\mathbf{x}$ denote the position of an electron relative, for example, to the center of mass of the nuclei. Let $\chi_R(\mathbf{x}) = 1$, if $\mathbf{x}$ lines within a sphere of radius R, and $= 0$ otherwise.

We are interested in the expression

$$\begin{aligned}&\text{Prob}\,[|\mathbf{x}_1|\leqslant R,\ldots,|\mathbf{x}_N|\leqslant R]\\ &\qquad = \sum_{\sigma_1,\ldots,\sigma_N}\int\left(\prod_{i=1}^{N}\mathrm{d}^3\mathbf{x}_i\chi_R(\mathbf{x}_i)\right)|\Psi(\mathbf{x}_1\sigma_1,\ldots,\mathbf{x}_N\sigma_N)|^2\end{aligned} \tag{4.23}$$

which gives the probability of finding all the electrons within the sphere of radius R. Then clearly for the probability of the electrons to lie within such a sphere we have

$$\begin{aligned}\text{Prob}\,[|\mathbf{x}_1| \leqslant R, \ldots, |\mathbf{x}_N| \leqslant R] \leqslant \text{Prob}\,[|\mathbf{x}_1| \leqslant R] \\ = \frac{1}{N} \int \mathrm{d}^3\mathbf{x}\, \chi_R(\mathbf{x})\, \rho(\mathbf{x}) \\ \leqslant \frac{1}{N} \left(\int \mathrm{d}^3\mathbf{x}\, \rho^{5/3}(\mathbf{x}) \right)^{3/5} (v_R)^{2/5}\end{aligned} \tag{4.24}$$

where in the last inequality, we have used Hölder's inequality, to obtain

$$\int \mathrm{d}^3\mathbf{x}\, \chi_R(\mathbf{x})\, \rho(\mathbf{x}) \leqslant \left(\int \mathrm{d}^3\mathbf{x}\, \rho^{5/3}(\mathbf{x}) \right)^{3/5} \left(\int \mathrm{d}^3\mathbf{x}\, \chi_R(\mathbf{x}) \right)^{2/5} \tag{4.25}$$

where $\chi_R^{5/2}(\mathbf{x}) = \chi_R(\mathbf{x})$, and

$$\int \mathrm{d}^3\mathbf{x}\, \chi_R(\mathbf{x}) = v_R = \frac{4\pi R^3}{3} \tag{4.26}$$

with v_R denoting the volume of a sphere of radius R.

From (4.24), we obtain

$$\begin{aligned}\text{Prob}\,[|\mathbf{x}_1| \leqslant R, \ldots, |\mathbf{x}_N| \leqslant R] \leqslant \text{Prob}\,[|\mathbf{x}_1| \leqslant R] \\ \leqslant \frac{(v_R)^{2/5}}{N} \left(\int \mathrm{d}^3\mathbf{x}\, \rho^{5/3}(\mathbf{x}) \right)^{3/5}\end{aligned} \tag{4.27}$$

and from (4.21) we also have

$$\begin{aligned}\int \mathrm{d}^3\mathbf{x}\, \rho^{5/3}(\mathbf{x}) <& \underline{q}^{2/3} \left(\frac{2}{\pi}\right)^{2/3} \left(\frac{2m}{\hbar^2}\right) \frac{1.89}{3} \left(\frac{me^4}{\hbar^2}\right) N\,(1+Z_{\max})^{4/3} \\ =& \frac{(2)(1.89)\,\underline{q}^{2/3}}{3} \left(\frac{2}{\pi}\right)^{2/3} \left(\frac{m^2e^4}{\hbar^4}\right) N\,(1+Z_{\max})^{4/3}\end{aligned}$$

$$=0.932447\,\underline{q}^{2/3}\left(\frac{m^2e^4}{\hbar^4}\right)N\,(1+Z_{\max})^{4/3}$$

$$\therefore\quad \int \mathrm{d}^3\mathbf{x}\,\rho^{5/3}(\mathbf{x}) < 0.932447\,\underline{q}^{2/3}\left(\frac{m^2e^4}{\hbar^4}\right)N\,(1+Z_{\max})^{4/3} \tag{4.28}$$

where

$$\frac{(2)(1.89)}{3}\left(\frac{2}{\pi}\right)^{2/3} = 0.932447. \tag{4.29}$$

Thus we obtain the following bound

$$\left(\int \mathrm{d}^3\mathbf{x}\,\rho^{5/3}(\mathbf{x})\right)^{3/5} < (0.932447)^{3/5}\underline{q}^{2/5}\left(\frac{m^2e^4}{\hbar^4}\right)^{3/5}N^{3/5}\,(1+Z_{\max})^{4/5}$$

$$=0.958902\,\underline{q}^{2/5}\left(\frac{1}{a_0^2}\right)^{3/5}N^{3/5}\,(1+Z_{\max})^{4/5}$$

$$\therefore\quad \left(\int \mathrm{d}^3\mathbf{x}\,\rho^{5/3}(\mathbf{x})\right)^{3/5} < 0.958902\,\underline{q}^{2/5}\left(\frac{1}{a_0^2}\right)^{3/5}N^{3/5}\,(1+Z_{\max})^{4/5} \tag{4.30}$$

where $a_0 = \hbar^2/me^2$ is the Bohr radius.

Substitute (4.30) into the right-hand side of the equalities (4.24), to obtain

$$\text{Prob}\,[|\mathbf{x}_1| \leqslant R, \ldots, |\mathbf{x}_N| \leqslant R] < 0.958902\,\underline{q}^{2/5}\left(\frac{1}{a_0^2}\right)^{3/5}\frac{v_R^{2/5}}{N}N^{3/5}\,(1+Z_{\max})^{4/5}$$

$$= 0.958902\,\underline{q}^{2/5}\left(\frac{1}{a_0^2}\right)^{3/5}\left(\frac{v_R}{N}\right)^{2/5}(1+Z_{\max})^{4/5}$$

$$\text{Prob}\,[|\mathbf{x}_1| \leqslant R, \ldots, |\mathbf{x}_N| \leqslant R] < 0.958902\,\underline{q}^{2/5}\left(\frac{1}{a_0^2}\right)^{3/5}\left(\frac{v_R}{N}\right)^{2/5}(1+Z_{\max})^{4/5}. \tag{4.31}$$

From (4.31), we then have the main result of this chapter :

$$\text{Prob}\left[|\mathbf{x}_1| \leqslant R, \ldots, |\mathbf{x}_N| \leqslant R\right] \left(\frac{N}{v_R}\right)^{2/5} < 0.958902\, \underline{q}^{2/5} \left(\frac{1}{a_0^2}\right)^{3/5} (1 + Z_{\max})^{4/5}\,. \tag{4.32}$$

We may infer from (4.32) the inescapable fact that *necessarily* for a non-vanishing probability of having the electrons within a sphere of radius R, the corresponding volume v_R grows not any slower than the first power of N for $N \to \infty$, since otherwise the left-hand side of (4.32) would go to infinity and would be in contradiction with the finite upper bound on its right-hand side. That is, *necessarily*, the radius R grows not any slower than $N^{1/3}$ for $N \to \infty$, establishing the result stated above. No wonder why matter occupies so large a volume! In turn, the infinite density limit $N/v_R \to \infty$ does not arise as the probability on the left-hand side of (4.32) would go to zero in this limit upon multiplying (4.32) first by $(v_R/N)^{2/5}$.

From (4.27) and (4.21), we may also write

$$\begin{aligned} \frac{1}{N}\int \mathrm{d}^3\mathbf{x}\, \chi_R(\mathbf{x})\rho(\mathbf{x}) &= \text{Prob}\left[|\mathbf{x}| \leqslant R\right] \\ &< 0.958902\, \underline{q}^{2/5} \left(\frac{1}{a_0^2}\right)^{3/5} \left(\frac{v_R}{N}\right)^{2/5} (1 + Z_{\max})^{4/5}\,. \end{aligned} \tag{4.33}$$

This will be used in the next section to obtain a lower bound to measure of the extension of matter.

4.4 Non-Zero Lower Bound for a Measure of the Extension of Matter

As a measure of the extension of matter, we introduce the expectation value :

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle = \sum \sigma_1, \ldots, \sigma_N \int \mathrm{d}^3\mathbf{x}_1 \ldots \mathrm{d}^3\mathbf{x}_N \left(\sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N}\right) |\Psi(\mathbf{x}_1\sigma_1, \ldots, \mathbf{x}_N\sigma_N)|^2$$

$$= \frac{1}{N} \int \mathrm{d}^3\mathbf{x}\, |\mathbf{x}| \rho(\mathbf{x}). \tag{4.34}$$

Now we use the fact that

$$\frac{1}{N} \int \mathrm{d}^3\mathbf{x}\, |\mathbf{x}|\, \rho(\mathbf{x}) \geqslant \frac{1}{N} \int\limits_{|\mathbf{x}|>R} \mathrm{d}^3\mathbf{x}\, |\mathbf{x}|\, \rho(\mathbf{x}) \geqslant \frac{R}{N} \int\limits_{|\mathbf{x}|>R} \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})$$

$$= R \text{ Prob}\left[|\mathbf{x}| > R\right] \tag{4.35}$$

and

$$\text{Prob}\left[|\mathbf{x}| > R\right] = 1 - \text{Prob}\left[|\mathbf{x}| \leqslant R\right]. \tag{4.36}$$

From (4.26), (4.33), (4.34) and (4.36) we then the bounds

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle > R \text{ Prob}\left[|\mathbf{x}| > R\right]$$

$$= R\left[1 - \text{Prob}\left[|\mathbf{x}| \leqslant R\right]\right]$$

$$\geqslant R\left[1 - 0.958902\, \underline{q}^{2/5} \left(\frac{1}{a_0^2}\right)^{3/5} \left(\frac{v_R}{N}\right)^{2/5} (1 + Z_{\max})^{4/5}\right]$$

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle > R\left[1 - 0.958902\, \underline{q}^{2/5} \left(\frac{1}{a_0^2}\right)^{3/5} \left(\frac{4\pi R^3}{3N}\right)^{2/5} (1 + Z_{\max})^{4/5}\right]. \tag{4.37}$$

Upon optimizing the right-hand side of the above inequality over R, we get

$$0 = 1 - 0.958902\, \underline{q}^{2/5} \left(\frac{1}{a_0^2}\right)^{3/5} \left(\frac{4\pi}{3N}\right)^{2/5} \frac{11\, R^{6/5}}{5} (1 + Z_{\max})^{4/5} \tag{4.38}$$

leading to

$$R^{6/5} = \frac{1}{0.958902\, \underline{q}^{2/5}} \left(\frac{5}{11}\right) \left(\frac{3N}{4\pi}\right)^{2/5} \frac{a_0^{6/5}}{(1 + Z_{\max})^{4/5}} \tag{4.39}$$

and

$$R = \left(\frac{1}{0.958902\, \underline{q}^{2/5}} \right)^{5/6} \left(\frac{5}{11} \right)^{5/6} \left(\frac{3N}{4\pi} \right)^{1/3} \frac{a_0}{(1+Z_{\max})^{2/3}}. \tag{4.40}$$

Substitute (4.40) into the right-hand side of inequality (4.36), we obtain

$$\begin{aligned}
\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle > & \left[\left(\frac{1}{0.958902\, \underline{q}^{2/5}} \right)^{5/6} \left(\frac{5}{11} \right)^{5/6} \left(\frac{3N}{4\pi} \right)^{1/3} \frac{a_0}{(1+Z_{\max})^{2/3}} \right. \\
& -0.958902\, \underline{q}^{2/5} \left(\frac{1}{a_0^2} \right)^{3/5} \left(\frac{4\pi}{3N} \right)^{2/5} (1+Z_{\max})^{4/5} \\
& \left. \times \left(\left(\frac{1}{0.958902\, \underline{q}^{2/5}} \right)^{5/6} \left(\frac{5}{11} \right)^{5/6} \left(\frac{3N}{4\pi} \right)^{1/3} \frac{a_0}{(1+Z_{\max})^{2/3}} \right)^{6/5} \right] \\
= & \left[\left(\frac{1}{0.958902\, \underline{q}^{2/5}} \right)^{5/6} \left(\frac{5}{11} \right)^{5/6} \left(\frac{3N}{4\pi} \right)^{1/3} \frac{a_0}{(1+Z_{\max})^{2/3}} - \left(\frac{5}{11} \right)^{5/6} \right] \\
= & \left[0.333022\, \frac{1}{\underline{q}^{1/3}} \frac{a_0\, N^{1/3}}{(1+Z_{\max})^{2/3}} - \left(\frac{5}{11} \right)^{5/6} \right]
\end{aligned} \tag{4.41}$$

where

$$\left(\frac{1}{0.958902\, \underline{q}^{2/5}} \right)^{5/6} \left(\frac{5}{11} \right)^{5/6} \left(\frac{3}{4\pi} \right)^{1/3} = 0.333022\, \frac{1}{\underline{q}^{1/3}}. \tag{4.42}$$

Eq.(4.41) then leads to non-zero lower the explicit bound

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle > 0.333022\, \frac{a_0}{\underline{q}^{1/3}}\, \frac{N^{1/3}}{[1+Z_{\max}]^{2/3}}. \tag{4.43}$$

The method developed above has been also used to analyse the localizability and stability of other quantum mechanical systems (Manoukian, 2006).

CHAPTER V

STABILITY AND INFLATION OF MATTER IN $2D$

5.1 Introduction

There has been much interest in recent years in physics in $2D$, e.g. (Geyer, 1995; Badhuri, 1996; Semenoff, 1987; Forte, 1992), and the role of the spin and statistics theorem. Two dimensional matter is physically relevant. It has thus become important to investigate the nature of matter in $2D$ with the exclusion principle. As a matter of fact, it is an important theoretical question to investigate if the change of the dimensionality of space will change matter from a stable to an unstable or an explosive phase. We show that matter *is* stable in $2D$. [Some of the present field theories speculate that at early stages of our universe the dimensionality of space was not necessarily coinciding with three, and by a process which may be referred to as compactification of space, the present three-dimensional character of space arose upon the evolution and the cooling down of the universe.] We do not wish to speculate on higher dimensions than three until a detailed rigorous study of this is carried out as done here in two dimensions. A preliminary study of this shows that the Thomas–Fermi density is too singular at the origin leading to serious problems with normalizability conditions in conformity with earlier studies (Kventzel and Katriel, 1981).

In Sect. 5.2, a detailed study of the Thomas–Fermi (TF) atom is carried out in $2D$. Some very preliminary study of this was also carried out (Kventzel and Katriel, 1981). The TF energy, however, was neither computed in the latter reference nor it was shown that it provides the smallest possible energy value for the TF energy functional. A lower bound for the expectation value of the exact kinetic energy is then derived in Sec. 5.3 which will be needed in Sects. 5.5, 5.6. The No-binding Theorem [cf.(Lieb and Thirring, 1975)] is established in Sect. 5.4 in $2D$ from which a lower bound to the electron–electron potential is obtained. A lower bound to the exact-ground-state energy of matter in $2D$ is derived in Sect. 5.5. The inflation of matter is investigated in Sect. 5.6, where it is shown that for a non-vanishing probability of having the electrons within a circle of radius R, the latter, necessarily, does not grow any slower than $N^{1/2}$ for large N. A non-zero lower bound for a measure of an extension of such matter is derived in Sect. 5.7.

5.2 The Thomas-Fermi Atom in $2D$

The semi-classical Green function part $G_{\sigma\sigma'}(\mathbf{x}t;\mathbf{x}'0)$ with spin indices σ, σ', with potential $V(\mathbf{x})$ is given by (Manoukian, 2006)

$$G_{\sigma\sigma'}\left(\mathbf{x}\tau;\mathbf{x}'0\right) = \delta_{\sigma\sigma'}\int \frac{\mathrm{d}^D\mathbf{p}}{(2\pi\hbar)^D}\ \exp\mathrm{i}\left[\frac{\mathbf{p.(x-x')}}{\hbar} - \frac{\mathbf{p}^2}{2m}\tau - V(\mathbf{x})\tau\right] \tag{5.1}$$

and for coincident space points $\mathbf{x} = \mathbf{x}'$, we obtain

$$G_{\sigma\sigma'}(\mathbf{x}\tau;\mathbf{x}0) = \delta_{\sigma\sigma'}\int \frac{\mathrm{d}^D\mathbf{p}}{(2\pi\hbar)^D}\ \exp\left[-\mathrm{i}\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{x})\right)\tau\right]. \tag{5.2}$$

where $\tau = t/\hbar$.

The particle density $n(\mathbf{x})$ may be expressed in terms of the Green function $G_{\sigma\sigma'}(\mathbf{x}\tau;\mathbf{x}0)$ for coincident space points as

$$n(\mathbf{x}) = \frac{\underline{q}}{2\pi\mathrm{i}}\int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon}\ G_{\sigma\sigma}\left(\mathbf{x}\tau;\mathbf{x}0\right)\mathrm{e}^{\mathrm{i}\xi\tau}\ , \qquad \epsilon \to +0 \tag{5.3}$$

where $\underline{q} = \sum_{\sigma} 1$ is the spin multiplicity. Substitute (5.2) into (5.3), to obtain

$$n(\mathbf{x}) = \frac{\underline{q}}{2\pi\mathrm{i}}\int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon}\ \int \frac{\mathrm{d}^D\mathbf{p}}{(2\pi\hbar)^D}\ \exp\mathrm{i}\left[\xi\tau - \frac{\mathbf{p}^2}{2m}\tau - V(\mathbf{x})\tau\right] \tag{5.4}$$

which upon using the integral representation of the step function

$$\Theta(\xi) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \, \mathrm{e}^{\mathrm{i}\xi\tau} \tag{5.5}$$

and

$$\Theta\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \, \exp \mathrm{i}\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right)\tau \tag{5.6}$$

with

$$\Theta\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right) = 1 \tag{5.7}$$

for $0 < p < \sqrt{2m(\xi - V(\mathbf{x}))}$, when $p = |\mathbf{p}|$.

By using (5.6) and (5.7), as applied to the right-hand side of (5.4), we obtain

$$\begin{aligned}
n(\mathbf{x}) =& \underline{q} \int \frac{\mathrm{d}^D\mathbf{p}}{(2\pi\hbar)^D} \, \Theta\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right) \\
=& \frac{\underline{q}}{(2\pi\hbar)^D} \int_0^{\sqrt{2m(\xi - V)}} p^{D-1} \, \mathrm{d}p \int \mathrm{d}\Omega_\nu \\
=& \frac{\underline{q}}{(2\pi\hbar)^D} \frac{2\pi^{D/2}}{\Gamma\left(D/2\right)} \int_0^{\sqrt{2m(\xi - V(\mathbf{x}))}} p^{D-1} \, \mathrm{d}p \\
=& \frac{\underline{q}}{(2\pi\hbar)^D} \frac{2\pi^{D/2}}{\Gamma\left(D/2\right)} \frac{\left(\sqrt{2m(\xi - V(\mathbf{x}))}\right)^D}{D} \\
=& \frac{\underline{q} \, 2\pi^{D/2}}{D \, \Gamma\left(D/2\right)} \left(\frac{2m(\xi - V(\mathbf{x}))}{(2\pi\hbar)^2}\right)^{D/2} .
\end{aligned} \tag{5.8}$$

From (5.8), $V(\mathbf{x}) = 0$ and $n = 0$ at the boundary, we get $\xi = 0$. So that the density of electrons in D-dimensions is

$$n(\mathbf{x}) = \frac{\underline{q} \, 2\pi^{D/2}}{D \, \Gamma\left(D/2\right)} \left(\frac{-2mV(\mathbf{x})}{(2\pi\hbar)^2}\right)^{D/2} . \tag{5.9}$$

The relationship between the particle density $n(\mathbf{x})$ and the potential $V(\mathbf{x})$ in 2-dimensions, i.e., for $D = 2$ is then given by

$$\begin{aligned} n(\mathbf{x}) =& \frac{\underline{q}\; 2\pi}{2\,\Gamma\,(1)} \left(\frac{-2mV(\mathbf{x})}{(2\pi\hbar)^2} \right) \\ =& -\frac{\underline{q}\; m}{2\pi\hbar^2}\, V(\mathbf{x}). \end{aligned} \tag{5.10}$$

We may also rewrite (5.10) as

$$V(\mathbf{x}) = -\frac{2\pi\hbar^2}{\underline{q}\; m}\, n(\mathbf{x}) \tag{5.11}$$

To obtain the sum of the kinetic energies of the electrons in D-dimensions $(T[n])$, we use the relationship between the kinetic energy and the Green's function :

$$\begin{aligned} T[n] =& \sum_\sigma \int \mathrm{d}^D\mathbf{x}\, \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \left[\mathrm{i}\frac{\partial}{\partial \tau} - V(\mathbf{x}) \right] G_{\sigma\sigma'}(\mathbf{x}t;\mathbf{x}0) \\ =& \underline{q} \int \mathrm{d}^D\mathbf{x}\, \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \left[\mathrm{i}\frac{\partial}{\partial \tau} - V(\mathbf{x}) \right] G_{\sigma\sigma'}(\mathbf{x}t;\mathbf{x}0) \\ =& \underline{q} \int \mathrm{d}^D\mathbf{x}\, \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \left[\mathrm{i}\frac{\partial}{\partial \tau} - V(\mathbf{x}) \right] \int \frac{\mathrm{d}^D\mathbf{p}}{(2\pi\hbar)^D} \exp\left[-\mathrm{i}\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \right)\tau \right] \\ =& \underline{q} \int \mathrm{d}^D\mathbf{x}\, \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \int \frac{\mathrm{d}^D\mathbf{p}}{(2\pi\hbar)^D}\, \frac{\mathbf{p}^2}{2m}\, \exp\left[-\mathrm{i}\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \right)\tau \right]. \end{aligned} \tag{5.12}$$

Upon using the integral representation of the step function

$$\Theta(\xi) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon}\, \mathrm{e}^{\mathrm{i}\xi\tau} \tag{5.13}$$

we obtain

$$\Theta\left(-\frac{\mathbf{p^2}}{2m} - V(\mathbf{x}) \right) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon}\, \exp \mathrm{i} \left(-\frac{\mathbf{p^2}}{2m} - V(\mathbf{x}) \right) \tau \tag{5.14}$$

and

$$\Theta\left(-\frac{\mathbf{p^2}}{2m} - V(\mathbf{x})\right) = 1 \tag{5.15}$$

for $0 < p < \sqrt{-2mV(\mathbf{x})}$.

By using (5.14) and (5.15), as applied to the right-hand side of (5.12), we obtain

$$\begin{aligned}
T[n] =& \underline{q} \int \mathrm{d}^D\mathbf{x} \int \frac{\mathrm{d}^D\mathbf{p}}{(2\pi\hbar)^D} \frac{\mathbf{p}^2}{2m} \Theta\left(-\frac{\mathbf{p^2}}{2m} - V(\mathbf{x})\right) \\
=& \frac{\underline{q}}{(2\pi\hbar)^D} \int \mathrm{d}^D\mathbf{x} \int_0^{\sqrt{-2mV(\mathbf{x})}} \mathrm{d}^D p \, p^{D-1} \frac{p^2}{2m} \int \mathrm{d}\Omega \\
=& \frac{\underline{q}}{2m(2\pi\hbar)^D} \frac{2\pi^{D/2}}{\Gamma(D/2)} \int \mathrm{d}^D\mathbf{x} \int_0^{\sqrt{-2mV(\mathbf{x})}} \mathrm{d}p \, p^{D+1} \\
=& \frac{\underline{q}}{2m(2\pi\hbar)^D} \frac{2\pi^{D/2}}{\Gamma(D/2)} \int \mathrm{d}^D\mathbf{x} \left. \frac{p^{D+2}}{D+2} \right|_0^{\sqrt{-2mV(\mathbf{x})}} \\
=& \frac{\underline{q}}{2m(2\pi\hbar)^D} \frac{2\pi^{D/2}}{\Gamma(D/2)} \int \mathrm{d}^D\mathbf{x} \frac{(-2mV(\mathbf{x}))^{(D+2)/2}}{D+2} \\
=& \frac{\underline{q}}{2m(D+2)} \frac{2\pi^{D/2}}{\Gamma(D/2)} \int \mathrm{d}^D\mathbf{x} \frac{(-2mV(\mathbf{x}))^{(D+2)/2}}{(2\pi\hbar)^D} \\
=& \frac{\underline{q}}{2m(D+2)} \frac{2\pi^{D/2}}{\Gamma(D/2)} \int \mathrm{d}^D\mathbf{x} \, (-2mV(\mathbf{x})) \left(\frac{-2mV(\mathbf{x})}{(2\pi\hbar)^2}\right)^{D/2}.
\end{aligned} \tag{5.16}$$

The relationship between the kinetic energy T and the potential V in 2-dimensions, is then given by

$$\begin{aligned}
T[n] =& \frac{\underline{q}}{8m} \frac{2\pi}{\Gamma(1)} \int \mathrm{d}^2\mathbf{x} \, (-2mV(\mathbf{x})) \left(\frac{-2mV(\mathbf{x})}{(2\pi\hbar)^2}\right) \\
=& \frac{\underline{q}}{8m} \frac{2\pi}{\Gamma(1)} \int \mathrm{d}^2\mathbf{x} \left(\frac{4m^2[V(\mathbf{x})]^2}{(2\pi\hbar)^2}\right) \\
=& \frac{\underline{q}\, m}{4\pi\hbar^2} \int \mathrm{d}^2\mathbf{x} \, [V(\mathbf{x})]^2.
\end{aligned} \tag{5.17}$$

Substitute (5.11) into the right-hand side of (5.17), to obtain

$$T[n] = \frac{\underline{q}\, m}{4\pi\hbar^2} \int d^2\mathbf{x}\, [V(\mathbf{x})]^2$$

$$= \frac{\pi\hbar^2}{\underline{q}\, m} \int d^2\mathbf{x}\ [n(\mathbf{x})]^2 . \tag{5.18}$$

The Hamiltonian of a neutral atom consisting of Z electrons and a nucleus of charge $Z|e|$ is taken to be

$$H = \sum_{i=1}^{Z} \left(\frac{\mathbf{p}_i^2}{2m} - Ze^2 V(\mathbf{x}) \right) + \sum_{i<j}^{Z} e^2 V(\mathbf{x} - \mathbf{x}') \tag{5.19}$$

where $V(\mathbf{x})$ is the scaled potential satisfying the Poisson's equation given below :

$$\boldsymbol{\nabla}^2 2 \ln \frac{|\mathbf{x}|}{A} = 4\pi\delta^2(\mathbf{x}). \tag{5.20}$$

This is,

$$V(\mathbf{x}) = 2 \ln \frac{|\mathbf{x}|}{A} \tag{5.21}$$

for any dimensional scale factor A.

The expectation value of the Hamiltonian of a neutral atom consisting of Z electrons and a nucleus of charge $Z|e|$ in 2-dimensions is

$$\langle\psi|\, H\, |\psi\rangle = \langle\psi| \sum_{i=1}^{Z} \frac{\mathbf{p}_i^2}{2m} |\psi\rangle + 2Ze^2 \langle\psi| \sum_{i=1}^{Z} \ln \frac{|\mathbf{x}|}{A} |\psi\rangle$$

$$- 2e^2 \langle\psi| \sum_{i<j}^{Z} \ln \frac{|\mathbf{x} - \mathbf{x}'|}{B} |\psi\rangle \tag{5.22}$$

where

$$\langle\psi|\psi\rangle = \int d^2\mathbf{x}\ \psi^*(\mathbf{x}\sigma)\ \psi(\mathbf{x}\sigma)$$

$$= \int \mathrm{d}^2\mathbf{x}\, |\psi(\mathbf{x}\sigma)|^2$$

$$=1, \tag{5.23a}$$

$$\int \mathrm{d}^2\mathbf{x}\; n(\mathbf{x}) = Z. \tag{5.23b}$$

Here A and B are dimensional scale factors which will be determined below. Form (5.18), we obtain the first term on the right-hand side of (5.22), corresponding to the kinetic energy term $T[n] = \frac{\pi\hbar^2}{\underline{q}\; m} \int \mathrm{d}^2\mathbf{x}\; [n(\mathbf{x})]^2$.

Consider the second term on the right-hand side of (5.22). This is given by

$$2Ze^2 \langle\psi| \sum_{i=1}^{Z} \ln \frac{|\mathbf{x}|}{A} |\psi\rangle = 2Ze^2 \langle\psi| \, Z \ln \frac{|\mathbf{x}|}{A} |\psi\rangle$$

$$= 2Ze^2 \langle\psi| \int \mathrm{d}^2\mathbf{x}\, n(\mathbf{x}) \ln \frac{|\mathbf{x}|}{A} |\psi\rangle$$

$$= 2Ze^2 \int \mathrm{d}^2\mathbf{x}\; \ln \frac{|\mathbf{x}|}{A}\, n(\mathbf{x}). \tag{5.24}$$

Consider the third term on the right-hand side of (5.23). This is given by

$$2e^2 \langle\psi| \sum_{i<j}^{Z} \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B} |\psi\rangle = 2\frac{e^2}{2} \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}' n(\mathbf{x})\, n(\mathbf{x}') \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B} \langle\psi|\psi\rangle$$

$$= e^2 \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}'\; n(\mathbf{x})\, n(\mathbf{x}') \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}. \tag{5.25}$$

Substitute (5.18), (5.24) and (5.25) into (5.22), to obtain

$$\langle\psi| H |\psi\rangle = \frac{\pi\hbar^2}{\underline{q}\; m} \int \mathrm{d}^2\mathbf{x}\, [n(\mathbf{x})]^2 + 2Ze^2 \int \mathrm{d}^2\mathbf{x}\; \ln \frac{|\mathbf{x}|}{A}\, n(\mathbf{x})$$

$$- e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\; n(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\, n(\mathbf{x}'). \tag{5.26}$$

Referring to (5.18), (5.24) and (5.25), one may define the interaction of the electron-nucleus system in terms of the electron density, and add to it the kinetic energy term . Let $F[n]$ denote the *energy* functional in 2-dimensions as a function of the density $n(\mathbf{x})$. From (5.26) we obtain

$$F[n] = \frac{\pi\hbar^2}{\underline{q}\, m}\int \mathrm{d}^2\mathbf{x}\,[n(\mathbf{x})]^2 + 2Ze^2\int \mathrm{d}^2\mathbf{x}\;\ln\frac{|\mathbf{x}|}{A}\,n(\mathbf{x})$$

$$- e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\,n(\mathbf{x})\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\,n(\mathbf{x}'). \tag{5.27}$$

Optimize (5.27) with respect to $n(\mathbf{x})$, to obtain

$$0 = \frac{\delta F[n]}{\delta n(\mathbf{x})}$$

$$= \frac{2\pi\hbar^2}{\underline{q}\, m}[n(\mathbf{x})] + 2Ze^2\ln\frac{|\mathbf{x}|}{A} - 2e^2\int \mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\,n(\mathbf{x}')$$

$$-\frac{\pi\hbar^2}{\underline{q}\, m}[n(\mathbf{x})] = Ze^2\ln\frac{|\mathbf{x}|}{A} - e^2\int \mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\,n(\mathbf{x}') \tag{5.28}$$

with solution $n(\mathbf{x}) = n_{TF}(\mathbf{x})$ satisfying

$$n_{TF}(\mathbf{x}) = -\frac{\underline{q}\, mZe^2}{\pi\hbar^2}\ln\frac{|\mathbf{x}|}{A} + \frac{\underline{q}\, me^2}{\pi\hbar^2}\int \mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\,n_{TF}(\mathbf{x}'). \tag{5.29}$$

From (5.10), we obtain the relationship between $n_{TF}(\mathbf{x})$ and $V_{TF}(\mathbf{x})$ as

$$n_{TF}(\mathbf{x}) = \frac{\underline{q}\;2\pi}{2\,\Gamma(1)}\left(\frac{-2mV_{TF}(\mathbf{x})}{(2\pi\hbar)^2}\right)$$

$$= -\frac{\underline{q}\, m}{2\pi\hbar^2}\,V_{TF}(\mathbf{x}). \tag{5.30}$$

Substitute (5.29) into (5.30) to obtain

$$V_{TF}(\mathbf{x}) = Ze^2\left(2\ln\frac{|\mathbf{x}|}{A}\right) - e^2\int \mathrm{d}^2\mathbf{x}'\left(2\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\right)\,n_{TF}(\mathbf{x}') \tag{5.31}$$

and

$$\nabla^2 V_{TF}(\mathbf{x}) = Ze^2\nabla^2\left(2\ln\frac{|\mathbf{x}|}{A}\right) - e^2\nabla^2\int \mathrm{d}^2\mathbf{x}'\left(2\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\right) n_{TF}(\mathbf{x}')$$
$$\equiv F_1 - F_2 \tag{5.32}$$

where

$$F_1 = Ze^2\nabla^2\left(2\ln\frac{|\mathbf{x}|}{A}\right)$$
$$= Ze^2 4\pi\delta^2(\mathbf{x}) \tag{5.33}$$

and

$$F_2 = e^2\nabla^2\int \mathrm{d}^2\mathbf{x}'\left(2\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\right) n_{TF}(\mathbf{x}')$$
$$= e^2\int \mathrm{d}^2\mathbf{x}'\, n_{TF}(\mathbf{x}')\, \nabla^2\left(2\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\right)$$
$$= e^2\int \mathrm{d}^2\mathbf{x}'\, n_{TF}(\mathbf{x}')\, 4\pi\delta^2(\mathbf{x}-\mathbf{x}')$$
$$= 4\pi e^2 n_{TF}(\mathbf{x}). \tag{5.34}$$

Substitute (5.33) and (5.34) into (5.32), to obtain

$$\nabla^2 V_{TF}(\mathbf{x}) = F_1 - F_2$$
$$= 4\pi Ze^2\delta^2(\mathbf{x}) - 4\pi e^2 n_{TF}(\mathbf{x}). \tag{5.35}$$

For the integral of the left-hand side of (5.35) over $\mathbf{x}$, we have

$$\int \mathrm{d}^2\mathbf{x}\, \nabla^2 V_{TF}(\mathbf{x}) = \int \mathrm{d}^2\mathbf{x} 4\pi Z e^2 \delta^2(\mathbf{x}) - 4\pi e^2 \int \mathrm{d}^2\mathbf{x}\, n_{TF}(\mathbf{x}). \tag{5.36}$$

The first term on the right-hand side of (5.36) is easily evaluated giving by

$$\int \mathrm{d}^2\mathbf{x}\, 4\pi Z e^2 \delta^2(\mathbf{x}) = 4\pi Z e^2. \tag{5.37}$$

For the second-term of the right-hand side of (5.36), we obtain

$$4\pi e^2 \int \mathrm{d}^2\mathbf{x}\, n_{TF}(\mathbf{x}) = 4\pi Z e^2. \tag{5.38}$$

Substitute (5.37) and (5.38) into (5.36), to obtain

$$\int \mathrm{d}^2\mathbf{x}\, \nabla^2 V_{TF}(\mathbf{x}) = 4\pi Z e^2 - 4\pi Z e^2 = 0. \tag{5.39}$$

Apply Laplacian operator to the left-hand side of (5.29), to obtain

$$\begin{aligned}
\nabla^2 n_{TF}(\mathbf{x}) =& \nabla^2 \left[-\frac{\underline{q}\, mZe^2}{\pi\hbar^2} \ln \frac{|\mathbf{x}|}{A} + \frac{\underline{q}\, me^2}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}'\ \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ n_{TF}(\mathbf{x}') \right] \\
=& -\frac{\underline{q}\, mZe^2}{\pi\hbar^2} \nabla^2 \ln \frac{|\mathbf{x}|}{A} + \frac{\underline{q}\, me^2}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}'\, n_{TF}(\mathbf{x}')\, \nabla^2 \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B} \\
=& -\frac{\underline{q}\, mZe^2}{\pi\hbar^2} 2\pi\delta^2(\mathbf{x}) + \frac{\underline{q}\, me^2}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}'\, n_{TF}(\mathbf{x}')\, 2\pi\delta^2(\mathbf{x}-\mathbf{x}') \\
=& -\frac{\underline{q}\, mZe^2}{\hbar^2} \delta^2(\mathbf{x}) + \frac{\underline{q}\, me^2}{\hbar^2} \int \mathrm{d}^2\mathbf{x}'\, n_{TF}(\mathbf{x}')\, \delta^2(\mathbf{x}-\mathbf{x}') \\
=& -\frac{\underline{q}\, mZe^2}{\hbar^2} \delta^2(\mathbf{x}) + \frac{\underline{q}\, me^2}{\hbar^2}\, n_{TF}(\mathbf{x})
\end{aligned}$$

$$\therefore \quad n_{TF}(\mathbf{x}) = Z\delta^2(\mathbf{x}) + \frac{\hbar^2}{\underline{q}\, me^2} \nabla^2 n_{TF}(\mathbf{x}). \tag{5.40}$$

Integraling the latter over $vecx$ gives

$$\int \mathrm{d}^2\mathbf{x}\, n_{TF}(\mathbf{x}) = \int \mathrm{d}^2\mathbf{x}\, Z\, \delta^2(\mathbf{x}) + \frac{\hbar^2}{\underline{q}\, me^2} \int \mathrm{d}^2\mathbf{x}\, \nabla^2 n_{TF}(\mathbf{x}). \tag{5.41}$$

From (5.30), we have for the second term

$$\int \mathrm{d}^2\mathbf{x}\, \nabla^2 n_{TF}(\mathbf{x}) = -\frac{\underline{q}\, m}{2\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}\, \nabla^2 V_{TF}(\mathbf{x}) = 0. \tag{5.42}$$

Substitute (5.42) into the second term on the right-hand side of (5.41), to obtain

$$\int \mathrm{d}^2\mathbf{x}\, n_{TF}(\mathbf{x}) = Z \tag{5.43}$$

as expected.

To obtain the exact expressions for the scaling dimensionless constant A and B in the definition of $F[n]$ in (5.29), first, apply taking the Laplacian to the left-hand side of (5.29), to obtain

$$\begin{aligned} \nabla^2 n_{TF}(\mathbf{x}) =& \nabla^2 \left[-\frac{\underline{q}\, mZe^2}{\pi\hbar^2} \ln \frac{|\mathbf{x}|}{A} + \frac{\underline{q}\, me^2}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}'\, \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\, n_{TF}(\mathbf{x}') \right] \\ =& -\frac{\underline{q}\, mZe^2}{\pi\hbar^2} \nabla^2 \ln \frac{|\mathbf{x}|}{A} + \frac{\underline{q}\, me^2}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}'\, n_{TF}(\mathbf{x}')\, \nabla^2 \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B} \end{aligned} \tag{5.44}$$

Consider the first term on right-hand side of (5.44), to get

$$\begin{aligned} \frac{\underline{q}\, mZe^2}{\pi\hbar^2} \nabla^2 \ln \frac{|\mathbf{x}|}{A} =& \frac{\underline{q}\, mZe^2}{\pi\hbar^2} (2\pi\delta^2(\mathbf{x})) \\ =& \frac{\underline{q}\, mZe^2}{\hbar^2} \delta^2(\mathbf{x}) \end{aligned} \tag{5.45}$$

Consider the second term on the right-hand side of (5.44), to get

$$\frac{\underline{q}\, me^2}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}'\, n_{TF}(\mathbf{x}')\, \nabla^2 \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B} = \frac{\underline{q}\, me^2}{\pi\hbar^2} 2\pi \int \mathrm{d}^2\mathbf{x}'\, n_{TF}(\mathbf{x}')\, \delta^2(\mathbf{x}-\mathbf{x}')$$

$$= \frac{\underline{q}2me^2}{\hbar^2}\, n_{TF}(\mathbf{x}). \tag{5.46}$$

Substitute (5.45) and (5.46) into (5.44), to obtain

$$\nabla^2 n_{TF}(\mathbf{x}) = -\frac{\underline{q}\; mZe^2}{\hbar^2}\delta^2(\mathbf{x}) + \frac{\underline{q}2me^2}{\hbar^2}\, n_{TF}(\mathbf{x}) \tag{5.47}$$

which upon multiplying (5.47) by r^2, we obtain

$$\begin{aligned}
r^2\nabla^2 n_{TF}(\mathbf{x}) =& -\frac{\underline{q}\; mZe^2}{\hbar^2} r^2\delta^2(\mathbf{x}) + \frac{\underline{q}2me^2}{\hbar^2}\, r^2\, n_{TF}(\mathbf{x}) \\
=& -\frac{\underline{q}\; mZe^2}{\hbar^2} r^2\frac{\delta(r)}{2\pi r} + \frac{\underline{q}2me^2}{\hbar^2}\, r^2\, n_{TF}(\mathbf{x}) \\
=& -\frac{\underline{q}\; mZe^2}{\hbar^2}\frac{r\;\delta(r)}{2\pi} + \frac{\underline{q}2me^2}{\hbar^2}\, r^2\, n_{TF}(\mathbf{x}) \\
=& \frac{\underline{q}\; me^2}{\hbar^2}\, r^2\, n_{TF}(\mathbf{x}) \\
0 =& r^2\nabla^2 n_{TF}(\mathbf{x}) - \frac{\underline{q}2me^2}{\hbar^2}\, r^2\, n_{TF}(\mathbf{x}) \\
0 =& \left(r^2\nabla^2 - \frac{\underline{q}2me^2 r^2}{\hbar^2}\right) n_{TF}(\mathbf{x})
\end{aligned} \tag{5.48}$$

where

$$\int_0^\infty r\;\delta(r)\;\mathrm{d}r = 0, \tag{5.49a}$$

$$r\,\delta(r) = 0. \tag{5.49b}$$

We set

$$\frac{r}{r_0} = R. \tag{5.50}$$

The general solution of (5.48) is given by

$$n_{TF}(R) = C_1 K_0(R) + C_2 I_0(R) \tag{5.51}$$

where K_0 and I_0 are modified Bessel functions and

$$r_0 = \left(\frac{\hbar^2}{2\underline{q}me^2}\right)^{1/2}. \tag{5.52}$$

Consider the large R behavior, $I_0(R) \to \infty$ for $R \to \infty$ so we have to choose $C_2 = 0$ and the solution of (5.48) becomes

$$n_{TF}(R) = C_1 K_0(R). \tag{5.53}$$

To obtain C_1, substitute (5.53) into (5.43), we get

$$\begin{aligned} Z =& C_1 \int \mathrm{d}^2\mathbf{x}\ K_0(R) \\ =& C_1 \int_0^\infty \mathrm{d}r \int_0^{2\pi} \mathrm{d}\theta\ r\ K_0(R) \\ =& 2\pi r_0^2\ C_1 \int_0^\infty \mathrm{d}R\ \ R\ K_0(R) \\ =& 2\pi r_0^2\ C_1 \\ =& 2\pi \left(\frac{\hbar^2}{2\underline{q}me^2}\right)\ C_1 \end{aligned}$$

$$C_1 = \left(\frac{\underline{q}mZe^2}{\pi\hbar^2}\right) \tag{5.54}$$

where

$$\int_0^\infty \mathrm{d}R\ R\ K_0(R) = 1. \tag{5.55}$$

Substitute (5.55) into (5.54), to obtain

$$n_{TF}(R) = \left(\frac{\underline{\underline{q}}mZe^2}{\pi\hbar^2}\right) K_0(R) \quad , \quad R = \frac{r}{r_0}. \tag{5.56}$$

To obtain A and B, by substitute (5.56) into (5.29) , to obtain

$$\left(\frac{\underline{\underline{q}}mZe^2}{\pi\hbar^2}\right) K_0\left(\frac{r}{r_0}\right) = -\frac{\underline{\underline{q}}\, mZe^2}{\pi\hbar^2} \ln\frac{|\mathbf{x}|}{A} + \frac{\underline{\underline{q}}\, me^2}{\pi\hbar^2}\int \mathrm{d}^2\mathbf{x}' \ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\, n_{TF}(\mathbf{x}')$$

$$= Q_1(\mathbf{x}) + Q_2(\mathbf{x}) \tag{5.57}$$

where

$$Q_1(\mathbf{x}) = -\frac{\underline{\underline{q}}\, mZe^2}{\pi\hbar^2} \ln\frac{|\mathbf{x}|}{A} \tag{5.58}$$

and

$$Q_2(\mathbf{x}) = \frac{\underline{\underline{q}}\, me^2}{\pi\hbar^2}\int \mathrm{d}^2\mathbf{x}' \ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\, n_{TF}(\mathbf{x}'). \tag{5.59}$$

Let $\mathbf{x} = 0$, the left-hand side of (5.56) will become

$$\left(\frac{\underline{\underline{q}}mZe^2}{\pi\hbar^2}\right) K_0(R) \simeq -\left(\frac{\underline{\underline{q}}mZe^2}{\pi\hbar^2}\right) \ln R. \tag{5.60}$$

The first term on the right-hand side of (5.57) becomes

$$Q_1(\mathbf{x}) \simeq -\left(\frac{\underline{\underline{q}}\, mZe^2}{\pi\hbar^2}\right)\left(\ln\frac{Rr_0}{A}\right). \tag{5.61}$$

The second term on right-hand side of (5.57) becomes

$$Q_2(0) = \frac{\underline{\underline{q}}\, me^2}{\pi\hbar^2}\left[\int \mathrm{d}^2\mathbf{x}' \ \ln\frac{|\mathbf{x}'|}{B}\, n_{TF}(\mathbf{x}')\right]$$

$$
\begin{aligned}
=&\frac{\underline{q}\, me^2}{\pi\hbar^2}\left[\int \mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}'|}{r_0}\,n_{TF}(\mathbf{x}') + \int \mathrm{d}^2\mathbf{x}'\;\ln\frac{r_0}{B}\,n_{TF}(\mathbf{x}')\right]\\
=&\frac{\underline{q}\, me^2}{\pi\hbar^2}\left[\int \mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}'|}{r_0}\,n_{TF}(\mathbf{x}') + Z\ln\frac{r_0}{B}\right]\\
=&\frac{\underline{q}\, me^2}{\pi\hbar^2}(r_0^2)(2\pi)\int \mathrm{d}R'\;R'\;\ln R'\,n_{TF}(R') + \frac{\underline{q}\, me^2}{\pi\hbar^2}Z\ln\frac{r_0}{B}\\
=&\frac{\underline{q}\, me^2}{\pi\hbar^2}\left(\frac{\hbar^2}{\underline{q}2me^2}\right)(2\pi)\left(\frac{\underline{q}mZe^2}{\pi\hbar^2}\right)\int \mathrm{d}R'\;R'\;\ln R'\;K_0(R')\\
&+\frac{\underline{q}\, me^2}{\pi\hbar^2}Z\ln\frac{r_0}{B}\\
=&\frac{\underline{q}\, me^2}{\pi\hbar^2}Z\int \mathrm{d}R'\;R'\;\ln R'\;K_0(R') + \frac{\underline{q}\, me^2}{\pi\hbar^2}Z\ln\frac{r_0}{B}\\
=&\frac{\underline{q}\, me^2}{\pi\hbar^2}Z[-\gamma+\ln 2] + \frac{\underline{q}\, me^2}{\pi\hbar^2}Z\ln\frac{r_0}{B}. \qquad (5.62)
\end{aligned}
$$

Referring to (5.60)–(5.62), for $R\simeq 0$ we obtain

$$
\begin{aligned}
Q_1(0)+Q_2(0) &= \left(\frac{\underline{q}mZe^2}{\pi\hbar^2}\right)K_0(0)\\
\ln 2+\ln\frac{r_0}{B} &\simeq -\left(\frac{\underline{q}mZe^2}{\pi\hbar^2}\right)\ln R + \frac{\underline{q}\, mZe^2}{\pi\hbar^2}\left[\ln\frac{Rr_0}{A}+\gamma\right]\\
-\ln B &= -\ln(2r_0) \qquad (5.63)
\end{aligned}
$$

giving

$$
B = 2r_0. \qquad (5.64)
$$

To obtain A, substitute (5.64) into (5.57), to obtain

$$
\left(\frac{\underline{q}mZe^2}{\pi\hbar^2}\right)K_0(R) = -\frac{\underline{q}\, mZe^2}{\pi\hbar^2}\ln\frac{|\mathbf{x}|}{A} + \frac{\underline{q}\, me^2}{\pi\hbar^2}\int \mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\,n_{TF}(\mathbf{x}')
$$

$$
\begin{aligned}
&= -\frac{\underline{q}\, mZe^2}{\pi\hbar^2} \ln\frac{|\mathbf{x}|}{2r_0} + \frac{\underline{q}\, me^2}{\pi\hbar^2}\int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{A}\ n_{TF}(\mathbf{x}') \\
&= Q_3(\mathbf{x}) + Q_4(\mathbf{x})
\end{aligned} \tag{5.65}
$$

where

$$
Q_3(\mathbf{x}) = -\frac{\underline{q}\, mZe^2}{\pi\hbar^2}\ln\frac{|\mathbf{x}|}{2r_0} \tag{5.66}
$$

and

$$
Q_4(\mathbf{x}) = \frac{\underline{q}\, me^2}{\pi\hbar^2}\int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{A}\ n_{TF}(\mathbf{x}'). \tag{5.67}
$$

Let $\mathbf{x} = 0$, the left-hand side of (5.65) becomes

$$
\left(\frac{\underline{q}mZe^2}{\pi\hbar^2}\right) K_0(R) \simeq -\left(\frac{\underline{q}mZe^2}{\pi\hbar^2}\right)\ln R. \tag{5.68}
$$

The first term on right-hand side of (5.65) becomes

$$
Q_3(\mathbf{x}) \simeq -\frac{\underline{q}\, mZe^2}{\pi\hbar^2}\left(\ln\frac{Rr_0}{2r_0}\right). \tag{5.69}
$$

For the second term on right-hand side of (5.65) becomes

$$
\begin{aligned}
Q_4(0) =& \frac{\underline{q}\, me^2}{\pi\hbar^2}\left[\int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}'|}{A}\ n_{TF}(\mathbf{x}')\right] \\
=& \frac{\underline{q}\, me^2}{\pi\hbar^2}\left[\int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}'|}{r_0}\ n_{TF}(\mathbf{x}') + \int \mathrm{d}^2\mathbf{x}'\ \ln\frac{r_0}{A}\ n_{TF}(\mathbf{x}')\right] \\
=& \frac{\underline{q}\, me^2}{\pi\hbar^2}\left[\int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}'|}{r_0}\ n_{TF}(\mathbf{x}') + Z\ln\frac{r_0}{A}\right] \\
=& \frac{\underline{q}\, me^2}{\pi\hbar^2}(r_0^2)(2\pi)\int \mathrm{d}R'\ R'\ \ln R'\ n_{TF}(R') + \frac{\underline{q}\, me^2}{\pi\hbar^2} Z\ln\frac{r_0}{A}
\end{aligned}
$$

$$
\begin{aligned}
=&\frac{\underline{q}\, me^2}{\pi\hbar^2}\left(\frac{\hbar^2}{\underline{q}2me^2}\right)(2\pi)\left(\frac{qmZe^2}{\pi\hbar^2}\right)\int \mathrm{d}R'\ R'\ \ln R'\ K_0(R') \\
&+\frac{\underline{q}\, me^2}{\pi\hbar^2}Z\ln\frac{r_0}{A} \\
=&\frac{\underline{q}\, me^2}{\pi\hbar^2}Z\int \mathrm{d}R'\ R'\ \ln R'\ K_0(R')+\frac{\underline{q}\, me^2}{\pi\hbar^2}Z\ln\frac{r_0}{A} \\
=&\frac{\underline{q}\, me^2}{\pi\hbar^2}Z[-\gamma+\ln 2]+\frac{\underline{q}\, me^2}{\pi\hbar^2}Z\ln\frac{r_0}{A}.
\end{aligned}
\tag{5.70}
$$

Referring to (5.68)- (5.70), for $R\simeq 0$ we obtain

$$
\begin{aligned}
Q_3(0)+Q_4(0)=&\left(\frac{\underline{q}mZe^2}{\pi\hbar^2}\right)K_0(0) \\
\ln 2+\ln\frac{r_0}{A}\simeq&-\left(\frac{\underline{q}mZe^2}{\pi\hbar^2}\right)\ln R+\frac{\underline{q}\, mZe^2}{\pi\hbar^2}\left[\ln\frac{Rr_0}{A}+\gamma\right] \\
-\ln A=&-\ln(2r_0)
\end{aligned}
\tag{5.71}
$$

giving

$$
A=2r_0. \tag{5.72}
$$

Substituting the values obtained for B and A in (5.64) and (5.72), into (5.27), we obtain the energy functional $F[n]$ as

$$
\begin{aligned}
F[n]=\frac{\pi\hbar^2}{qm}&\int\mathrm{d}^2\mathbf{x}\ \left[n(\mathbf{x})\right]^2+2Ze^2\int\mathrm{d}^2\mathbf{x}\ \ln\left(\frac{|\mathbf{x}|}{2r_0}\right)n(\mathbf{x}) \\
&-e^2\int\mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ n(\mathbf{x})\ln\left(\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\right)n(\mathbf{x}').
\end{aligned}
\tag{5.73}
$$

From (5.73), with $n=n_{TF}$, we obtain the TF energy functional $F[n_{TF}]$:

$$
F[n_{TF}]=\frac{\pi\hbar^2}{\underline{q}\ m}\int\mathrm{d}^2\mathbf{x}\,[n_{TF}(\mathbf{x})]^2+2Ze^2\int\mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{2r_0}\ n_{TF}(\mathbf{x})
$$

$$- e^2 \int d^2\mathbf{x}\, d^2\mathbf{x}'\, n_{TF}(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\, n_{TF}(\mathbf{x}'). \tag{5.74}$$

To obtain the ground-state energy of the TF atom $F[n_{TF}] \equiv E_{TF}(Z)$, we refer to (5.29) and (5.74) for the kinetic energy term $T[n_{TF}]$, given by

$$T[n_{TF}] = \frac{\pi\hbar^2}{\underline{q}\, m} \int d^2\mathbf{x}\, [n_{TF}(\mathbf{x})]^2 \,. \tag{5.75}$$

Substitute (5.56) into (5.75), to obtain

$$\begin{aligned} T[n_{TF}] =& \frac{\pi\hbar^2}{\underline{q}\, m} \int d^2\mathbf{x}\, [n_{TF}(\mathbf{x})]^2 \\ =& \frac{\pi\hbar^2}{\underline{q}\, m} 2\pi \int_0^\infty dr\, r\; [n_{TF}(r)]^2 \\ =& \frac{\pi\hbar^2}{\underline{q}\, m} 2\pi r_0^2 \int_0^\infty dR\, R\, \left(\frac{\underline{q} m Z e^2}{\pi\hbar^2}\right)^2 [K_0(R)]^2 \\ =& \frac{2\pi^2\hbar^2}{\underline{q}\, m} \left(\frac{\hbar^2}{\underline{q} 2me^2}\right) \left(\frac{\underline{q} m Z e^2}{\pi\hbar^2}\right)^2 \int_0^\infty dR\, R\; [K_0(R)]^2 \\ =& \frac{1}{2} Z^2 e^2 \end{aligned} \tag{5.76}$$

where

$$\int_0^\infty dR\, R\; [K_0(R)]^2 = \frac{1}{2}. \tag{5.77}$$

For the electron-nucleus interaction part, we have

$$\begin{aligned} E_{e-n}[n_{TF}] =& 2Ze^2 \int d^2\mathbf{x}\; \ln \frac{|\mathbf{x}|}{2r_0}\, n_{TF}(\mathbf{x}) \\ =& Ze^2 4\pi \int_0^\infty dr\, r\; \ln \frac{r}{2r_0}\, n_{TF}(r) \end{aligned}$$

$$
\begin{aligned}
=&Ze^2 4\pi \int_0^\infty \mathrm{d}r\; r\; \ln\frac{r}{r_0}\, n_{TF}(r) - 2Ze^2 \int \mathrm{d}^2\mathbf{x}\; \ln 2\, n_{TF}(\mathbf{x}) \\
=&Ze^2 4\pi r_0^2 \int_0^\infty \mathrm{d}R\; R\; \ln(R)\; \left(\frac{2\underline{q}mZe^2}{2\pi\hbar^2}\right)\; K_0(R) - 2Z^2e^2 \ln 2 \\
=&Ze^2 4\pi r_0^2 \frac{Z}{2\pi r_0^2} \int_0^\infty \mathrm{d}R\; R\; \ln R\; K_0(R) - 2Z^2e^2 \ln 2 \\
=&2Z^2e^2 \left[\int_0^\infty \mathrm{d}R\; R\; \ln R\; K_0(R) - \ln 2\right] \\
=&2Z^2e^2 \left[-\gamma + \ln 2 - \ln 2\right] \\
=&-2\gamma Z^2 e^2
\end{aligned} \tag{5.78}
$$

where

$$
\int_0^\infty \mathrm{d}R\; R\; \ln R\; K_0(R) = -\gamma + \ln 2, \tag{5.79a}
$$

$$
\gamma = 0.57722, \tag{5.79b}
$$

$$
\int_0^\infty \mathrm{d}R\; R\; K_0(R) = 1. \tag{5.79c}
$$

The electron-electron interaction part is given by

$$
\begin{aligned}
E_{e-e}[n_{TF}] =& -e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\; n_{TF}(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\; n_{TF}(\mathbf{x}') \\
=& -e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\; n_{TF}(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\; n_{TF}(\mathbf{x}') \\
=& +4\pi^2 e^2 C^2 r_0^4 \ln 2 \int \mathrm{d}R\; R\; K_0(\mathbf{R}) \int \mathrm{d}R'\; R'\;\; K_0(\mathbf{R}') \\
& - e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}' n_{TF}(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{r_0}\; n_{TF}(\mathbf{x}')
\end{aligned}
$$

$$= + e^2 Z^2 \ln 2 - e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, n_{TF}(\mathbf{x}) \ln \frac{|\mathbf{x} - \mathbf{x}'|}{r_0}\, n_{TF}(\mathbf{x}')$$

$$= e^2 Z^2 \ln 2 + I_1 \tag{5.80}$$

where

$$I_1 = -e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, n_{TF}(\mathbf{x}) \ln \frac{|\mathbf{x} - \mathbf{x}'|}{r_0}\, n_{TF}(\mathbf{x}'). \tag{5.81}$$

By setting $\mathbf{x}/r_0 = \mathbf{R}$, we obtain

$$\int \mathrm{d}^2\mathbf{x}\,(.) = \int_0^\infty r\, \mathrm{d}r \int_0^{2\pi} \mathrm{d}\theta\,(.)$$

$$= r_0^2 \int_0^\infty R\, \mathrm{d}R \int_0^{2\pi} \mathrm{d}\theta\,(.)$$

$$= r_0^2 \int \mathrm{d}^2\mathbf{R}\,(.). \tag{5.82}$$

Substitute (5.82) into (5.81), to obtain

$$I_1 = - e^2 r_0^4 \int \mathrm{d}^2\mathbf{R}\, \mathrm{d}^2\mathbf{R}'\, n_{TF}(\mathbf{R}) \ln |\mathbf{R} - \mathbf{R}'|\, n_{TF}(\mathbf{R}')$$

$$= - 2\pi e^2 \left(\frac{\hbar^2}{\underline{q}2me^2}\right)^2 \left(\frac{\underline{q}mZe^2}{\pi\hbar^2}\right)^2 \left(\int_0^\infty \mathrm{d}R\, R\, K_0(R) \int_0^\infty \mathrm{d}R'\, R'\, K_0(R')\right.$$

$$\left. \times \int_0^{2\pi} \mathrm{d}\theta\, \ln(R^2 - 2RR' \cos\theta + R'^2)^{1/2}\right)$$

$$= - \frac{e^2 Z^2}{2\pi} \left[\int_0^\infty \mathrm{d}R\, R\, K_0(R) \int_0^\infty \mathrm{d}R'\, R'\, K_0(R')\right.$$

$$\left. \times \int_0^{2\pi} \mathrm{d}\theta\, \ln(R^2 - 2RR' \cos\theta + R'^2)^{1/2}\right]$$

$$= - \frac{e^2 Z^2}{2} \int_0^\infty \mathrm{d}R\, R\, K_0(R) \int_0^\infty \mathrm{d}R'\, R'\, K_0(R')\, \ln R_>^2$$

$$= -\frac{e^2 Z^2}{2}\int_0^\infty dR\, R\, K_0(R)\, f(R) \tag{5.83}$$

where

$$\int_0^{2\pi} d\theta\ \ln(R^2 - 2RR'\cos\theta + R'^2)^{1/2} = \pi \ln R_>^2 \tag{5.84}$$

and

$$\begin{aligned} f(R) &= \int_0^\infty dR'\, R'\, K_0(R')\, \ln R_>^2 \\ &= \ln R^2 \int_0^R dR'\, R'\, K_0(R') + \int_R^\infty dR'\, R'\, K_0(R')\, \ln R'^2 \\ &= \ln R^2 [1 - R\, K_1(R)] + \int_R^\infty dR'\, R'\, K_0(R')\, \ln R'^2 \\ &= \ln R^2 - R\, K_1(R)\, \ln R^2 + \int_R^\infty dR'\, R'\, K_0(R')\, \ln R'^2. \end{aligned} \tag{5.85}$$

Substitute (5.85) into (5.83), to obtain

$$\begin{aligned} I_1 = &-\frac{e^2 Z^2}{2}\int_0^\infty dR\, R\, K_0(R)\, \ln R^2 \\ &+ \frac{e^2 Z^2}{2}\int_0^\infty dR\, R^2\, K_0(R)\, K_1(R)\, \ln R^2 \\ &- \frac{e^2 Z^2}{2}\int_0^\infty dR\, R\, K_0(R) \int_R^\infty dR'\, R'\, K_0(R')\, \ln R'^2 \\ = &-\frac{e^2 Z^2}{2}[-2\gamma + 2\ln 2] + \frac{e^2 Z^2}{2}[-\frac{1}{2} - \gamma + \ln 2] - (0.615932)\frac{e^2 Z^2}{2} \\ = &-e^2 Z^2 0.61593 \end{aligned} \tag{5.86}$$

where

$$\int_0^{\infty} \mathrm{d}R\, R\, K_0(R) \int_R^{\infty} \mathrm{d}R'\, R'\, K_0(R')\, \ln R'^2$$

$$= \int_0^{\infty} \mathrm{d}R\, R\, K_0(R) \int_0^{\infty} \mathrm{d}R'\, R'\, K_0(R')\, \ln R'^2$$

$$- \int_0^{\infty} \mathrm{d}R\, R\, K_0(R) \int_0^{R} \mathrm{d}R'\, R'\, K_0(R')\, \ln R'^2$$

$$= -\,2\gamma + 2\ln 2 - (-0.384068)$$

$$=0.615931. \tag{5.87}$$

Substitute (5.87) into (5.80), to obtain the value for the ground-state energy of the TF atom $E_{TF}(n_{TF})$ in 2-dimensions

$$E_{TF}[n_{TF}] = T(n_{TF}) + E_{en}(n_{TF}) + E_{e-e}(n_{TF})$$

$$E_{TF}[n_{TF}] = \left(\frac{1}{2} Z^2 e^2\right) - \left(2\gamma Z^2 e^2\right) + \left(Z^2 e^2 \ln 2 - (0.61593) Z^2 e^2\right)$$

$$= -\,(0.576486) Z^2 e^2. \tag{5.88}$$

For the TF potential energy $V_{\mathrm{TF}}(\mathbf{x})$ we have from (5.20) and (5.35)

$$\boldsymbol{\nabla}^2 V_{\mathrm{TF}}(\mathbf{x}) = 4\pi\, Z e^2\, \delta^2(\mathbf{x}) - 4\pi\, e^2 n_{\mathrm{TF}}(\mathbf{x}) \tag{5.89}$$

with the first term corresponding to the nucleus at the origin, while the second term corresponds to the electron density. Upon integration over $\mathbf{x}$, and using (5.43), we obtain

$$\int \mathrm{d}^2\mathbf{x}\ \boldsymbol{\nabla}^2 V(\mathbf{x}) = 0 \tag{5.90}$$

verifying the neutrality of the TF atom.

It remains to show that $n_{\rm TF}$ provides the smallest possible value for $F[n]$ in (5.73), that is

$$F[\sigma] \geqslant F[n_{\rm TF}]. \tag{5.91}$$

To the above end, define a priori a density functional for an arbitrary density $\rho(\mathbf{x}) \geqslant 0$ by

$$\begin{aligned} F[\rho] =& A \int \mathrm{d}^2\mathbf{x}\,[\rho(\mathbf{x})]^2 + 2Ze^2 \int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\,\rho(\mathbf{x}) \\ & - e^2 \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\,\rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\,\rho(\mathbf{x}') \end{aligned} \tag{5.92}$$

where

$$A = \frac{\pi\hbar^2}{\underline{q}\,m}. \tag{5.93}$$

We define the Fourier transform for real function $\rho(\mathbf{x})$

$$\rho(\mathbf{x}) = \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2}\,\tilde{\rho}(\mathbf{p})\,\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar}, \tag{5.94a}$$

$$\tilde{\rho}^*(\mathbf{p}) = \int \mathrm{d}^2\mathbf{x}\,\rho^*(\mathbf{x})\,\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar} = \int \mathrm{d}^2\mathbf{x}\,\rho(\mathbf{x})\,\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar}. \tag{5.94b}$$

We show that the third term on the right-hand side of (5.92) is positive, we start from the solution of the Poisson's equation in (5.20), giving

$$\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B} = 2\pi\left(\boldsymbol{\nabla}^2\right)^{-1}\delta^2(\mathbf{x}-\mathbf{x}'). \tag{5.95}$$

Substitute into the third term on the right-hand side of (5.92), to obtain

$$\begin{aligned} & -\int \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}'\rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\,\rho(\mathbf{x}') \\ & \qquad = -2\pi \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\rho(\mathbf{x})\left(\boldsymbol{\nabla}^2\right)^{-1}\delta^2(\mathbf{x}-\mathbf{x}')\,\rho(\mathbf{x}'). \end{aligned} \tag{5.96}$$

We use an integral representation of the delta function in 2-dimensions in (5.95) and the Fourier transform of $\tilde{\rho}(\mathbf{p})$ in (5.94), then apply to (5.96), to obtain

$$
\begin{aligned}
-&\int d^2\mathbf{x}\, d^2\mathbf{x}' \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}') \\
&= -2\pi \int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \int d^2\mathbf{x}\, d^2\mathbf{x}' \rho(\mathbf{x})\ \rho(\mathbf{x}')\ \left(\boldsymbol{\nabla}^2\right)^{-1}\ e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')} \\
&= -2\pi \int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \int d^2\mathbf{x}\, d^2\mathbf{x}' \rho(\mathbf{x})\ \rho(\mathbf{x}')\ e^{-i\mathbf{p}\cdot\mathbf{x}'/\hbar}\ \left(\boldsymbol{\nabla}^2\right)^{-1} e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}. \qquad (5.97)
\end{aligned}
$$

The Fourier transform of $\rho(\mathbf{x})$ is

$$
\tilde{\rho}(\mathbf{p}) = \int d^2\mathbf{x}'\ \rho(\mathbf{x}')\ e^{-i\mathbf{p}\cdot\mathbf{x}'/\hbar}. \qquad (5.98)
$$

and

$$
\boldsymbol{\nabla}^2 e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} = -\left(\frac{\mathbf{p}}{\hbar}\right)^2 e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}, \qquad (5.99a)
$$

$$
\left(\boldsymbol{\nabla}^2\right)^{-1} e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} = -\left(\frac{\hbar}{\mathbf{p}}\right)^2 e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}. \qquad (5.99b)
$$

Apply (5.98) and (5.99) into (5.97), to get

$$
\begin{aligned}
-&\int d^2\mathbf{x} d^2\mathbf{x}' \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}') \\
&= 2\pi \int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \int d^2\mathbf{x}\, d^2\mathbf{x}'\ \rho(\mathbf{x})\ \rho(\mathbf{x}')\ e^{-i\mathbf{p}\cdot\mathbf{x}'/\hbar}\ \left(\frac{\hbar}{\mathbf{p}}\right)^2\ e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} \\
&= 2\pi \int \frac{d^2\mathbf{p}}{(2\pi)^2} \int d^2\mathbf{x}\ \rho(\mathbf{x})\ \tilde{\rho}(\mathbf{p}) \frac{1}{\mathbf{p}^2}\ e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}. \qquad (5.100)
\end{aligned}
$$

Since $\rho(\mathbf{x})$ is real function, i.e., $\rho(\mathbf{x}) = \rho^*(\mathbf{x})$, we have

$$
\rho(\mathbf{x}) = \int \frac{d^2\mathbf{p}'}{(2\pi\hbar)^2}\ \tilde{\rho}^*(\mathbf{p}')\ e^{-i\mathbf{p}'\cdot\mathbf{x}}. \qquad (5.101)
$$

Substitute (5.101) into (5.100), to obtain

$$-\int d^2\mathbf{x} d^2\mathbf{x}' \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\, \rho(\mathbf{x}')$$

$$=2\pi \int \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} \int \frac{d^2\mathbf{p}'}{(2\pi)^2} \int d^2\mathbf{x}\, e^{-i\mathbf{p}'\cdot\mathbf{x}}\, \tilde{\rho}^*(\mathbf{p}')\, \tilde{\rho}(\mathbf{p}) \frac{1}{\mathbf{p}^2}\, e^{i\mathbf{p}\cdot\mathbf{x}/\hbar}$$

$$=2\pi \int \frac{d^2\mathbf{p}}{(2\pi)^2} \int \frac{d^2\mathbf{p}'}{(2\pi\hbar)^2}\, \tilde{\rho}^*(\mathbf{p}')\, \tilde{\rho}(\mathbf{p}) \frac{1}{\mathbf{p}^2} \int d^2\mathbf{x}\, e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{x}}. \tag{5.102}$$

By using an integral representation of the delta function in 2-dimensions :

$$\delta^2(\mathbf{p}-\mathbf{p}') = \int \frac{d^2\mathbf{x}}{(2\pi\hbar)^2}\, e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{x}}, \tag{5.103a}$$

$$F(\mathbf{p}) = \int d^2\mathbf{p}'\, F(\mathbf{p}')\, \delta^2(\mathbf{p}-\mathbf{p}'). \tag{5.103b}$$

Applying into (5.102), to obtain

$$-\int d^2\mathbf{x} d^2\mathbf{x}' \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\, \rho(\mathbf{x}')$$

$$=2\pi \int \frac{d^2\mathbf{p}}{(2\pi)^2}\, \tilde{\rho}(\mathbf{p})\, \frac{1}{\mathbf{p}^2}\, (2\pi\hbar)^2 \int \frac{d^2\mathbf{p}'}{(2\pi\hbar)^2}\, \tilde{\rho}^*(\mathbf{p}')\, \delta^2(\mathbf{p}-\mathbf{p}')$$

$$=2\pi \int \frac{d^2\mathbf{p}}{(2\pi)^2}\, \tilde{\rho}(\mathbf{p})\, \frac{1}{\mathbf{p}^2}\, \tilde{\rho}^*(\mathbf{p})$$

$$=2\pi \int \frac{d^2\mathbf{p}}{(2\pi)^2}\, |\tilde{\rho}(\mathbf{p})|^2\, \frac{1}{\mathbf{p}^2}. \tag{5.104}$$

So that, from (5.104), we have

$$-e^2 \int d^2\mathbf{x}\, d^2\mathbf{x}' \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\, \rho(\mathbf{x}') \geqslant 0 \tag{5.105}$$

Let

$$\rho(\mathbf{x}) = t\rho_1(\mathbf{x}) + \beta\rho_2(\mathbf{x}) \equiv t\rho_1 + \beta\rho_2 \; (= \rho), \tag{5.106a}$$

$$\rho(\mathbf{x}') = t\rho_1(\mathbf{x}') + \beta\rho_2(\mathbf{x}') \equiv t\rho_1' + \beta\rho_2' \; (= \rho'), \tag{5.106b}$$

$$1 = t + \beta, \tag{5.106c}$$

$$\beta = (1 - t), \tag{5.106d}$$

where $0 \leqslant t \leqslant 1$ and $\rho_1, \rho_2 \geqslant 0$.

For any real ρ_1, ρ_2, we obtain the inequality

$$t^2(\rho_1 - \rho_2)^2 \leqslant t(\rho_1 - \rho_2)^2$$

$$t^2(\rho_1^2 - 2\rho_1\rho_2 + \rho_2^2) \leqslant t(\rho_1^2 - 2\rho_1\rho_2 + \rho_2^2)$$

$$t^2\rho_1^2 - 2t^2\rho_1\rho_2 + t^2\rho_2^2 \leqslant t\rho_1^2 - 2t\rho_1\rho_2 + t\rho_2^2. \tag{5.107}$$

Subtracting the both-sides of (5.107) by $2t\rho_2^2$, gives

$$t^2\rho_1^2 - 2t^2\rho_1\rho_2 + t^2\rho_2^2 - 2t\rho_2^2 \leqslant t\rho_1^2 - 2t\rho_1\rho_2 + t\rho_2^2 - 2t\rho_2^2$$

$$t^2\rho_1^2 - 2t^2\rho_1\rho_2 + t^2\rho_2^2 - 2t\rho^2 \leqslant t\rho_1^2 - 2t\rho_1\rho_2 - t\rho_2^2. \tag{5.108}$$

Add to both-sides of (5.108) the expressions $\rho_2^2 + 2t\rho_1\rho_2$, to obtain

$$t^2\rho_1^2 - 2t^2\rho_1\rho_2 + t^2\rho_2^2 - 2t\rho^2 + \rho_2^2 + 2t\rho_1\rho_2 \leqslant t\rho_1^2 - t\rho_2^2 + \rho_2^2. \tag{5.109}$$

The left-hand side of (5.109) can be rewritten as

$$t^2\rho_1^2 - 2t^2\rho_1\rho_2 + t^2\rho_2^2 - 2t\rho^2 + \rho_2^2 + 2t\rho_1\rho_2$$

$$=t^2\rho_1^2 + (1+t^2-2t)\rho_2^2 + 2t(1-t)\rho_1\rho_2$$

$$=t^2\rho_1^2 + (1-t)^2\rho_2^2 + 2t(1-t)\rho_1\rho_2$$

$$=(t\rho_1 + (1-t)\rho_2)^2. \tag{5.110}$$

Also the right-hand side of (5.109) is given by

$$t\rho_1^2 - t\rho_2^2 + \rho_2^2 = t\left(\rho_1\right)^2 + (1-t)\left(\rho_2\right)^2. \tag{5.111}$$

Substitute (5.110) and (5.111), to obtain the elementary inequality

$$\big(t\rho_1 + (1-t)\rho_2\big)^2 \leqslant t\left(\rho_1\right)^2 + (1-t)\left(\rho_2\right)^2. \tag{5.112}$$

Also

$$\begin{aligned}\big[t\rho_1 + (1-t)\rho_2\big]\big[t\rho_1' + (1-t)\rho_2'\big] =& t^2\rho_1\rho_1' + (1-t)^2\rho_2\rho_2' + t(1-t)\rho_1\rho_2' \\ &+ t(1-t)\rho_1'\rho_2 \\ =& t^2\rho_1\rho_1' + \rho_2\rho_2' - t^2\rho_2\rho_2' + t\rho_1\rho_2' - t\rho_1'\rho_2 \\ &+ t\rho_1'\rho_2 - t^2\rho_1'\rho_2 \\ =& t^2\rho_1\rho_1' + \rho_2\rho_2' - t^2\rho_2\rho_2' + t\rho_1\rho_2' - t\rho_1'\rho_2 \\ &+ t\rho_1'\rho_2 - t^2\rho_1'\rho_2 + t\rho_1\rho_1' - t\rho_1\rho_1' \\ =& t\rho_1\rho_1' + (1-t)\rho_2\rho_2' \\ &- t(1-t)(\rho_1-\rho_2)(\rho_1'-\rho_2')\end{aligned}$$

$$\therefore \quad \big[t\rho_1 + (1-t)\rho_2\big]\big[t\rho_1' + (1-t)\rho_2'\big] = t\rho_1\rho_1' + (1-t)\rho_2\rho_2' - t(1-t)(\rho_1 - \rho_2)(\rho_1' - \rho_2'). \quad (5.113)$$

From (5.105), replace $\rho(\mathbf{x})$ by $\big[\rho_1(\mathbf{x}) - \rho_2(\mathbf{x})\big]$ and replace $\rho(\mathbf{x}')$ by $\big[\rho_1(\mathbf{x}') - \rho_2(\mathbf{x}')\big]$, to obtain

$$-\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\,\big[\rho_1(\mathbf{x}) - \rho_2(\mathbf{x})\big]\,\ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\big[\rho_1(\mathbf{x}') - \rho_2(\mathbf{x}')\big] \geqslant 0. \quad (5.114)$$

From (5.92) and (5.106), replace $\rho(\mathbf{x})$ by $\big[t\rho_1 + (1-t)\rho_2\big]$ and $\rho(\mathbf{x}')$ by $\big[t\rho_1' + (1-t)\rho_2'\big]$, to obtain

$$\begin{aligned} F\big[t\rho_1 + (1-t)\rho_2\big] = & A\int \mathrm{d}^2\mathbf{x}\big[t\rho_1 + (1-t)\rho_2\big]^2 \\ & + 2Ze^2\int \mathrm{d}^2\mathbf{x}\;\ln\frac{|\mathbf{x}|}{A}\,\big[t\rho_1 + (1-t)\rho_2\big] \\ & - e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\big[t\rho_1 + (1-t)\rho_2\big]\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\,\big[t\rho_1' + (1-t)\rho_2'\big]. \end{aligned} \quad (5.115)$$

Consider the first term on the right-hand side of (5.115), by using, in the process, the elementary inequality in (5.112) giving

$$\begin{aligned} A\int \mathrm{d}^2\mathbf{x}\big[t\rho_1 + (1-t)\rho_2\big]^2 \leqslant & A\int \mathrm{d}^2\mathbf{x}\;\big(t\,(\rho_1)^2 + (1-t)\,(\rho_2)^2\big) \\ = & A\int \mathrm{d}^2\mathbf{x}\,t\,(\rho_1)^2 + A\int \mathrm{d}^2\mathbf{x}\,(1-t)\,(\rho_2)^2 \end{aligned}$$

$$\therefore \;\; A\int \mathrm{d}^2\mathbf{x}\big[t\rho_1 + (1-t)\rho_2\big]^2 \leqslant t\left(A\int \mathrm{d}^2\mathbf{x}\;(\rho_1)^2\right) + (1-t)\left(A\int \mathrm{d}^2\mathbf{x}\;(\rho_2)^2\right). \quad (5.116)$$

Consider the second term on the right-hand side of (5.115) we may write

$$
\begin{aligned}
2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \big[t\rho_1+(1-t)\rho_2\big] =& 2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ t\rho_1 \\
&+ 2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ (1-t)\rho_2 \\
=& t\left(2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \rho_1\right) \\
&+ (1-t)\left(2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \rho_2\right). \qquad (5.117)
\end{aligned}
$$

Consider the third term on the right-hand side of (5.115), by using (5.113), to obtain

$$
\begin{aligned}
&-e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\big[t\rho_1+(1-t)\rho_2\big]\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \big[t\rho_1'+(1-t)\rho_2'\big] \\
&\quad= -e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ t\rho_1\rho_1' - e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ (1-t)\rho_2\rho_2' \\
&\qquad+ e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \big(t(1-t)(\rho_1-\rho_2)(\rho_1'-\rho_2')\big). \qquad (5.118)
\end{aligned}
$$

From (5.114), the left-hand side of (5.118) is positive, so that (5.118) can be rewritten as

$$
\begin{aligned}
&-e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\big[t\rho_1+(1-t)\rho_2\big]\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \big[t\rho_1'+(1-t)\rho_2'\big] \\
&\quad\leqslant -t\left(e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho_1\rho_1'\right) \\
&\qquad-(1-t)\left(e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho_2\rho_2'\right). \qquad (5.119)
\end{aligned}
$$

Substitute (5.116), (5.117) and (5.119) into (5.115), to obtain

$$
\begin{aligned}
F\big[t\rho_1+(1-t)\rho_2\big] \leqslant\, & t\left(A\int \mathrm{d}^2\mathbf{x}\ (\rho_1)^2\right)+(1-t)\left(A\int \mathrm{d}^2\mathbf{x}\ (\rho_2)^2\right)\\
&+t\left(2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \rho_1\right)\\
&+(1-t)\left(2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \rho_2\right)\\
&-t\left(e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho_1\rho_1'\right)\\
&-(1-t)\left(e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho_2\rho_2'\right)\\
=&t\left(A\int \mathrm{d}^2\mathbf{x}\ (\rho_1)^2+2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \rho_1\right.\\
&\left.-e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho_1\rho_1'\right)\\
&+(1-t)\left(A\int \mathrm{d}^2\mathbf{x}\ (\rho_2)^2+2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \rho_2\right.\\
&\left.-e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho_2\rho_2'\right).
\end{aligned}
\tag{5.120}
$$

Refer to (5.92), to write

$$
\begin{aligned}
F[\rho_1]=&A\int \mathrm{d}^2\mathbf{x}\ (\rho_1)^2+2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \rho_1\\
&-e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho_1\,\rho_1'
\end{aligned}
\tag{5.121}
$$

and

$$
F[\rho_2]=A\int \mathrm{d}^2\mathbf{x}\ (\rho_2)^2+2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \rho_2
$$

$$- e^2 \int d^2\mathbf{x}\, d^2\mathbf{x}' \; \ln \frac{|\mathbf{x} - \mathbf{x}'|}{B} \; \rho_2 \, \rho_2'. \tag{5.122}$$

Substitute (5.120) and (5.122) into the right- hand side of inequality (5.120), to derive the bound :

$$F\big[t\rho_1 + (1-t)\rho_2\big] \leqslant tF[\rho_1] + (1-t)F[\rho_2]. \tag{5.123}$$

Also, from (5.115), we have

$$\begin{aligned} \frac{d}{dt} F\big[t\rho_1 + (1-t)\rho_2\big] =& 2A \int d^2\mathbf{x} \; \big[t\rho_1 + (1-t)\rho_2\big](\rho_1 - \rho_2) \\ & + 2Ze^2 \int d^2\mathbf{x} \; \ln \frac{|\mathbf{x}|}{2r_0} \, (\rho_1 - \rho_2) \\ & - 2e^2 \int d^2\mathbf{x}\, d^2\mathbf{x}' \; \ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0} \; \big[t\rho_1' + (1-t)\rho_2'\big](\rho_1 - \rho_2) \end{aligned} \tag{5.124}$$

and

$$\begin{aligned} & \frac{d}{dt} F\big[t\rho_1 + (1-t)\rho_2\big]\Big|_{t=0} \\ & \quad = \int d^2\mathbf{x} \, (\rho_1 - \rho_2) \left[2A\rho_2 + Ze^2 \ln \frac{|\mathbf{x}|}{2r_0} - e^2 \int d^2\mathbf{x}' \; \rho_2' \; \ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0} \right]. \end{aligned} \tag{5.125}$$

By choosing $\rho_2 = n_{\mathrm{TF}}$, and $\rho_1 = \sigma \geqslant 0$ arbitrary, we conclude from (5.29) and (5.43) that the expression within the square brackets in (5.117) is zero, thus

$$\frac{d}{dt} F\big[t\sigma + (1-t)n_{\mathrm{TF}}\big]\Big|_{t=0} = 0. \tag{5.126}$$

Also (5.107) leads to the bound

$$F\big[\sigma\big] - F\big[n_{\mathrm{TF}}\big] \geqslant \frac{F\big[t\sigma + (1-t)n_{\mathrm{TF}}\big] - F\big[n_{\mathrm{TF}}\big]}{t}. \tag{5.127}$$

Since the left-hand side of (5.127) is independent of t, we may take the limit

$t \to 0$, leading to

$$F\left[\sigma\right] - F\left[n_{\mathrm{TF}}\right] \geqslant \lim_{t\to 0}\left(\frac{F\left[t\sigma + (1-t)n_{\mathrm{TF}}\right] - F\left[n_{\mathrm{TF}}\right]}{t}\right) \tag{5.128}$$

and use (5.126) to conclude that

$$F\left[\sigma\right] \geqslant F\left[n_{\mathrm{TF}}\right] \tag{5.129}$$

with the TF density n_{TF} providing the smallest possible value for the energy functional in (5.92).

5.3 Lower Bound to the Expectation Value of The Exact Kinetic Energy

From earlier equations, (2.1)–(2.13), for $\rho \geqslant 0$, in particular we recall that

$$\begin{aligned}\int \mathrm{d}^{\nu}\mathbf{x}\,\langle\mathbf{x}|\,A^{\rho}\,|\mathbf{x}\rangle \geqslant \frac{1}{g^{\rho}} \times [&\text{Number of all } g'\text{'s as eigenvalues of } A\\ &\text{in } 0 < g' \leqslant g \text{ for which } H_0 - g'v(\mathbf{x})\\ &\text{has the eigenvalue } = -\xi]\end{aligned} \tag{5.130}$$

and the Schwinger inequality (2.20) :

$$N_{-\xi}\left(H_0 - gv(\mathbf{x})\right) \leqslant g^{\rho} \int \mathrm{d}^{\nu}\mathbf{x}\,\langle\mathbf{x}|\,A^{\rho}\,|\mathbf{x}\rangle\,. \tag{5.131}$$

In two dimensions $(\nu = 2)$, we choose $\rho = 2$ on the right-hand side of (5.130). Thus with the definition of A in (2.13), we obtain for the right-hand side of (5.130) with

$g = 1$

$$\int \mathrm{d}^2\mathbf{x} \, \langle \mathbf{x}| \, A^2 \, |\mathbf{x}\rangle = \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}' \, \langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle \, \langle \mathbf{x}'| \, A \, |\mathbf{x}\rangle$$

$$= \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}' \, \langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle \, \langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle^*$$

$$= \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}' \, |\langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle|^2$$

$$= \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^3\mathbf{x}' \, v(\mathbf{x}) \, v(\mathbf{x}') \left| \left\langle \mathbf{x} \left| \frac{1}{\left[\frac{\mathbf{p}^2}{2m} + \xi\right]} \right| \mathbf{x}' \right\rangle \right|^2 . \tag{5.132}$$

For $\left\langle \mathbf{x} \left| \left[\frac{\mathbf{p}^2}{2m} + \xi\right]^{-1} \right| \mathbf{x}' \right\rangle$, denote $\left[\frac{\mathbf{p}^2}{2m} + \xi\right]^{-1}$ by $\hat{A}(\mathbf{p})$, to obtain

$$\left\langle \mathbf{x} \left| \frac{1}{\left[\frac{\mathbf{p}^2}{2m} + \xi\right]} \right| \mathbf{x}' \right\rangle = \left\langle \mathbf{x} \left| \hat{A}(\mathbf{p}) \right| \mathbf{x}' \right\rangle$$

$$= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \frac{\mathrm{d}^2\mathbf{p}'}{(2\pi\hbar)^2} \, \langle \mathbf{x} \mid \mathbf{p} \rangle \left\langle \mathbf{p} \left| \hat{A}(\mathbf{p}) \right| \mathbf{p}' \right\rangle \langle \mathbf{p}' \mid \mathbf{x}' \rangle$$

$$= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \frac{\mathrm{d}^2\mathbf{p}'}{(2\pi\hbar)^2} \, \mathrm{e}^{\mathrm{i}\frac{\mathbf{p}}{\hbar}\cdot\mathbf{x}} \left\langle \mathbf{p} \left| \hat{A}(\mathbf{p}) \right| \mathbf{p}' \right\rangle \mathrm{e}^{-\mathrm{i}\frac{\mathbf{p}'}{\hbar}\cdot\mathbf{x}'}$$

$$= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \frac{\mathrm{d}^2\mathbf{p}'}{(2\pi\hbar)^2} \, \mathrm{e}^{\mathrm{i}(\mathbf{p}\cdot\mathbf{x} - \mathbf{p}'\cdot\mathbf{x}')/\hbar} \left\langle \mathbf{p} \left| \hat{A}(\mathbf{p}) \right| \mathbf{p}' \right\rangle$$

$$= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \frac{\mathrm{d}^2\mathbf{p}'}{(2\pi\hbar)^2} \, \mathrm{e}^{\mathrm{i}(\mathbf{p}\cdot\mathbf{x} - \mathbf{p}'\cdot\mathbf{x}')/\hbar} \, \hat{A}(\mathbf{p}) \, (2\pi\hbar)^2 \, \delta^2\left(\mathbf{p} - \mathbf{p}'\right)$$

$$= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \, \hat{A}(\mathbf{p}) \, (2\pi\hbar)^2 \int \frac{\mathrm{d}^2\mathbf{p}'}{(2\pi\hbar)^2} \, \mathrm{e}^{\mathrm{i}(\mathbf{p}\cdot\mathbf{x} - \mathbf{p}'\cdot\mathbf{x}')/\hbar} \delta^2\left(\mathbf{p} - \mathbf{p}'\right)$$

$$= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \, \hat{A}(\mathbf{p}) \, \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot(\mathbf{x} - \mathbf{x}')/\hbar}$$

$$= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \frac{\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot(\mathbf{x} - \mathbf{x}')/\hbar}}{\left[\frac{\mathbf{p}^2}{2m} + \xi\right]}, \quad \boldsymbol{\eta} = |\mathbf{x} - \mathbf{x}'|$$

$$=\frac{1}{(2\pi\hbar)^2}\int_0^\infty \frac{p\,\mathrm{d}p}{\left(\frac{p^2}{2m}+\xi\right)}\int_0^{2\pi}\mathrm{d}\theta\,\mathrm{e}^{\mathrm{i}\eta p\cos\theta/\hbar}. \tag{5.133}$$

The angular part is given by

$$\int_0^{2\pi}\mathrm{d}\theta\,\mathrm{e}^{\mathrm{i}\eta p\cos\theta/\hbar}=2\pi\;J_0(\frac{p\eta}{\hbar}) \tag{5.134}$$

where $J_0(x)$ is the Bessel function of order zero. On other hand,

$$\int_0^\infty \mathrm{d}x\;\frac{x}{(x^2+a^2)}J_0(x)=K_0(ax) \tag{5.135}$$

where $K_0(ax)$ is the modified Bessel function of order zero.

Apply (5.134) and (5.135) to (5.133), to obtain

$$\left\langle \mathbf{x}\left|\frac{1}{\left[\frac{\mathbf{p}^2}{2m}+\xi\right]}\right|\mathbf{x}'\right\rangle=\frac{1}{(2\pi\hbar)^2}\int_0^\infty \frac{p\,\mathrm{d}p}{\left(\frac{p^2}{2m}+\xi\right)}\int_0^{2\pi}\mathrm{d}\theta\,\mathrm{e}^{\mathrm{i}\eta p\;\cos\theta/\hbar},\;\;\boldsymbol{\eta}=|\mathbf{x}-\mathbf{x'}|$$

$$=\frac{m}{\pi\hbar^2}K_0\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\hbar}\right)\sqrt{2m\xi}. \tag{5.136}$$

Substitute (5.136) into (5.132), to obtain

$$\int \mathrm{d}^2\mathbf{x}\,\langle\mathbf{x}|\,A^2\,|\mathbf{x}\rangle$$

$$=\int \mathrm{d}^2\mathbf{x}\int \mathrm{d}^3\mathbf{x'}\;v(\mathbf{x})\;v(\mathbf{x}')\left(\frac{m}{\pi\hbar^2}K_0\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\hbar}\right)\sqrt{2m\xi}\right)^2$$

$$=\left(\frac{m}{\pi\hbar^2}\right)^2\int \mathrm{d}^2\mathbf{x}\int \mathrm{d}^3\mathbf{x'}\;v(\mathbf{x})\;v(\mathbf{x}')\left(K_0\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\hbar}\right)\sqrt{2m\xi}\right)^2. \tag{5.137}$$

We use Young's inequality

$$\left|\int \mathrm{d}^2\mathbf{x}\int \mathrm{d}^2\mathbf{x}' f(\mathbf{x})g(\mathbf{x}-\mathbf{x'})h(\mathbf{x}')\right|\leqslant\left\{\int \mathrm{d}^2\mathbf{x}\,|f(\mathbf{x})|^p\right\}^{1/p}\left\{\int \mathrm{d}^2\mathbf{x}\,|g(\mathbf{x})|^q\right\}^{1/q}$$

$$\times \left\{ \int \mathrm{d}^2\mathbf{x} |h(\mathbf{x})|^s \right\}^{1/s} \tag{5.138}$$

with $p = 2,\ s = 2,\ q = 1$ and

$$f(\mathbf{x}) = v(\mathbf{x}), \tag{5.139}$$

$$g(\mathbf{x} - \mathbf{x'}) = \left(K_0 \left(\frac{|\mathbf{x} - \mathbf{x}'|}{\hbar} \right) \sqrt{2m\xi} \right)^2, \tag{5.140}$$

$$h(\mathbf{x}') = v(\mathbf{x}'), \tag{5.141}$$

to obtain

$$\left| \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x'}\ \ v(\mathbf{x})\, \frac{\mathrm{e}^{-2|\mathbf{x}-\mathbf{x'}|\sqrt{2m\xi}/\hbar}}{|\mathbf{x} - \mathbf{x'}|^2}\, v(\mathbf{x}') \right|$$

$$\leqslant \left(\int \mathrm{d}^2\mathbf{x}\, |v(\mathbf{x})|^2 \right)^{1/2} \left(\int \mathrm{d}^2\mathbf{x}\, \left| \left(K_0 \left(\frac{|\mathbf{x} - \mathbf{x}'|}{\hbar} \right) \sqrt{2m\xi} \right)^2 \right| \right)$$

$$\times \left(\int \mathrm{d}^2\mathbf{x}\, |v(\mathbf{x})|^2 \right)^{1/2}$$

$$= \left(\int \mathrm{d}^2\mathbf{x}\, (v(\mathbf{x}))^2 \right)^{1/2} \left(\int \mathrm{d}^2\mathbf{x}\, (v(\mathbf{x}))^2 \right)^{1/2}$$

$$\times \left(\int \mathrm{d}^2\mathbf{x}\, \left| \left(K_0 \left(\frac{|\mathbf{x} - \mathbf{x}'|}{\hbar} \right) \sqrt{2m\xi} \right)^2 \right| \right)$$

$$\therefore \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}'\ v(\mathbf{x}) \frac{\mathrm{e}^{-2|\mathbf{x}-\mathbf{x'}|\sqrt{2m\xi}/\hbar}}{|\mathbf{x} - \mathbf{x'}|^2}\ v(\mathbf{x}')$$

$$\leqslant \left(\int \mathrm{d}^2\mathbf{x}\, (v(\mathbf{x}))^2 \right) \left(\int \mathrm{d}^2\mathbf{x}\, \left| \left(K_0 \left(\frac{|\mathbf{x} - \mathbf{x}'|}{\hbar} \right) \sqrt{2m\xi} \right)^2 \right| \right). \tag{5.142}$$

By using the integral

$$\int \mathrm{d}^2\mathbf{x} \left[K_0\left(\frac{|\mathbf{x}|}{\hbar}\sqrt{2m\xi}\right)\right]^2 = \frac{\pi\hbar^2}{2m\xi} \tag{5.143}$$

we then have

$$\int \mathrm{d}^2\mathbf{x} \, \langle\mathbf{x}|\, A^2 \,|\mathbf{x}\rangle = \frac{m}{2\hbar^2}\frac{1}{\pi\xi}\int \mathrm{d}^2\,\mathbf{x} v^2(\mathbf{x}). \tag{5.144}$$

From (5.131), this gives

$$N_{-\xi}\left(H_0 - gv(\mathbf{x})\right) \leqslant \frac{m}{2\hbar^2}\frac{1}{\pi\xi}\int \mathrm{d}^2\mathbf{x}\, v^2(\mathbf{x}). \tag{5.145}$$

From (5.145) we have $N_{-\xi}\left(H_0 - v(\mathbf{x})\right) < 1$ if we choose

$$\xi = \frac{m}{2\hbar^2}\frac{(1+\delta)}{\pi}\int \mathrm{d}^2\mathbf{x}\, v^2(\mathbf{x}), \quad \delta > 0 \tag{5.146}$$

or

$$-\xi = -\frac{m}{2\hbar^2}\frac{(1+\delta)}{\pi}\int \mathrm{d}^2\mathbf{x}\, v^2(\mathbf{x}). \tag{5.147}$$

On the other hand, $N_{-\xi}(\mathbf{p}^2/2m - v(\mathbf{x})) < 1$, implies that $N_{-\xi}(\mathbf{p}^2/2m - v(\mathbf{x})) = 0$, since $N_{-\xi}$ must be a natural number, and the right-hand side of (5.147) provides a lower bound to the spectrum of $[\mathbf{p}^2/2m - v(\mathbf{x})]$ since its spectrum would then be empty for energies $-\xi$. That is, (5.147) gives the following lower bound for the ground-state energy of the Hamiltonian,

$$-\frac{m}{2\hbar^2}\frac{(1+\delta)}{\pi}\int \mathrm{d}^2\mathbf{x}\, v^2(\mathbf{x}). \tag{5.148}$$

For one particle systems, we first obtain a lower bound for T. First we consider the one particle state with normalization condition $\int \mathrm{d}^2\mathbf{x}\, \rho(\mathbf{x}) = 1$ and define the positive function

$$v(\mathbf{x}) = \gamma \frac{\rho^{\alpha}(\mathbf{x})}{\int \mathrm{d}^2\mathbf{x}\, \rho^{\alpha+1}(\mathbf{x})} T \tag{5.149}$$

where α, γ are to be determined, and $v(\mathbf{x})$ is not the potential energy for any Hamiltonian. It is just introduced in order to be able to obtain a lower bound for T. Substitution (5.149) into $\langle \psi \,| H_0 - v(\mathbf{x}) |\, \psi \rangle$, to obtain

$$\left\langle \psi \left| \frac{\mathbf{p}^2}{2m} - v(\mathbf{x}) \right| \psi \right\rangle = -(\gamma - 1)\, T \tag{5.150}$$

and in reference to the bound in (5.148), we have

$$\left\langle \psi \left| \frac{\mathbf{p}^2}{2m} - v(\mathbf{x}) \right| \psi \right\rangle \geqslant - \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \int \mathrm{d}^2\mathbf{x}\, v^2(\mathbf{x}). \tag{5.151}$$

From (5.150) and (5.151), we may infer that

$$\begin{aligned} -(\gamma - 1)\, T \geqslant\; & - \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \int \mathrm{d}^2\mathbf{x}\, v^2(\mathbf{x}) \\ & = - \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \int \mathrm{d}^2\mathbf{x} \left(\gamma \frac{\rho^{\alpha}(\mathbf{x})}{\int \mathrm{d}^2\mathbf{x}\, \rho^{\alpha+1}(\mathbf{x})} T \right)^2 \\ & = - T^2 \gamma^2 \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \frac{\int \mathrm{d}^2\mathbf{x}\, \rho^{2\alpha}(\mathbf{x})}{\left(\int \mathrm{d}^2\mathbf{x}\, \rho^{\alpha+1}(\mathbf{x}) \right)^2} \end{aligned}$$

$$(\gamma - 1)\, T \leqslant T^2 \gamma^2 \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \frac{\int \mathrm{d}^2\mathbf{x}\, \rho^{2\alpha}(\mathbf{x})}{\left(\int \mathrm{d}^2\mathbf{x}\, \rho^{\alpha+1}(\mathbf{x}) \right)^2}. \tag{5.152}$$

This suggests to choose $2\alpha = \alpha + 1$, giving $\alpha = 1$. So the inequality in (5.152) becomes

$$\begin{aligned} (\gamma - 1)\, T & \leqslant T^2 \gamma^2 \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \frac{\int \mathrm{d}^2\mathbf{x}\, \rho^{2}(\mathbf{x})}{\left(\int \mathrm{d}^2\mathbf{x}\, \rho^{2}(\mathbf{x}) \right)^2} \\ & = T^2 \gamma^2 \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \frac{1}{\int \mathrm{d}^2\mathbf{x}\, \rho^{2}(\mathbf{x})} \end{aligned}$$

$$T \geqslant \frac{(\gamma-1)}{\gamma^2}\frac{2\hbar^2\pi}{m(1+\delta)}\int \mathrm{d}^2\mathbf{x}\,\rho^2(\mathbf{x}). \tag{5.153}$$

Optimizing (5.153) over γ

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\gamma}\frac{\gamma-1}{\gamma^2} =&0\\ \frac{-1}{\gamma^2}+\frac{2}{\gamma^3} =&0\end{aligned} \tag{5.154}$$

gives

$$\gamma =2. \tag{5.155}$$

Substitute γ from (5.155) into (5.153), to obtain the following bound for the expectation value of the kinetic energy T (for one particle systems)

$$T \geqslant \frac{\pi}{(1+\delta)}\frac{\hbar^2}{2m}\int \mathrm{d}^2\mathbf{x}\,\rho^2(\mathbf{x}) \tag{5.156}$$

for arbitrary small $\delta > 0$. From (5.156), we may rewrite the expectation value of the kinetic energy T (for one particle systems), whose the particle number density is denoted by $\rho(\mathbf{x})$in the form

$$T \geqslant B_n\left(\frac{\hbar^2}{2m}\right)\left(\int \mathrm{d}^n\mathbf{x}\,\rho^{p/(p-1)}(\mathbf{x})\right)^{2(p-1)/n} \tag{5.157}$$

where

$$B_n =\frac{n}{(1+\delta)}\left(\frac{\pi}{2}\right)^{2(p-1)/n} \tag{5.158}$$

and $n=2, p=2$.

For multi-particle systems, consider N identical fermions, each of mass m and introduce the particle number density in two dimensions :

$$\rho(\mathbf{x}) = N \sum_{\sigma_1,\ldots,\sigma_N} \int \mathrm{d}^2\mathbf{x}_2 \ldots \mathrm{d}^2\mathbf{x}_N \, |\psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, \ldots, \mathbf{x}_N\sigma_N)|^2 \quad , \tag{5.159}$$

where $\sigma_1, \ldots, \sigma_N$ specify spin projection values each taking $\underline{q}$ values for a particle of spin s.

The total number of particles N is given self consistently from the normalization condition

$$\int \mathrm{d}^2\mathbf{x} \, \rho(\mathbf{x}) = N. \tag{5.160}$$

The wavefunctions $\psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, \ldots, \mathbf{x}_N\sigma_N)$ are assumed to satisfy the appropriate statistics which in this case are anti-symmetric in the exchange of any two particles which amounts into the interchange of the position-spin labeling : $(\mathbf{x}_i\sigma_i) \Leftrightarrow (\mathbf{x}_j\sigma_j)$

In reference to (5.149), with $\gamma = 2, \ \alpha = 1$, we obtain the expression for the positive function $v(\mathbf{x})$

$$v(\mathbf{x}) = 2 \frac{\rho(\mathbf{x})}{\int \mathrm{d}^2\mathbf{x} \, \rho^2(\mathbf{x})} T \tag{5.161}$$

where

$$T = \left\langle \psi \left| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \right| \psi \right\rangle . \tag{5.162}$$

It is easily verified that

$$\left\langle \psi \left| \sum_{i=1}^{N} v(\mathbf{x}_i) \right| \psi \right\rangle = 2T \tag{5.163}$$

where $\sum_{i=1}^{N} v(\mathbf{x}_i) = v(\mathbf{x})$ and $v(\mathbf{x})$ is not the potential energy for any Hamiltonian. It is just introduced in order to be able to obtain the expectation value of the kinetic energy

T (for N identical fermions) in two dimensions.

We consider the operator

$$\sum_{i=1}^{N}\left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i)\right] \tag{5.164}$$

defining a hypothetical Hamiltonian of N non-interacting fermions which, however, interact with the external "potential" $v(\mathbf{x})$.

From (5.162) and (5.163), we have

$$\left\langle \psi \left| \sum_{i=1}^{N}\left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i)\right] \right| \psi \right\rangle = -\,T. \tag{5.165}$$

To obtain a lower bound to the spectrum of the "Hamiltonian" (operator) in (5.164), we note that, allowing for multiplicity and spin degeneracy, we can put the N fermions in the lowest energy of levels of the "Hamiltonian" in conformity with Pauli's exclusion principle, if N is the number of such levels. If N is larger than this number of levels, the remaining free fermions may be chosen to have arbitrary small $(\to 0)$ kinetic energies, and be infinitely separated, to define the lowest energy of the Hamiltonian in (5.164). That is, in all cases, the Hamiltonian (5.164) is bounded below by $\underline{q}$ times the ground-state energy in (5.148). From (5.151), (for N identical fermions) we thus have

$$\left\langle \psi \left| \sum_{i=1}^{N}\left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i)\right] \right| \psi \right\rangle \geqslant -\frac{\underline{q}\, m}{2\hbar^2}\frac{(1+\delta)}{\pi}\int \mathrm{d}^2\mathbf{x}\; v^2(\mathbf{x}). \tag{5.166}$$

Substituting (5.161), (5.165) into (5.166) and using the normalization condition $\int \mathrm{d}^2\mathbf{x}\;\rho(\mathbf{x}) = N$, we obtain for the expectation value of the kinetic energy T (for N identical fermions)

$$\begin{aligned} -T \geqslant\; & -\frac{\underline{q}\, m}{2\hbar^2}\frac{(1+\delta)}{\pi}\int \mathrm{d}^2\mathbf{x}\;\left(2\frac{\rho(\mathbf{x})}{\int \mathrm{d}^2\mathbf{x}\,\rho^2(\mathbf{x})}T\right)^2 \\ =\; & -\;4T^2\frac{\underline{q}\, m}{2\hbar^2}\frac{(1+\delta)}{\pi}\frac{1}{\int \mathrm{d}^2\mathbf{x}\,\rho^2(\mathbf{x})} \end{aligned}$$

$$T \geqslant \frac{1}{\underline{q}} \frac{\pi}{(1+\delta)} \frac{\hbar^2}{2m} \int \mathrm{d}^2\mathbf{x}\, \rho^2(\mathbf{x}) \tag{5.167}$$

From (5.167), the expectation value of the kinetic energy T as

$$T \geqslant \frac{B_n}{\underline{q}} \left(\int \mathrm{d}^n\mathbf{x}\, \rho^{p/(p-1)}(\mathbf{x}) \right)^{2(p-1)/n} \tag{5.168}$$

where B_n is defined in (5.158) and $n = 2, p = 2$.

5.4 A Thomas-Fermi Energy Functional and a Lower Bound for The Electron-Electron Interaction

For anti-symmetric normalized functions $\Psi(\mathbf{x}_1\sigma_1, \ldots, \mathbf{x}_N\sigma_N)$ of N electrons, we have for the expectation value of the Hamiltonian H

$$\begin{aligned} \langle\Psi| H |\Psi\rangle =& \sum_{i=1}^{N} \langle\Psi| \frac{\mathbf{p}_i^2}{2m} |\Psi\rangle + 2\sum_{i=1}^{N}\sum_{j=1}^{k} Z_j e^2 \langle\Psi| \ln\frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0} |\Psi\rangle \\ & - 2\sum_{i<j}^{N} e^2 \langle\Psi| \ln\frac{|\mathbf{x}_i - \mathbf{x}_j|}{2r_0} |\Psi\rangle \\ & - 2\sum_{i<j}^{k} Z_i Z_j e^2 \langle\Psi| \ln\frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} |\Psi\rangle \end{aligned} \tag{5.169}$$

To derive a lower bound to this expectation value, we recall the definition of electron density

$$\rho(\mathbf{x}) = N \sum_{\sigma_1,\ldots,\sigma_N} \int \mathrm{d}^2\mathbf{x}_2 \ldots \mathrm{d}^2\mathbf{x}_N \left|\Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, \ldots, \mathbf{x}_N\sigma_N)\right|^2 \tag{5.170}$$

normalized to

$$\int \mathrm{d}^2\mathbf{x}\, \rho(\mathbf{x}) = N \tag{5.171}$$

and

$$\langle\Psi|\Psi\rangle = \int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2 ... \mathrm{d}^2\mathbf{x}_N \ \Psi^*(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N) \ \Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N)$$

$$= \sum_{\sigma_1,...,\sigma_N}^{n} \int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2 ... \mathrm{d}^2\mathbf{x}_N \, |\Psi(\mathbf{x}\sigma_1, \mathbf{x}_2\sigma_2, ..., \mathbf{x}_N\sigma_N)|^2$$

$$=1. \tag{5.172}$$

The lower bound (5.18) to the expectation value of the kinetic energy for particles of mass βm is then given by :

$$\sum_{i=1}^{N} \langle\Psi| \frac{\mathbf{p}_i^2}{2m\beta} |\Psi\rangle > \frac{\pi\hbar^2}{\underline{q}\ m\beta} \frac{1}{1+\delta} \int \mathrm{d}^2\mathbf{x} \ [\rho(\mathbf{x})]^2 \tag{5.173}$$

where $\beta > 0$.

In reference to the second term on the right-hand side of (5.169), substitute (5.170) into (5.169), giving

$$2 \sum_{i=1}^{N} \sum_{j=1}^{k} Z_j e^2 \langle\Psi| \ln \frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0} |\Psi\rangle$$

$$=2 \int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N \ \Psi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\sum_{i=1}^{N} \sum_{j=1}^{k} e^2 Z_j \ln \frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0} \right) \Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$=2 \sum_{j=1}^{k} \sum_{i=1}^{N} \int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N \ \Psi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(e^2 Z_j \ln \frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0} \right) \Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$=2 \sum_{j=1}^{k} \sum_{j=1}^{N} \int \mathrm{d}^2\mathbf{x} \ e^2 Z_j \ln \frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0}$$

$$\times \sum_{\sigma_1,\ldots,\sigma_N} \int \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N \, |\Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2$$

$$= 2\sum_{j=1}^{k} \int \mathrm{d}^2\mathbf{x} \, e^2 Z_j \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} \, \frac{\rho(\mathbf{x})}{N}$$

$$+ 2\sum_{j=1}^{k} \int \mathrm{d}^2\mathbf{x}_2 \, e^2 Z_j \ln \frac{|\mathbf{x}_2 - \mathbf{R}_j|}{2r_0} \, \frac{\rho(\mathbf{x}_2)}{N}$$

$$+ \ldots + 2\sum_{j=1}^{k} \int \mathrm{d}^2\mathbf{x}_N \, e^2 Z_j \ln \frac{|\mathbf{x}_N - \mathbf{R}_j|}{2r_0} \, \frac{\rho(\mathbf{x}_N)}{N}. \tag{5.174}$$

In reference to the third term on the right-hand side of (5.169), we first note that

$$-2\sum_{i<j}^{N} e^2 \, \langle\Psi| \ln \frac{|\mathbf{x}_i - \mathbf{x}_j|}{2r_0} \, |\Psi\rangle = -e^2 \int \mathrm{d}^2\mathbf{x}' \int \mathrm{d}^2\mathbf{x} \, \rho(\mathbf{x}) \ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0} \, \rho(\mathbf{x}') \tag{5.175}$$

and for the fourth term on the right-hand side of (5.169) , we may write

$$-2\sum_{i<j}^{k} Z_i Z_j e^2 \, \langle\Psi| \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} \, |\Psi\rangle = -2\sum_{i<j}^{k} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} \, \langle\Psi \mid \Psi\rangle$$

$$= -2\sum_{i<j}^{k} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}. \tag{5.176}$$

From (5.173)–(5.176), we obtain the following lower bound for (5.169)

$$\langle\Psi| \, H \, |\Psi\rangle > \frac{\pi\hbar^2}{\underline{q} \, m\beta} \int \mathrm{d}^2\mathbf{x} \, \left[\rho(\mathbf{x})\right]^2 + 2\sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^2\mathbf{x} \, \rho(\mathbf{x}) \, \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0}$$

$$- e^2 \int \mathrm{d}^2\mathbf{x} \, \mathrm{d}^2\mathbf{x}' \, \rho(\mathbf{x}) \ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0} \, \rho(\mathbf{x}')$$

$$- 2\sum_{i<j}^{k} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} \tag{5.177}$$

by closing δ arbitrary small.

We define an *energy* functional in 2-dimensions by

$$F[\rho; Z_1, \dots, Z_k, \mathbf{R}_1, \dots, \mathbf{R}_j] = \frac{\pi\hbar^2}{\underline{q}\, m\beta} \int \mathrm{d}^2\mathbf{x}\ [\rho(\mathbf{x})]^2$$
$$+ 2\sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\, \rho(\mathbf{x})\ \ln \frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}$$
$$- e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\, \rho(\mathbf{x}')$$
$$- 2\sum_{i<j}^{k} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0} \tag{5.178}$$

depending on positive parameters $Z_1, \dots, Z_k$ and $\mathbf{R}_1, \dots, \mathbf{R}_j$.

Optimize (5.178) over $\rho(\mathbf{x})$, by taking the functional derivative of (5.178), with respect to $\rho(\mathbf{x})$, equal to zero, to obtain

$$0 = \frac{\delta F[\rho]}{\delta \rho(\mathbf{x})}$$
$$= \frac{2\pi\hbar^2}{\underline{q}\, m\beta}\rho(\mathbf{x}) + 2e^2 \sum_{j=1}^{k} Z_j\ \ln \frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}$$
$$- 2e^2 \int \mathrm{d}^2\mathbf{x}'\ \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\, \rho(\mathbf{x}'). \tag{5.179}$$

Let $\rho(x) = \rho_0(\mathbf{x}; k)$ satisfy the equation (5.179), this is

$$\frac{2\pi\hbar^2}{\underline{q}\, m\beta} [\rho_0(\mathbf{x}; k)] = - 2e^2 \sum_{j=1}^{k} Z_j\ \ln \frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}$$
$$+ 2e^2 \int \mathrm{d}^2\mathbf{x}'\ \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\, \rho(\mathbf{x}'). \tag{5.180}$$

Refer to (5.106)–(5.129), which shows that the TF density actually provides the smallest value, we conclude that $\rho_0(\mathbf{x}; k)$ satisfying (5.180) provides the smallest value for the functional (5.178), with the corresponding solution, $\rho_0(\mathbf{x};k)$ satisfying the normalization condition

$$\int \mathrm{d}^2\mathbf{x}\ \rho_0(\mathbf{x};k) = \sum_{j=1}^{k} Z_j. \tag{5.181}$$

From (5.129), we then have

$$F[\rho] \geqslant F[\rho_0]$$

$$F[\rho; Z_1,\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k] \geqslant F[\rho_0; Z_1,\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k]. \tag{5.182}$$

We introduce the functionals

$$F[\rho; \lambda Z_1,\ldots,\lambda Z_\ell,\ Z_{\ell+1},\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k] \tag{5.183}$$

and

$$F[\rho; \lambda Z_1,\ldots,\lambda Z_\ell,\mathbf{R}_1,\ldots,\mathbf{R}_\ell] \tag{5.184}$$

where $\ell < k$ and $\lambda > 0$ is arbitrary parameter.

Let $\rho_1(\mathbf{x}), \rho_2(\mathbf{x})$ be the corresponding solutions to (5.179) for the functionals in (5.183), (5.184), respectively. By referring to (5.179), we have

$$\begin{aligned} \frac{\pi\hbar^2}{\underline{q}\ m\beta}\rho_1(\mathbf{x}) = &- e^2\lambda\sum_{j=1}^{\ell} Z_j\ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} - e^2\sum_{j=\ell+1}^{k} Z_j\ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} \\ &+ e^2\int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho_1(\mathbf{x}') \end{aligned} \tag{5.185}$$

and

$$\frac{\pi\hbar^2}{\underline{q}\ m\beta}\rho_2(\mathbf{x}) = - e^2\lambda\sum_{j=1}^{\ell} Z_j\ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} + e^2\int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho_2(\mathbf{x}') \tag{5.186}$$

and for the simplicity of the notation only, we have suppressed the dependence of ρ_1, ρ_2 on λ, k, ℓ.

By subtracting (5.185) from (5.186), we obtain

$$Q_1(\mathbf{x}) - Q_2(\mathbf{x}) = -\, e^2 \sum_{j=\ell+1}^{\ell} Z_j \ln \frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} + e^2 \int \mathrm{d}^2\mathbf{x}' \ \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0} \left[\rho_1(\mathbf{x}') - \rho_2(\mathbf{x}')\right]$$

$$= -\, e^2 \sum_{j=\ell+1}^{\ell} Z_j \ln \frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}$$

$$+ \frac{e^2 \underline{q}\, m\beta}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}' \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0} \left[Q_1(\mathbf{x}') - Q_2(\mathbf{x}')\right] \tag{5.187}$$

where

$$Q_1(\mathbf{x}) = \frac{\pi\hbar^2 \rho_1(\mathbf{x})}{\underline{q}\, m\beta} \tag{5.188}$$

$$Q_2(\mathbf{x}) = \frac{\pi\hbar^2 \rho_2(\mathbf{x})}{\underline{q}\, m\beta}. \tag{5.189}$$

Since the sum over j in (5.187) is non-negative, $\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ cannot be strictly negative for all $\mathbf{x}$ otherwise this will be in contradiction with the equation (5.187) itself.

We introduce the set

$$S = \{\mathbf{x} | Q_1(\mathbf{x}) - Q_2(\mathbf{x}) < 0\} \tag{5.190}$$

which we will show that it is empty, thus concluding that $Q_1(\mathbf{x}) - Q_2(\mathbf{x}) \geqslant 0$.

We assume that S is non-empty and then run into a contradiction. As we move away from the boundary Ω of S, $\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ changes sign or vanishes, by definition of S, and we then have

$$\hat{\mathbf{n}} \cdot \boldsymbol{\nabla} \big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] \geqslant 0 \tag{5.191}$$

which $\hat{n}$ is a unit vector perpendicular to the boundary at $\mathbf{x}$, otherwise, we would run into a region beyond S where $\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ is still strictly negative. [If S is of infinite extension the non-negativity of $\hat{\mathbf{n}} \cdot \boldsymbol{\nabla}\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ on the boundary still holds.]

The application of the Laplacian to (5.187) gives

$$\begin{aligned}
\nabla^2\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] = -e^2\lambda \sum_{j=\ell+1}^{k} Z_j \nabla^2 \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} \\
+ \frac{e^2 \underline{q}\, m\beta}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}'\, \nabla^2 \ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0} \,[Q_1(\mathbf{x}') - Q_2(\mathbf{x}')] \\
= -4\pi e^2 \sum_{j=l+1}^{k} Z_j\, \delta^2(\mathbf{x} - \mathbf{R_j}) \\
+ \frac{e^2 \underline{q}\, m\beta}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}'\, \delta^2(\mathbf{x} - \mathbf{x}')\,[Q_1(\mathbf{x}') - Q_2(\mathbf{x}')] \\
= -4\pi e^2 \sum_{j=l+1}^{k} Z_j\, \delta^2(\mathbf{x} - \mathbf{R_j}) \\
+ 4\pi e^2 \frac{\underline{q}\, m\beta}{\pi\hbar^2}\,[Q_1(\mathbf{x}) - Q_2(\mathbf{x})]
\end{aligned} \tag{5.192}$$

and for $\mathbf{x}$ in the set S, the expression on the right-hand side of this equation is strictly negative since $\Big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\Big] < 0$ for such $\mathbf{x}$ by hypothesis.

Accordingly,

$$0 > \int_S \mathrm{d}^2\mathbf{x}\, \nabla^2\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] = \int_\Omega \mathrm{d}\Omega\, \hat{\mathbf{n}} \cdot \boldsymbol{\nabla}\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] \tag{5.193}$$

in contradiction with (5.191), hence S is empty and

$$Q_1(\mathbf{x}) - Q_2(\mathbf{x}) \geqslant 0 \tag{5.194}$$

as a function of $\mathbf{x}$.

In reference to the functional

$$F\left[\rho; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\right] \tag{5.195}$$

let $\rho_3(\mathbf{x})$ satisfy

$$\frac{\pi\hbar^2}{\underline{q}\; m\beta}\rho_3(\mathbf{x}) = -e^2 \sum_{j=\ell+1}^{k} Z_j \;\ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} + e^2 \int \mathrm{d}^2\mathbf{x}' \;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\;\rho_3(\mathbf{x}') \tag{5.196}$$

in analogy to (5.185), (5.186).

We define

$$\begin{aligned} g(\lambda) = F\big[&\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big] \\ &- F\big[\rho_2; \lambda Z_1, \ldots, \lambda Z_l, \mathbf{R}_1, \ldots, \mathbf{R}_l\big] \\ &- F\big[\rho_3; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\big] \end{aligned} \tag{5.197}$$

with $l < k$. Since for $\lambda = 0$, ρ_1 and ρ_3 denote the same density, and ρ_2, in (5.197) is obviously equal to zero for $\lambda = 0$, as the left-hand side of (5.197) is non-negative while the right-hand side is non-positive for $\lambda = 0$, and

$$\begin{aligned} g(0) = F\big[&\rho; Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big] \\ &- F\big[0; \ldots \mathbf{R}_1, \ldots, \mathbf{R}_l\big] \\ &- F\big[\rho; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\big] \end{aligned} \tag{5.198}$$

we may infer that

$$g(0) = 0. \tag{5.199}$$

For $\lambda = 1$, gives

$$g(1) = F\big[\rho; Z_1, \ldots, Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big]$$

$$- F\big[\rho_2; Z_1, \ldots, Z_l, \mathbf{R}_1, \ldots, \mathbf{R}_l\big]$$

$$- F\big[\rho; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\big]. \tag{5.200}$$

From (5.199) and (5.202), we may write

$$g(1) = \int_0^1 \mathrm{d}\lambda \; g'(\lambda) \tag{5.201}$$

we infer that ($F[\rho] \geqslant F[\rho_0]$)

$$g(1) \geqslant 0 \tag{5.202}$$

and hence to establish (5.202) it is sufficient to show that $g'(\lambda) \geqslant 0$ for $0 \leqslant \lambda \leqslant 1$.

To the above end, we note from (5.178) with $Z_1 \to \lambda Z_1, \ldots, Z_l \to \lambda Z_l$, $\rho \to \rho_1$, we obtain

$$F\big[\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big]$$

$$= \frac{\pi\hbar^2}{\underline{q}\; m\beta} \int \mathrm{d}^2\mathbf{x}\; [\rho_1(\mathbf{x})]^2$$

$$+ 2\lambda \sum_{j=1}^{\ell} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\, \rho_1(\mathbf{x})\; \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0}$$

$$+ 2 \sum_{j=\ell+1}^{k} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\, \rho_1(\mathbf{x})\; \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0}$$

$$- e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, \rho_1(\mathbf{x}) \ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0}\; \rho_1(\mathbf{x}')$$

$$- 2\lambda^2 \sum_{i=1}^{\ell-1} \sum_{j=\ell+1}^{\ell} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}$$

$$- 2 \sum_{i=1}^{\ell} \lambda Z_i \sum_{j=\ell+1}^{k} Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} \tag{5.203}$$

where

$$2 \sum_{i<j}^{k} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} = 2\lambda^2 \sum_{i=1}^{\ell-1} \sum_{j=\ell+1}^{\ell} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}$$

$$+ 2 \sum_{i=1}^{\ell} \lambda Z_i \sum_{j=\ell+1}^{k} Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}. \tag{5.204}$$

By setting the functional partial derivative of (5.203), with respect to λ, we obtain

$$\frac{\partial}{\partial \lambda} F\big[\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big]$$

$$= 2 \frac{\pi \hbar^2}{\underline{q}\, m\beta} \int \mathrm{d}^2\mathbf{x}\ \rho_1(\mathbf{x})\ \frac{\partial}{\partial \lambda} \rho_1(\mathbf{x})$$

$$+ 2\lambda \sum_{j=1}^{\ell} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} \frac{\partial}{\partial \lambda} \rho_1(\mathbf{x})$$

$$+ 2 \sum_{j=1}^{\ell} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\ \rho_1(\mathbf{x})\ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0}$$

$$+ 2 \sum_{j=\ell+1}^{k} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0}\ \frac{\partial}{\partial \lambda} \rho_1(\mathbf{x})$$

$$- 2e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}' \ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0}\ \rho_1(\mathbf{x}')\ \frac{\partial}{\partial \lambda} \rho_1(\mathbf{x})$$

$$- 4\lambda \sum_{i=1}^{\ell-1} \sum_{j=\ell+1}^{\ell} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}$$

$$- 2\sum_{i=1}^{\ell} Z_i \sum_{j=\ell+1}^{k} Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}. \tag{5.205}$$

Eq.(5.205) can be rewritten as

$$\frac{\partial}{\partial\lambda} F\left[\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\right]$$

$$= \int d^2\mathbf{x} \left[2\frac{\pi\hbar^2}{\underline{q}\, m\beta}\, \rho_1(\mathbf{x}) + 2\lambda \sum_{j=1}^{\ell} e^2 Z_j\ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} \right.$$

$$\left. +2\sum_{j=\ell+1}^{k} e^2 Z_j\ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} - 2e^2 \int d^2\mathbf{x}' \ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0}\, \rho_1(\mathbf{x}') \right] \frac{\partial}{\partial\lambda} \rho_1(\mathbf{x})$$

$$- e^2 \left[4\lambda \sum_{i=1}^{\ell-1} \sum_{j=\ell+1}^{\ell} Z_i Z_j \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} + 2\sum_{i=1}^{\ell} Z_i \sum_{j=\ell+1}^{k} Z_j \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} \right]$$

$$+ 2\sum_{j=1}^{\ell} e^2 Z_j \int d^2\mathbf{x}\, \rho_1(\mathbf{x})\ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} \tag{5.206}$$

Refer to (5.185), and note that the expression within the brackets of the $\mathbf{x}$-integral in the first term on the right-hand side of (5.206) is zero. So that (5.206) becomes

$$\frac{\partial}{\partial\lambda} F\left[\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\right]$$

$$= -e^2 \left[4\lambda \sum_{i=1}^{\ell-1} \sum_{j=\ell+1}^{\ell} Z_i Z_j \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} + 2\sum_{i=1}^{\ell} Z_i \sum_{j=\ell+1}^{k} Z_j \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} \right]$$

$$+ 2\sum_{j=1}^{\ell} e^2 Z_j \int d^2\mathbf{x}\, \rho_1(\mathbf{x})\ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0}. \tag{5.207}$$

Refer to (5.206), and in the same way as in (5.207), we obtain

$$\frac{\partial}{\partial\lambda} F\left[\rho_2; \lambda Z_1, \ldots, \lambda Z_l, \mathbf{R}_1, \ldots, \mathbf{R}_l\right]$$

$$= -e^2 \left[4\lambda \sum_{i=1}^{\ell-1} \sum_{j=\ell+1}^{\ell} Z_i Z_j \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} + 2 \sum_{i=1}^{\ell} Z_i \sum_{j=\ell+1}^{k} Z_j \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} \right]$$

$$+ 2 \sum_{j=1}^{\ell} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\, \rho_2(\mathbf{x})\ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0}. \tag{5.208}$$

Refer to (5.206), and in the same way as in (5.207), we obtain

$$\frac{\partial}{\partial \lambda} F\big[\rho_3; Z_l, \ldots, Z_k \mathbf{R}_{\ell+1}, \ldots, \mathbf{R}_k\big]$$

$$= -2e^2 \sum_{i=1}^{\ell} Z_i \sum_{j=\ell+1}^{k} Z_j \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}. \tag{5.209}$$

Finally refer to (5.200) and (5.207) to (5.209), to obtain

$$\begin{aligned}
\frac{\partial}{\partial \lambda} g(\lambda) =& 2 \sum_{j=1}^{\ell} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\, \rho_1(\mathbf{x})\ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} - 2 \sum_{j=1}^{\ell} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\, \rho_2(\mathbf{x})\ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} \\
&+ 2e^2 \sum_{i=1}^{\ell} Z_i \sum_{j=\ell+1}^{k} Z_j \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} \\
=& 2 \sum_{i=1}^{\ell} Z_i \left[\sum_{j=\ell+1}^{k} Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} + e^2 \int \mathrm{d}^2\mathbf{x}\, \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0}\ \left[\rho_1(\mathbf{x}) - \rho_2(\mathbf{x})\right] \right] \\
=& 2 \sum_{i=1}^{\ell} Z_i \left[Q_1(\mathbf{R}_i) - Q_2(\mathbf{R_i}) \right] \\
\geqslant& 0
\end{aligned} \tag{5.210}$$

where we have used (5.194).

Accordingly, from (5.197) and (5.202), we have

$$\begin{aligned}
F\big[\rho_1; Z_1, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big] \geqslant& F\big[\rho_2; Z_1, \ldots, Z_l, \mathbf{R}_1, \ldots, \mathbf{R}_\ell\big] \\
&+ F\big[\rho_3; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{\ell+1}, \ldots, \mathbf{R}_k\big]
\end{aligned} \tag{5.211}$$

for any $1 \leqslant \ell < k$, where ρ_1, ρ_2, ρ_3 are the densities which provide the smallest values for the corresponding functionals, respectively.

Accordingly, from (5.182) and (5.211), since ℓ, k (with $l < k$) are arbitrary natural numbers,we may conclude that

$$F\big[\rho_0; Z_1, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big] \geqslant \sum_{i=1}^{k} F\big[\rho^i_{\mathrm{TF}}; Z_i, \mathbf{R}_i\big] \tag{5.212}$$

where each $F\big[\rho^i_{\mathrm{TF}}; Z_i, \mathbf{R}_i\big]$ is a TF functional.

Consider the solution of the TF functional

$$-\frac{\pi\hbar^2}{\underline{q}\ m}\,[n_{TF}(\mathbf{x})] = Ze^2 \ln\frac{|\mathbf{x}|}{2r_0} - e^2 \int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ n_{TF}(\mathbf{x}') \tag{5.213}$$

where $n_{TF}(\mathbf{x})$ is the TF density.

The ground-state energy $E_{TF}(Z)$ of the TF atom is given from (5.88) to be

$$E_{TF}(Z) = -(0.576486)\ e^2 Z^2. \tag{5.214}$$

In TF density ρ^i_{TF} with nuclear charge $Z_i|e|$, situated at $\mathbf{R}_i$, and the mass m of each negatively charged particle simply scaled by β, we replace $\mathbf{x}$ by $\mathbf{x} + \mathbf{R}$ and set

$$\rho^i_{TF}(\mathbf{x} + \mathbf{R}_i) = n_{TF}(\mathbf{x})\big|_{m\to m\beta, Z\to Z_i}\,. \tag{5.215}$$

Substitute this into (5.213),giving

$$-\frac{\pi\hbar^2}{\underline{q}\ m\beta}\,\big[\rho^i_{TF}(\mathbf{x})\big] = Ze^2 \ln\frac{|\mathbf{x}-\mathbf{R}_i|}{2r_0} - e^2 \int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho^i_{TF}(\mathbf{x}'). \tag{5.216}$$

From (5.182),(5.212) and (5.214), we then have

$$F\big[\rho; Z_1, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big] \geqslant E_{\mathrm{TF}}(1) \sum_{i=1}^{k} Z_i^2 \tag{5.217}$$

where $E_{TF}(1) = -(0.576486)e^2$, independent to m.

The basic inequality in (5.211), shows that a system identified by the parameters $\left[Z_1, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\right]$ cannot have an (optimized) energy functional (5.178) less than the sum of the (optimized) energy functional of any two subsystems identified by parameters $\left[Z_1, \ldots, Z_l, \mathbf{R}_1, \ldots, \mathbf{R}_l\right]$, $\left[Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\right]$, $l < k$. Because of this last property, the Theorem embodied in the inequalities (5.211), (5.212) is referred to as a "No Binding Theorem".

We now deride a lower bound of the multi-particle repulsive coulomb potential energy. From (5.217) we note that

$$\frac{\pi\hbar^2}{\underline{q}\, m\beta} \int \mathrm{d}^2\mathbf{x}\,[\rho(\mathbf{x})]^2 + 2\sum_{j=1}^{k} Z_i e^2 \int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}\,\rho(\mathbf{x})$$
$$- e^2 \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\,\rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\,\rho(\mathbf{x}') - 2\sum_{i<j}^{k} Z_i Z_j e^2 \ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}$$
$$\geqslant E_{TF}(1)\sum_{i=1}^{N} Z_i^2. \tag{5.218}$$

The energy density functional, expressed in terms of the density $\rho(\mathbf{x})$ on the left-hand side of (5.218) is in the spirit of the TF energy functional, with the mass m of the electron replaced by $m\beta$, and with the further generalization of including k nuclei, with the last term, involving '$Z_i Z_j\, e^2$', describing their interactions.

The inequality in (5.218) gives rise to a lower bound to the (repulsive) Coulomb potential energy of k particles of charges $Z_1|e|, \ldots, Z_k|e|$, or charges $-Z_1|e|, \ldots, -Z_k|e|$, i.e., for charges of the same signs as follows :

$$-2\sum_{i<j}^{k} Z_i Z_j e^2 \ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0} \geqslant E_{TF}(1)\sum_{i=1}^{k} Z_i^2 - \frac{\pi\hbar^2}{\underline{q}\, m\beta}\int \mathrm{d}^2\mathbf{x}\,[\rho(\mathbf{x})]^2$$
$$- 2\sum_{j=1}^{k} Z_i e^2 \int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}\,\rho(\mathbf{x})$$

$$+ e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\, \rho(\mathbf{x}'). \qquad (5.219)$$

In particular for the interaction of N electrons we have, with substitutions $k \to N$, $Z_j \to 1$, $\mathbf{R}_j \to \mathbf{x}_j$ for $j = 1, \ldots, N$:

$$-2 \sum_{i<j}^{k} e^2 \ln \frac{|\mathbf{x}_i - \mathbf{x}_j|}{2r_0} \geqslant N E_{TF}(1) - \frac{\pi \hbar^2}{\underline{q}\, m\beta} \int \mathrm{d}^2\mathbf{x}\, [\rho(\mathbf{x})]^2$$

$$- 2 \sum_{i=1}^{N} e^2 \int \mathrm{d}^2\mathbf{x}\ \ln \frac{|\mathbf{x}-\mathbf{x}_j|}{2r_0}\, \rho(\mathbf{x})$$

$$+ e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\, \rho(\mathbf{x}') \qquad (5.220)$$

5.5 Lower Bound for the Exact Ground-state Energy

For anti-symmetric normalized functions $\Psi(\mathbf{x}_1\sigma_1, \ldots, \mathbf{x}_N\sigma_N)$ of N electrons, we have for the expectation value of the Hamiltonian H

$$\langle\Psi|\, H\, |\Psi\rangle = \sum_{i=1}^{N} \langle\Psi|\, \frac{\mathbf{p}_i^2}{2m}\, |\Psi\rangle + 2 \sum_{i=1}^{N} \sum_{j=1}^{k} Z_j e^2 \langle\Psi|\ln \frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0}\, |\Psi\rangle$$

$$- 2 \sum_{i<j}^{N} e^2 \langle\Psi|\ln \frac{|\mathbf{x}_i - \mathbf{x}_j|}{2r_0}\, |\Psi\rangle$$

$$- 2 \sum_{i<j}^{k} Z_i Z_j e^2 \langle\Psi|\ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}\, |\Psi\rangle \qquad (5.221)$$

with wavefunction and spin normalization condition.

The lower bound (5.167) to the expectation value of the kinetic energy for spin multiplicity $\underline{q}$:

$$\sum_{i=1}^{N} \langle\Psi|\, \frac{\mathbf{p}_i^2}{2m}\, |\Psi\rangle > \frac{\pi}{\underline{q}} \frac{\hbar^2}{2m} \int \mathrm{d}^2\mathbf{x}\, \rho^2(\mathbf{x}) \qquad (5.222)$$

for δ sufficiently small.

For the second term on the right-hand side of (5.221), substitute (5.170) into (5.221), we obtain

$$
\begin{aligned}
& 2\sum_{i=1}^{N}\sum_{j=1}^{k} Z_j e^2 \langle\Psi|\ln\frac{|\mathbf{x}_i-\mathbf{R}_j|}{2r_0}|\Psi\rangle \\
&= 2\int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N \; \Psi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N) \\
&\quad \times \left(\sum_{i=1}^{N}\sum_{j=1}^{k} e^2 Z_j \ln\frac{|\mathbf{x}_i-\mathbf{R}_j|}{2r_0}\right)\Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N) \\
&= 2\sum_{j=1}^{k}\sum_{i=1}^{N}\int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N \; \Psi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N) \\
&\quad \times \left(e^2 Z_j \ln\frac{|\mathbf{x}_i-\mathbf{R}_j|}{2r_0}\right)\Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N) \\
&= 2\sum_{j=1}^{k}\sum_{j=1}^{N}\int \mathrm{d}^2\mathbf{x}\, e^2 Z_j \ln\frac{|\mathbf{x}_i-\mathbf{R}_j|}{2r_0} \\
&\quad \times \sum_{\sigma_1,\ldots,\sigma_N}\int \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N \, |\Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2 \\
&= 2\sum_{j=1}^{k}\int \mathrm{d}^2\mathbf{x}\, e^2 Z_j \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}\;\frac{\rho(\mathbf{x})}{N} \\
&\quad + 2\sum_{j=1}^{k}\int \mathrm{d}^2\mathbf{x}_2\, e^2 Z_j \ln\frac{|\mathbf{x}_2-\mathbf{R}_j|}{2r_0}\;\frac{\rho(\mathbf{x}_2)}{N} \\
&\quad + \ldots + 2\sum_{j=1}^{k}\int \mathrm{d}^2\mathbf{x}_N\, e^2 Z_j \ln\frac{|\mathbf{x}_N-\mathbf{R}_j|}{2r_0}\;\frac{\rho(\mathbf{x}_N)}{N} \\
&= 2\sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\,\rho\;\ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}.
\end{aligned}
\tag{5.223}
$$

For the third term on the right-hand side of (5.221), we first note that

$$
\begin{aligned}
-2\sum_{i=1}^{N} e^2 \langle\Psi| \int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}-\mathbf{x}_j|}{2r_0}\,\rho(\mathbf{x})\,|\Psi\rangle \\
&= -\,2\sum_{j=1}^{N} e^2 \int \mathrm{d}^2\mathbf{x}', \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N\ \Psi^*(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N) \\
&\quad \times \left(\int \mathrm{d}^2\mathbf{x}\,\rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}_j|}{2r_0}\right)\ \Psi(\mathbf{x}', \mathbf{x}_2, \ldots \mathbf{x}_N) \\
&= -2\sum_{j=1}^{N} e^2 \int \mathrm{d}^2\mathbf{x}' \int \mathrm{d}^2\mathbf{x}\,\rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}_j|}{2r_0} \\
&\quad \times \sum_{\sigma_1,\ldots,\sigma_N} \int \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N\ |\Psi(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2 \\
&= -2\frac{e^2}{N} \int \mathrm{d}^2\mathbf{x}' \int \mathrm{d}^2\mathbf{x}\,\rho(\mathbf{x})\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho(\mathbf{x}') \\
&\quad + \frac{e^2}{N} \int \mathrm{d}^2\mathbf{x}_2 \int \mathrm{d}^2\mathbf{x}\,\rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}_2|}{2r_0}\ \rho(\mathbf{x}_2) \\
&\quad + \ldots + \frac{e^2}{N} \int \mathrm{d}^2\mathbf{x}_N \int \mathrm{d}^2\mathbf{x}\,\rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}_N|}{2r_0}\ \rho(\mathbf{x}_N) \\
&= -2e^2 \int \mathrm{d}^2\mathbf{x}' \int \mathrm{d}^2\mathbf{x}\,\rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho(\mathbf{x}')
\end{aligned}
\tag{5.224}
$$

and from (5.220)

$$
\begin{aligned}
-2\sum_{i<j}^{k} e^2 \langle\Psi| \ln\frac{|\mathbf{x}_i-\mathbf{x}_j|}{2r_0}\,|\Psi\rangle \geq{}& N E_{TF}(1) - \frac{\pi\hbar^2}{\underline{q}\, m\beta} \int \mathrm{d}^2\mathbf{x}\,[\rho(\mathbf{x})]^2 \\
& - e^2 \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\,\rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}').
\end{aligned}
\tag{5.225}
$$

From (5.222)–(5.225), we obtain the following lower bound for (5.221)

$$\begin{aligned}
\langle\Psi|\, H \,|\Psi\rangle \geq & \frac{\pi}{2}\frac{\hbar^2}{2m}\int \mathrm{d}^2\mathbf{x}\, \rho^2(\mathbf{x}) + 2\sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\, \rho\, \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} \\
& + \beta N E_{TF}(1) - \frac{\pi\hbar^2}{\underline{q}\, m\beta}\int \mathrm{d}^2\mathbf{x}\, [\rho(\mathbf{x})]^2 \\
& - e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, \rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\, \rho(\mathbf{x}') \\
& - 2\sum_{i<j}^{k} Z_i Z_j e^2 \langle\Psi| \ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}\, |\Psi\rangle\,. \qquad (5.226)
\end{aligned}$$

We set

$$\left(\frac{\pi}{2} - \frac{2\pi}{\underline{q}\beta}\right) \times \frac{\underline{q}}{2\pi} = \frac{\underline{q}}{4} - \frac{1}{\beta} = \frac{1}{\beta'} \qquad (5.227)$$

and for positive β' we have to choose $\beta > (4/\underline{q})$. Apply (5.227) to (5.226), to get

$$\begin{aligned}
\langle\Psi|\, H \,|\Psi\rangle \geq & \frac{2\pi}{\underline{q}\beta'}\frac{\hbar^2}{2m}\int \mathrm{d}^2\mathbf{x}\, \rho^2(\mathbf{x}) + 2\sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\, \rho\, \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} \\
& - e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, \rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\, \rho(\mathbf{x}') \\
& - 2\sum_{i<j}^{k} Z_i Z_j e^2 \langle\Psi| \ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}\, |\Psi\rangle + N E_{TF}(1). \qquad (5.228)
\end{aligned}$$

The sum of the first form on the right-hand side of inequality (5.226) then gives

$$\begin{aligned}
\langle\Psi|\, H \,|\Psi\rangle \geq & E_{TF}(1)\sum_{j=1}^{k} Z_j^2 + N E_{TF}(1) \\
= & E_{TF}(1)\left(N + \sum_{j=1}^{k} Z_j^2\right)
\end{aligned}$$

$$\langle\Psi| H |\Psi\rangle \geq -(0.576486)e^2 \left(N + \sum_{j=1}^{k} Z_j Z_{max}\right)$$

$$= -(0.576486)e^2 (N + NZ_{max})$$

$$= -(0.576486)e^2 N(1 + Z_{max})$$

$$\therefore \quad \langle\Psi| H |\Psi\rangle \geq -(0.576486)e^2 N(1 + Z_{max}) \tag{5.229}$$

where

$$Z_j Z_{max} \geq Z_j^2. \tag{5.230}$$

5.6 Inflation of Matter.

Let $|\Psi(m)\rangle$ denote any negative energy-state of matter, not necessarily the ground-state,

$$-\varepsilon_N[m] \leqslant \langle\Psi(m)| H |\Psi(m)\rangle \tag{5.231}$$

where $-\varepsilon_N[m] = E_N < 0$ is the ground-state energy, and we have emphasized its dependence on the mass m of the electron.

By definition of the ground-state energy, the state $|\Psi(m/2)\rangle$ cannot lead for $\langle\Psi(m/2)| H |\Psi(m/2)\rangle$ a numerical value lower than $-\varepsilon_N[m]$. That is,

$$-\varepsilon_N[m] \leqslant \langle\Psi(m/2)| H |\Psi(m/2)\rangle \tag{5.232}$$

where we note that the interaction part V of the Hamiltonian H in (5.221) is not explicitly dependent on m :

$$V = 2\sum_{i=1}^{N}\sum_{j=1}^{k} Z_j e^2 \ln\frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0} - 2\sum_{i<j}^{N} e^2 \ln\frac{|\mathbf{x}_i - \mathbf{x}_j|}{2r_0}$$

$$- 2\sum_{i<j}^{k} Z_i Z_j e^2 \ln\frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}. \tag{5.233}$$

Accordingly (5.232) implies that

$$-\varepsilon_N[2m] \leqslant \left\langle \Psi(m) \middle| \left(\sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{4m} + V \right) \middle| \Psi(m) \right\rangle. \tag{5.234}$$

Upon writing, trivially,

$$\sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + V = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{4m} + \left(\sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{4m} + V \right) \tag{5.235}$$

the extreme right-hand of the inequality (5.231) then leads to

$$\left\langle \Psi(m) \middle| \left(\sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{4m} \right) \middle| \Psi(m) \right\rangle < - \left\langle \Psi(m) \middle| \left(\sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{4m} + V \right) \middle| \Psi(m) \right\rangle \tag{5.236}$$

which upon multiplying by two, (5.234) gives

$$\left\langle \Psi(m) \middle| \left(\sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \right) \middle| \Psi(m) \right\rangle < 2\varepsilon_N \tag{5.237}$$

for all states $|\Psi(m)\rangle$ such that (5.231) is true including the ground-state.

Thus from (5.237), (5.230), (5.222), we have the following bounds for the expectation value T of the total kinetic energy of all the electrons in such states

$$\frac{\pi}{\underline{q}} \frac{\hbar^2}{2m} \int \mathrm{d}^2\mathbf{x}\, \rho^2(\mathbf{x}) < T < (1.152972) e^2 N (1 + Z_{max}) \tag{5.238}$$

To investigate the inflation of matter, let $\mathbf{x}$ denote the position of an electron relative, for example, to the center of mass of the nuclei. We define the set function

$$\chi_R(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{x} \text{ lies within a sphere of radius } R \\ 0, & \text{otherwise.} \end{cases} \tag{5.239}$$

We are interested in the expression

$$\text{Prob}\left[|\mathbf{x}_1| \leqslant R, \ldots, |\mathbf{x}_N| \leqslant R\right] = \sum_{\sigma_1,\ldots,\sigma_N} \int \left(\prod_{i=1}^{N} \mathrm{d}^2\mathbf{x}_i \; \chi_R(\mathbf{x}_i) \right) |\Psi(\mathbf{x}_1\sigma_1, \ldots, \mathbf{x}_N\sigma_N)|^2 \tag{5.240}$$

which gives the probability of finding all the electrons within a circle of radius R. Clearly,

$$\begin{aligned} \text{Prob}\left[|\mathbf{x}_1| \leqslant R, \ldots, |\mathbf{x}_N| \leqslant R\right] &\leqslant \text{Prob}\left[|\mathbf{x}_1| \leqslant R, \ldots, |\mathbf{x}_j| \leqslant R\right] \\ &\leqslant \ldots \leqslant \text{Prob}\left[|\mathbf{x}_1| \leqslant R\right] \\ &= \frac{1}{N} \int \mathrm{d}^2\mathbf{x} \; \chi_R(\mathbf{x}) \rho(\mathbf{x}) \end{aligned} \tag{5.241}$$

for $j < N$, with $\rho(\mathbf{x})$ given in (5.170).

By Hölder's inequality we have

$$\int \mathrm{d}^2\mathbf{x} \; \chi_R(\mathbf{x}) \rho(\mathbf{x}) \leqslant \left(\int \mathrm{d}^2\mathbf{x} \; \rho^2(\mathbf{x}) \right)^{1/2} \left(\int \mathrm{d}^2\mathbf{x} \; \chi_R^2(\mathbf{x}) \right)^{1/2} \tag{5.242}$$

where $\chi_R^2(\mathbf{x}) = \chi_R(\mathbf{x})$, and

$$\int \mathrm{d}^2\mathbf{x} \; \chi_R(\mathbf{x}) = A_R \tag{5.243}$$

denotes the area in which the electrons are confined.

Hence, in particular, (5.241) gives

$$\text{Prob}\,[|\mathbf{x}_1| \leqslant R, \dots, |\mathbf{x}_N| \leqslant R] \leqslant \text{Prob}\,[|\mathbf{x}_1| \leqslant R]$$
$$\leqslant \frac{(A_R)^{1/2}}{N} \left(\int \mathrm{d}^2\mathbf{x}\ \rho^2(\mathbf{x}) \right)^{1/2}$$
$$\leq \frac{(A_R)^{1/2}}{N} \left((1.152972) \frac{q}{\pi} \frac{2me^2}{\hbar^2} N(1 + Z_{\max} \right)^{1/2} \tag{5.244}$$

where (from (5.238))

$$\left(\int \mathrm{d}^2\mathbf{x}\ \rho^2(\mathbf{x}) \right)^{1/2} \leqslant \left[(1.152972) \frac{q}{\pi} \frac{2me^2}{\hbar^2} N(1 + Z_{max}) \right]^{1/2} \tag{5.245}$$

finally leads to the simple bound

$$\text{Prob}\,[|\mathbf{x}_1| \leqslant R, \dots, |\mathbf{x}_N| \leqslant R] \left(\frac{N}{A_R} \right)^{1/2} < (0.856741) \left[\frac{qme^2}{\hbar^2} (1 + Z_{\max}) \right]^{1/2} \tag{5.246}$$

where $a_0 = \hbar^2/me^2$ is the Bohr radius and $Z_{\max}$ is the maximum of the nuclear charges.

We immediately infer from (5.246) the inescapable fact the *necessarily*, given that there is a non-zero probability of electrons to be limit within a circle of radius R, then the corresponding area A_R grows not any slower than the first power of N for $N \to \infty$, since otherwise the left-hand side of (5.246) would go to infinite in this limit while the right-hand side is finite. That is, *necessarily*, the radius R *of spatial extension of matter grows not any slower than* $N^{1/2}$ *for* $N \to \infty$.

We note that N/A_R gives the electron density, and one may infer from (5.246), with a probability non-zero provide that electrons are limit within a circle of radius R, the infinite density limit $N/A_R \to \infty$, i.e., of the system collapsing onto itself, does not occur.

5.7 Non-Zero Lower Bound for a Measure of the Extension of Matter

We use define the expectation value

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle = \sum_{\sigma_1,\ldots,\sigma_N} \int \mathrm{d}^2\mathbf{x}_1 \ldots \mathrm{d}^2\mathbf{x}_N \left(\sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right) |\Psi(\mathbf{x}_1\sigma_1, \ldots, \mathbf{x}_N\sigma_N)|^2$$

$$= \frac{1}{N} \int \mathrm{d}^2\mathbf{x}\ |\mathbf{x}|\rho(\mathbf{x}) \tag{5.247}$$

as for a measure of the extension of matter. Using the facts that

$$\frac{1}{N} \int \mathrm{d}^2\mathbf{x}\ |\mathbf{x}|\rho(\mathbf{x}) \geqslant \frac{1}{N} \int_{|\mathbf{x}|>R} \mathrm{d}^2\mathbf{x}\ |\mathbf{x}|\rho(\mathbf{x}) \geqslant \frac{R}{N} \int_{|\mathbf{x}|>R} \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x})$$

$$= R\ \text{Prob}\left[|\mathbf{x}| > R\right] \tag{5.248}$$

$$\text{Prob}\left[|\mathbf{x}| > R\right] = 1 - \text{Prob}\left[|\mathbf{x}| \leqslant R\right] \tag{5.249}$$

$A_R = \pi R^2$, and (5.246) we obtain

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle \geqslant R \left[1 - \left(\frac{\pi R^2}{N} \right)^{1/2} (0.856741) \left[\frac{\underline{q} m e^2}{\hbar^2} (1 + Z_{\text{max}}) \right]^{1/2} \right]. \tag{5.250}$$

Upon optimizing the right-hand side of the above inequality over R, this gives

$$R = (0.583607) \left(\frac{N}{\pi} \frac{\hbar^2}{\underline{q} m e^2} \frac{1}{(1 + Z_{\text{max}})} \right)^{1/2}. \tag{5.251}$$

leading for (5.250) to the explicit non-zero lower bound

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle \geqslant (0.291803) N^{1/2} \left(\frac{\hbar^2}{\pi \underline{q} m e^2} \frac{1}{(1 + Z_{\text{max}})} \right)^{1/2}. \tag{5.252}$$

CHAPTER VI

CONCLUSION

We have carried out a detailed mathematically rigorous analysis of the stability of matter in bulk by invoking, in the process of the investigations, the Pauli exclusion principle at every stage. As is well know the practical effect of the exclusion principle, or more generally of the Spin and Statistics Theorem, prevails over the whole of science and provides the basis for explaining the periodic table of elements from which we are made of. Without the Spin and Statistics connection our world will be unstable and ceases to exits. As mentioned in the bulk of this thesis, the drastic difference between matter with the exclusion principle and so-called "bosonic matter", i.e., without exclusion principle, is that the ground-state energy E_N for the former $-E_N \sim N$, with N denoting the number of negative charges (the electrons), while for the latter $-E_N \sim N^\alpha$, with $\alpha > 1$. A power law behaviour with $\alpha > 1$ implies that of instability as the formation of single system consisting of $(2N + 2N)$ particles is favoured over two separated systems brought together, each consisting of $(N + N)$ particles, and the energy released upon the collapse of the two systems into one, being proportional to $[(2N)^\alpha - 2N^\alpha]$, will be overwhelmingly large for realistic large N, e.g., $N \sim 10^{23}$. Thus the actual demonstration of a single power of N for the ground-state energy of matter (i.e., with the exclusion principle) is essential. We note, in particular, that for matter, the energy $-E_N/N$ shared by a particle remains finite for large N in clear distinction with the "bosonic" one which increases without bound for large N.

To carry out our analysis of the stability of matter we have derived several lower *and* upper bounds for the exact ground-state energy as shown in Chapters II and III. The most relevant ones are embodied in the following double inequality given by :

$$-\underline{c}\left(\frac{me^4}{2\hbar^2}\right) N \left[1+\left(\sum_{i=1}^{k}\frac{Z_i^{7/3}}{N}\right)^{1/2}\right]^2 \leqslant E_N \leqslant -\bar{c}\left(\frac{me^4}{2\hbar^2}\right)\sum_{i=1}^{k} Z_i^2 \tag{6.1}$$

(see (2.388), (2.391), (3.437), (3.438)), where

$$\underline{c} = 4(0.68060)\left(\frac{4}{3\pi}\right)^{2/3} = 1.53749 \tag{6.2}$$

$$\bar{c} = (1.00000) \tag{6.3}$$

where $Z_1|e|, \ldots, Z_k|e|$ denote the nuclear charges. The numerical values of the constants $\underline{c}/\bar{c}$ given in (6.2)/(6.3) may be further decreased/increased giving a tighter interval bound for E_N, but all of our conclusions remain unaltered.

Our main conclusions are as follows :

Stability of matter : In nature, the nuclear charges $Z_1|e|, \ldots, Z_k|e|$ are bounded. Accordingly, let $Z = \max_i Z_i$. Then $Z_i \leqslant Z$. Also $\sum_{i=1}^{k} Z_i = N$.

Hence, (6.1) leads to the following double inequality

$$-\underline{c}\left(\frac{me^4}{2\hbar^2}\right) N \left[1+Z^{2/3}\right]^2 \leqslant E_N \leqslant -\bar{c}\left(\frac{me^4}{2\hbar^2}\right) N \tag{6.4}$$

with a single power of N appearing on both sides.

Fate of the nuclei: Let p be a positive number such that $2 \leq p \ll N$ (i.e., in particular, p is much smaller than the number of electrons). We conclude from (6.1) that for $Z_1 = \ldots = Z_p = N/p$, $Z_{p+1} = \ldots = Z_k = 0$, $-E_N$ grows not any slower than N^2, for $N \to \infty$, and is obviously quite relevant physically to the stability of matter. It leads to the conclusion that as more and more matter is put together, thus increasing the number N of electrons, the number k of nuclei in such matter, as separate clusters, would necessarily increase and not arbitrarily fuse together and their individual charges remain *bounded*. That is, as $N \to \infty$, then stability implies that $k \to \infty$ as well, and no nuclei may be found in matter that would carry arbitrarily large portions of the total charge available. As stated above the Z_i are bounded in nature.

Inflation (swelling) of matter: We have shown in (4.32) that for the probability of having the electrons within a sphere of radius R, with its center, say, at the center of mass of the nuclei, we have the bound

$$\text{Prob}\left[|\mathbf{x}_1| \leqslant R, \ldots, |\mathbf{x}_N| \leqslant R\right] \left(\frac{N}{v_R}\right)^{2/5} \leqslant 1.26528 \left(\frac{1}{a_0^2}\right)^{3/5} (1+Z)^{4/5}\,. \tag{6.5}$$

where $v_R = 4\pi R^3/3$ is the volume of the sphere, $a_0 = \hbar^2/me^2$ is the Bohr radius, and $Z = \max_i Z_i$, introduced above. We infer from (6.5) the inescapable fact that *necessarily* for a non-vanishing probability of having the electrons within a sphere of radius R, the corresponding volume grows (swells) not any slower than the first power of N for $N \to \infty$, since otherwise the left-hand side of (6.5) would go to infinity and would be in contradiction with the finite upper bound on its right-hand side. That is, necessarily, the radius R grows not any slower than $N^{1/3}$ for $N \to \infty$. No wonder why matter occupies so large a volume ! Here it is worth recalling part of the Ehrenfest–Pauli debate as stated by Ehrenfest : "*We take a piece of metal, or a stone. When we think about it, we are astonished that this quantity of matter should occupy so large a volume*". He went on by stating that the Pauli exclusion principle is the reason : *"Answer : only the Pauli principle, no two electrons in the same state"*. The method developed here has been also used to analyze the localizability and stability of other quantum systems (Manoukian, 2006).

Infinite density limit: We may rewrite the inequality in (6.5) as

$$\text{Prob}\left[|\mathbf{x}_1| \leqslant R, \ldots, |\mathbf{x}_N| \leqslant R\right] \leqslant \left(\frac{v_R}{N}\right)^{2/5} (1.26528) \left(\frac{1}{a_0^2}\right)^{3/5} (1+Z)^{4/5}\,. \tag{6.6}$$

Thus, in turn, the infinite density limit $N/v_R \to \infty$, i.e., $v_R/N \to 0$, does *not* arise as the probability on the left-hand side of (6.6) would go to zero in this limit, i.e., this does *not* happen.

Non-zero lower bound for a measure of extension of matter. As a measure of the extension of matter we introduce the expectation value $\left\langle \sum_{i=1}^{N} |\mathbf{x}|/N \right\rangle$, and we have established rigorously in (4.43), the following *non-zero* lower bound:

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}|}{N} \right\rangle > 0.26432\, a_0 \, \frac{N^{1/3}}{[1+Z]^{2/3}} \tag{6.7}$$

with the expectation value taken with respect to any state of matter, including the ground-state.

Two-dimensional matter: Due to the overwhelming interest recently in physics in two dimensions, we have also proved rigorously the stability and inflation of such matter in Chapter V.

Matter without the exclusion principle: Our methods developed in this thesis have led to new estimates on matter when the exclusion principle is revoked. These are worked out in detail in Appendices A and B. In particular, we have shown in (B.10), for the probability of finding the negative charges within a sphere of radius R, with center of the sphere, say, at the center of mass of the nuclei:

$$\text{Prob}\left[|\mathbf{x}_1| \leq R, \ldots, |\mathbf{x}_N| \leq R\right] \frac{1}{(v_R N)^{1/2}} < \left(\frac{1}{a_0^3}\right)^{1/2} 1.61\,[1+Z]\,. \tag{6.8}$$

where a_0 is the Bohr radius, $Z = \max_i Z_i$ as before. This is to be compared with (6.5). From this inequality we infer the inescapable fact that if deflation of “bosonic matter” occurs, upon collapse, then for a non-vanishing probability of having the N negatively charged particles within a sphere of radius R, the corresponding volume v_R, necessarily, cannot shrink faster than $1/N$ for $N \to \infty$, or R cannot decrease faster than $N^{-1/3}$, since otherwise the left-hand side of (6.8) would go to infinity and would be in contradiction with the finite upper bound on its right-hand side.

As stated earlier, although the mathematical intricacies and the corresponding intermediate estimates turn out to be quite tedious and involved, the final results are expressed in terms of simple expressions and are readily physically interpreted as we have just seen in this concluding chapter.

REFERENCES

REFERENCES

Balàzs, N. L. (1967). Formation of stable molecules within the statistical theory of atoms. **Physical Review** 156 (1): 42–47.

Bethe, H. A., Jackiw, R. W. (1986). **Intermediate quantum mechanics** 3^{rd} **edition**. New York, Addison–Wesley Publishing Company .

Bhaduri, R. K., Murthy, M. V. N. and Srivastava, M. K. (1996). Fractional exclusion statistics and two dimensional electron systems. **Physical Review Letters** 76 (2): 165–168.

Birman, M. Š. (1961). On the spectrum of singular boundary-value problems. **Matematicheskiĭ Sbornik** 55 (97): 125–174. English translation: Birman, M. Š. (1966). **The American Mathematical Society Transl.** 53 (2): 23–60.

Brown, L. and Schwinger, J. (1961). Spin and statistics. **Progress of Theoretical Physics** 26: 917–926.

Burgoyne, N. (1958). On the connection of spin and statistics. **Nuovo Cimento** 8: 607–609.

Casselman, B. (2004). The difficulties of kissing in three dimensions. **Notices of the American Mathematical Society** 51 (8): 884–885.

Conlon, J. G. (1984). The ground state energy of a classical gas. **Communications in Mathematical Physics** 94 (4): 439–458.

Conlon, J. G., Lieb, E. H. and Yau, H-T. (1988). The $N^{7/5}$ law for charged bosons. **Communications in Mathematical Physics** 116 (3): 417–448. Reprinted in Thirring (1991), pp. 435–466.

Croft, H. T., Falconer, K. J. and Guy, R. K. (1991). **Unsolved problems in geometry**. New York: Springer-Verlag.

de Wet, J. S. (1940). On the connection between the spin and statistics of elementary particles. **Physical Review** 57 (7): 646–652.

Dirac, P. A. M. (1930). Note on exchange phenomena in the Thomas atom. **Proceedings of the Cambridge Philosophical Society** 26: 376–385.

Duck, I. and Sudarshan, E. C. G. (eds.). (1997). **Pauli and the spin-statistics theorem**. Singapore: World Scientific.

Dyson, F. J. (1967). Ground-state energy of a finite system of charged particles. **Journal of Mathematical Physics** 8 (8): 1538–1545.

Dyson, F. J. and Lenard, A. (1967). Stability of matter. I. **Journal of Mathematical Physics** 8 (3): 423–434.

Dyson, F. J. and Lenard, A. (1968). Stability of matter. II. **Journal of Mathematical Physics** 9: 698.

Ehrenfest, P. (1959). Ansprache zur Verleihung der Lorentzmedaille an Professor Wolfgang Pauli am 31 Oktober 1931. (Address on award of Lorentz medal to Professor Wolfgang Pauli on 31 October 1931). In M. J. Klein (ed.). (1959). **Paul Ehrenfest: Collected scientific papers** (p. 617). Amsterdam: North-Holland. [The address appeared originally in P. Ehrenfest (1931). **Versl. Akad. Amsterdam** 40: 121–126.]

Fermi, E. (1927). Un metodo statistico per la determinazione di alcume prioretà dell'atome. (A statistical method for determining some properties of the atom. I). **Atti della Accademia Nazionale dei Lincei, Classe di Scienze Fisiche, Matematiche e Naturali, Rendiconti** 6: 602–607.

Fierz, M. (1939). Über die relativistiche Theorie kräftfreier Teilchen mit beliebegem Spin. (On the relativistic theory of non-interacting particles of arbitrary spin). **Helvetica Physica Acta** 12: 3–37.

Fisher, M. E. (1964). The free energy of a macroscopic system. **Archive for Rational Mechanics and Analysis** 17: 377–410.

Fock, V. (1930). Näherungsmethode zur Lösung des quantenmechanischen Mehrkörperproblems. **Zeitschrift für Physik** 61: 126–148. [See also Fock, V. (1930). "Self-consistent field" mit austausch für Natrium. ("Self-consistent field" with interchange for sodium). **Zeitschrift für Physik** 62: 795–805.]

Forte, S. (1992). Quantum mechanics and field theory with fractional spin and statistics. **Reviews of Modern Physics** 64 (1): 193–236.

Geyer, H. B. (ed.). (1995). **Field theory, topology and condensed matter physics: Proceedings of the ninth Chris Engelbrecht summer school in theoretical physics, held at Storms River Mouth, Tsitsikamma National Park, South Africa, 17–28 January 1994**. Berlin: Springer-Verlag.

Gombás, P. (1949). **Die statistischen Theorie des Atomes und ihre Anwendungen**. Berlin: Springer-Verlag.

Green, M. B., Schwarz, J. H. and Witten, E. (1988). **Superstring theory** (Vols. 1–2). Cambridge: Cambridge University Press.

Hall, R. L. (2000). General energy bounds for systems of bosons with soft cores. **Physical Review A** 62 (5): 052510.

Hall, D. and Wightman, A. S. (1957). A theorem on invariant analytic functions with applications to relativistic quantum field theory. **Mathematisk-Fysiske Meddelelser det Kongelige Danske Videnskabernes Selskab** 31 (5): 1–41.

Hartree, D. R. (1928). The wave mechanics of an atom with a non-Coulomb central field. I. Theory and methods. **Proceedings of the Cambridge Philosophical Society** 24: 89–110.

Heisenberg, W. (1927). Über den anschaulichen inhalt der quantentheoretischen Kinematik und Mechanik. (The Actual Content of Quantum Theoretical Kinematics and Mechanics). **Zeitschrift für Physik** 43: 172–198.

Helffer, B. and Robert, D. (1990). Riesz means of bounded states and semi-classical limit connected with a Lieb-Thirring conjecture. II. **Annales de l' Institut Henri Poincaré** 53 (2): 139–147.

Hertel, P., Lieb, E. H. and Thirring, W. (1975). Lower bound to the energy of complex atoms. **Journal of Chemical Physics** 62 (8): 3355–3356. Reprinted in Thirring (1991), pp. 63–64.

Hoffmann-Ostenhof, M. and Hoffmann-Ostenhof, T. (1977). "Schrödinger inequalities" and asymptotic behavior of the electron density of atoms and molecules. **Physical Review A** 16 (5): 1782–1785.

Hundertmark, D., Laptev, A and Weidl, T. (1999). New bounds on the Lieb-Thirring constants. **ArXiv: math-ph/9906013** [On-line]. Available: `http://lanl.arxiv.org/abs/math-ph/9906013`

Iwanenko, D. and Sokolow, A. (1937). Note on the second quantization of the Dirac equation. **Physikalische Zeitschrift der Sowjetunion** 11: 590.

Jost, R. (1960). Das Pauli-prinzip und die Lorentz-gruppe. In M. Fierz and V. F. Weisskopf (eds.). **Theoretical physics in the twentieth century; a memorial volume to Wolfgang Pauli** (pp. 107–136). New York: Interscience.

Kato, T. (1951). Fundamental properties of Hamiltonian operators of Schrödinger type. **Transactions of the American Mathematical Society** 70: 195–211.

Kato, T. (1972). Schrödinger operators with singular potentials. **Israel Journal of Mathematics** 13: 135–148.

Kirzhnits, D. A. (1957). **Zhurnal Eksperimental'noi i Teoreticheskoi Fiziki** 32: 115–123. English translation: (1957). Quantum corrections to the Thomas-Fermi equations. **Journal of Experimental and Theoretical Physics** 5: 64–71.

Kobayashi, S., Matsukuma, T., Nagai, S. and Umeda, K. (1955). Accuate value of initial slope of the ordinary TF function. **Journal of the Physical Society of Japan** 10 (9): 759-762.

Kompaneets, A. S. and Pavlovskii, E. S. (1956), **Zhurnal Eksperimental'noi i Teoreticheskoi Fiziki** 31: 427–438. English translation: (1957). The self-consistent field equations in an atom. **Journal of Experimental and Theoretical Physics** 4: 328–336.

Kventzel, G. F. and Katriel, J. (1981). Thomas-Fermi atom in *n* dimensions. **Physical Review A**. 24, 2299.

Laptev, A. and Weidl, T. (1999). Sharp Lieb-Thirring inequalities in high dimensions. **ArXiv: math-ph/9903007** [On-line]. Available: http://lanl.arxiv.org/abs/math-ph/9903007

Lenard, A. and Dyson, F. J. (1968). Stability of matter. II. **Journal of Mathematical Physics** 9 (5): 698–711.

Lenz, W. (1932). Über die Anwendbarkeit der statistischen Methode auf ionengitter. (Applicability of the statistical method to ionic lattices). **Zeitschrift für Physik** 77: 713–721.

Lieb, E. H. (1976a). The stability of matter. **Reviews of Modern Physics** 48 (4): 553–569. Reprinted in Thirring (1991), pp. 483–499.

Lieb, E. H. (1976b). Bounds on the eigenvalues of the Laplace and Schrödinger operators. **Bulletin of the American Mathematical Society** 82: 751–753.

Lieb E. H., Thirring W., (1976). **In studies in mathematical physics**, (Lieb E. H., Simon B., Wightman A. S., Eds.). Princeton University Press, New Jersey , 279.

Lieb, E. H. (1979). The $N^{5/3}$ law for bosons. **Physics Letters A** 70 (2): 71–73. Reprinted in Thirring (1991), pp. 327–329.

Lieb, E. H. (1980). The number of bound states of one-body Schrödinger operators and the Weyl problem. **Proceedings of the American Mathematical Society Symposia in Pure Math.** 36: 241–252. Reprinted in Thirring (1991), pp. 173–184.

Lieb, E. H. (1983). On the lowest eigenvalue of the Laplacian for the intersection of two domains. **Invention mathematicae** 74: 441–448.

Lieb, E. H. (1990). The stability of matter: from atoms to stars, 1989 Gibbs Lecture. **Bulletin of the American Mathematical Society** 22: 1–49. Reprinted in Thirring (1991), pp. 11–59.

Lieb, E. H. and Lebowitz, J. L. (1972). The constitution of matter: Existence of thermodynamics for systems composed of electrons and nuclei. **Advances in Mathematics** 9 (3): 316–398.

Lieb, E. H. and Simon, B. (1974). On solutions to the Hartree-Fock problem for atoms and molecules. **Journal of Chemical Physics** 61 (2): 735–736.

Lieb, E. H. and Simon, B. (1977). The Thomas-Fermi theory of atoms, molecules and solids. **Advances in Mathematics** 23 (1): 22–116. [See also Lieb, E. H. and Simon, B. (1973). The Thomas-Fermi theory revisited, **Physical Review Letters** 31 (11): 681–683.]

Lieb, E. H. and Thirring, W. E. (1975). Bound for the kinetic energy of fermions which proves the stability of matter. **Physical Review Letters** 35 (11): 687–689. Errata: **Physical Review Letters** 35 (16): 1116. Reprinted in Thirring (1991), pp. 323–326.

Lieb, E. H. and Thirring, W. (1976). Inequalities for the moments of the eigenvalues of the Schrödinger Hamiltonian and their relation to Sobolev inequalities. In E. H. Lieb, B. Simon and A. S. Wightman (eds.). **Studies in mathematical physics: Essays in honor of Valentine Bargmann** (pp. 269–303). Princeton, New Jersey: Princeton University Press. Reprinted in Thirring (1991), pp. 135–169.

Lüders, G. and Zumino, B. (1958). Connection between spin and statistics. **Physical Review** 110 (6): 1450–1453.

Manoukian, E. B. (1985). Quantum action principle and path integrals for long-range interactions. **Nuovo Cimento A** 90 (11): 295–307.

Manoukian, E. B. (1986). Action principle and quantization of gauge fields. **Physical Review** 34 (12), 3739–3749.

Manoukian E. B. (2006). **Quantum theory: A wide spectrum**. Dordrecht, Berlin, New York, Springer: Sects. 3.1-3.4, 7.1, 14.3.

Manoukian, E. B. and Muthaporn, C. (2002). The collapse of “bosonic matter”. **Progress of Theoretical Physics** 107 (5): 927–939.

Manoukian, E. B. and Muthaporn, C. (2003a). Is ‘bosonic matter’ unstable in 2D?. **Journal of Physics A** 36 (3): 653–663.

Manoukian, E. B. and Muthaporn, C. (2003b). $N^{5/3}$ Law for bosons for arbitrary large N. **Progress of Theoretical Physics** 110 (2): 385–391.

Manoukian, E. B. and Sirininlakul, S. (2004). Rigorous lower bounds for the ground-state energy of matter. **Physics Letters A** 332 (1–2): 54–59. Errata: **Physics Letters A** 337 (4–6) 496.

Manoukian, E. B. and Sirininlakul, S. (2005). High-Density Limit and Inflation of Matter **Physical Review Letters** 95: 190402-1.

Manoukian, E.B. and Limboonsong, K. (2006). Number of eigenvalues of a given potentail: Explicit functional expressions. **Progress of Theoretical Physics** 115(4): 833–837 L.

Manoukian, E. B., Muthaporn, C. and Sirininlakul, S. (2006b). Collapsing stage of “bosonic matter”. **Physics Letters A** 352: 488–490.

Manoukian, E. B. and Sirininlakul, S. (2006b). Stability of Matter in 2D. **Reports on Mathematical Physics** 57:xx.

Miller, A. I. (ed.). (1994). **Early quantum electrodynamics: A source book**. Cambridge: Cambridge University Press.

Mitrinović, D. S., Pečarić, J. E. and Fink, A. M. (1993). **Classical and new inequalities in analysis**. Dordrecht: Kluwer Academic.

Muthaporn, C. and Manoukian, E. B. (2004a). N^2 Law for Bosons in $2D$. **Reports on Mathematical Physics** 53 (3): 415–424.

Muthaporn, C. and Manoukian, E. B. (2004b). Instability of “bosonic matter” in all dimensions. **Physics Letters A** 321 (3): 152–154.

Muthaporn, C. (2005). The Collapse of “Bosonic Matter”. **A Thesis Submitted in Partical Fulfillment of the Requirements for the Degee of Doctor of Philosophy in Physics**, Suranaree University of Technology, Acadamic Year 2004.

Ni, G.-J., Wang, Y.-P. (1983). Vacuum instability and the critical value of the coupling parameter in scalar QED. **Physical Review D** 27 (4): 969–975.

Oka, T. (1997). The Story of Spin. **University of Chicago Press**, Chicago.

Pauli, W. (1925). Über den Zusammenhang des Abschlusses der Elektronengruppen im Atom mit der Komplexstruktur der Spektren. (On the Connexion between the Completion of Electron Groups in an Atom with the Complex Structure of Spectra). **Zeitschrift für Physik** 31: 765.

Pauli, W. (1936). Quantized theory of particles obeying Bose-Einstein statistics. **Annales de l' Institut Henri Poincaré** 6, 137.

Pauli, W. (1950). On the connection between spin and statistics. **Progress of Theoretical Physics** 5: 526–543.

Pauli, W. and Belinfante, F. J. (1940). On the statistical behaviour of known and unknown elementary particles. **Physica** 7 (3): 177–192.

Pauli, W. and Weisskopf, V. F. (1934). The quantization of the scalar relativistic wave equation, **Helvetica Physica Acta** 7: 709–731. Reprinted in english translation in Miller (1994), pp. 188–205.

Perez, J. F., Malta, C. P. and Coutinho, F. A. B. (1988). A lower bound for the ground-state energy of many particles moving in one dimension. **Journal of Physics A** 21 (8): 1847–1856.

Pfender, F. and Ziegler, G. M. (2004). Kissing numbers, sphere packings, and some unexpected proofs. **Notices of the American Mathematical Society** 51 (8): 873–883.

Rosen, G. (1971). Minimum value for c in the Sobolev inequality $\|\Phi\|_3 \leq c\,\|\nabla\Phi\|^3$. **SIAM Journal on Applied Mathematics** 21: 30–32.

Schwarz, J. H. (ed.). (1985). **Superstrings: The first 15 years of superstring theory** (Vols. 1–2). Singapore: World Scientific.

Schwinger, J. (1951a). On the Green's functions of quantized fields I. **Proceedings of the National Academy of Sciences of the United States of America** 37 (7): 452–455. Reprinted in Schwinger (1958c), pp. 379–382.

Schwinger, J. (1951b). The theory of quantized fields I. **Physical Review** 82 (6): 914–927. Reprinted in Schwinger (1958c), pp. 342–355.

Schwinger, J. (1953). The theory of quantized fields II. **Physical Review** 91 (3): 713–728. Reprinted in Schwinger (1958c), pp. 356–371.

Schwinger, J. (1954). The theory of quantized fields V. **Physical Review** 93 (3): 615–628.

Schwinger, J. (1958a). Spin, statistics, and the TCP theorem. **Proceedings of the National Academy of Sciences of the United States of America** 44 (2): 223–228.

Schwinger, J. (1958b). Addendum to spin, statistics and the TCP theorem. **Proceedings of the National Academy of Sciences of the United States of America** 44 (6): 617–619.

Schwinger, J. (ed.). (1958c). **Selected papers in quantum electrodynamics**. New York: Dover.

Schwinger, J. (1961). On the bound states of a given potential. **Proceedings of the National Academy of Sciences of the United States of America** 47 (1): 122–129.

Schwinger, J. (1988). **Particles, sources and fields** (Vols. 1–3). Redwood City, California: Addison-Wesley.

Scott, J. M. C. (1952). The binding energy of the Thomas Fermi atom. **Philosophical Magazine** 43: 859.

Semenoff, G. W. and Wijewardhana, L. C. R. (1987). Induced fractional spin statistics in three-dimensional QED. **Physics Letters B** 184 (4): 397–402.

Sheldon, J. W. (1955). Use of the statistical field approximation in molecular physics. **Physical Review** 99 (4): 1291–1301.

Slater, J. C. (1930). The theory of complex spectra. **Physical Review** 34 (10): 1293–1322.

Sobolev, S. L. (1938). On a theorem in functional analysis **Matematicheskiĭ Sbornik** 46: 471–497. [See also Sobolev, S. L. (1963). Applications of functional analysis in mathematical physics. **The American Mathematical Society Transl.** 34: 39–68.]

Sommerfeld, A. (1932). Asymptotische Integration der Differential-gleichung des Thomas-Fermischen Atoms. **Zeitschrift für Physik** 78: 283–308.

Stoner, E. C. (1924). The distribution of electrons among atomic levels. **Philosophical Magazine** 48 (286): 719–736.

Stein, E. M. (1971). **Singular integrals and differentiability properties of functions**. Princeton, New Jersey: Princeton University Press.

Teller, E. (1962). On the stability of molecules in the Thomas-Fermi theory. **Review of Modern Physics** 34 (4): 627–631.

Thirring, W. E. (1983). **A course in mathematical physics: Quantum mechanics of large systems (Course in mathematical physics)**. Berlin: Springer-Verlag.

Thirring, W. E. (ed.). (1991). **The stability of matter: from atoms to stars: Selecta of Elliot H. Lieb and subsequent editions**. Berlin: Springer-Verlag.

Thomas, L. H. (1927). The calculation of atomic fields. **Proceedings of the Cambridge Philosophical Society** 23: 542–548.

Tomonaga, S-I. (1997). **The story of spin**. Translated by T. Oka. Chicago: University of Chicago Press.

von Weizsäcker, C. F. (1935). Zur Theorie der Kernmassen. **Zeitschrift für Physik** 96: 431–458.

Woan, G. (2000). **The Cambridge handbook of physics formulas**. Cambridge: Cambridge University Press.

Watson, G. N. (1966). **A treatise on the theory of Bessel functions** (2nd ed.). Cambridge: Cambridge University Press.

Weidl, T. (1996). On the Lieb-Thirring constants for $L_{\gamma,1}$ for $\gamma \geqq 1/2$. **Communications in Mathematical Physics** 178 (1): 135–146.

Yosida, K. (1980). **Functional analysis** (6th ed.). Berlin: Springer-Verlag.

APPENDICES

APPENDIX A

LOWER BOUND FOR THE EXACT GROUND-STATE ENERGY OF MATTER WITHOUT THE EXCLUSION PRINCIPLE

Although it is sufficient to obtain an upper bound for the ground-state energy for bosonic matter to infer its instability, the knowledge of a lower bound is also important to get an actual estimate of a range for the ground-state energy. As a byproduct of their analysis of the stability of fermionic matter, Manoukian and Sirininlakul (2005) were able to obtain a lower bound to the exact ground-state energy of "bosonic" matter. At present it is the best bound obtained in the literature even better than the one given by Lieb (1978). Here for completeness, we sketch over derivation of the lower bound.

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + V_1 + V_2 - \sum_{i=1}^{N}\sum_{j=1}^{k} Z_j e^2 |\mathbf{x}_i - \mathbf{R}_j|^{-1}, \tag{A.1}$$

where

$$V_1 = \sum_{i<j}^{N} e^2 |\mathbf{x}_i - \mathbf{x}_j|^{-1} \qquad , \tag{A.2}$$

$$V_2 = \sum_{i<j}^{k} Z_i Z_j e^2 |\mathbf{R}_i - \mathbf{R}_j|^{-1}\ , \quad \sum_{i=1}^{k} Z_i = N, \quad k \geq 2 \tag{A.3}$$

with fixed positive charges, and $\mathbf{x}_i$, $\mathbf{R}_j$ refer to the position of negative and positive charges, respectively. We note that for $k = 1$, the V_2 term in (A.3) will be absent in the expression for *H* and one would be dealing with an atom. Throughout, we are interested in the case for which $k \neq 1$ relevant to matter.

A rigorous study of the instability and stability of such systems for bosons and fermions, respectively, began several years ago in some remarkable work giving rise to the respective famous $N^{5/3}$ and N power laws for the ground-state energy (Dyson and Lenard, 1967). Much simplified derivations with tremendous improvements of the corresponding estimates have been given for bosonic cases (Lieb and Thirring, 1975; Manoukian and Sirininlakul, 2004)

$$-c_B N^{5/3}\left[1+\left(\sum_{i=1}^{k}\frac{Z_i^{7/3}}{N}\right)^{1/2}\right]^2, \tag{A.4}$$

in units of $me^4/2\hbar^2$, where c_B is some positive constant.

Motivated by the lower bound of the repulsive part of the Coulomb potential derived below (Hertel, Lieb and Thirring, 1975), rigorous lower bounds are derived for the ground-state energies of the above systems by using, in the process, lower bounds for the kinetic energies as some power of an integral of ρ^2 rather than of the familiar $\rho^{5/3}$, where ρ is the particle density.

Consider a real function $v(\mathbf{x})$, $\mathbf{x}$ is vector in 3-dimensions, we have

$$v(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\widetilde{v}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{A.5}$$

$$\widetilde{v}(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}\,v(\mathbf{x})\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{A.6}$$

such that $v(\mathbf{x}) \geq 0$ and $v(0) < \infty$, and such that its Fourier transform $\widetilde{v}(\mathbf{k}) \geq 0$ as well. Let $\phi(\mathbf{x})$ be a real function, and

$$\phi(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\widetilde{\phi}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$$

$$\phi(\mathbf{x}_j) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\widetilde{\phi}(\mathbf{k})\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \tag{A.7}$$

$$\widetilde{\phi}(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}\, \phi(\mathbf{x})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{A.8}$$

Let $A_1, \ldots, A_k \ (k \geq 2)$ be real and positive numbers. We have

$$\begin{aligned}
A_1\phi(\mathbf{x}_1) =& A_1 \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\phi}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_1} \\
A_2\phi(\mathbf{x}_2) =& A_2 \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\phi}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_2} \\
&\vdots \\
A_k\phi(\mathbf{x}_k) =& A_k \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\phi}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_k}
\end{aligned} \tag{A.9}$$

and

$$A_1\phi(\mathbf{x}_1) + A_2\phi(\mathbf{x}_2) + \ldots + A_k\phi(\mathbf{x}_k) = \sum_{j=1}^{k} A_j\phi\left(\mathbf{x}_j\right). \tag{A.10}$$

Substitute $\phi\left(\mathbf{x}_j\right) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\phi}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j}$ into $\sum_{j=1}^{k} A_j\phi\left(\mathbf{x}_j\right)$, to obtain

$$\sum_{j=1}^{k} A_j\phi\left(\mathbf{x}_j\right) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\phi}(\mathbf{k}) \left(\sum_{j=1}^{k} A_j\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \right). \tag{A.11}$$

Multiply the integrand on the right-hand side (A.11) by $\frac{\sqrt{\widetilde{v}(\mathbf{k})}}{\sqrt{\widetilde{v}(\mathbf{k})}}$, givingThen we may write

$$\sum_{j=1}^{k} A_j\phi\left(\mathbf{x}_j\right) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \frac{\widetilde{\phi}(\mathbf{k})}{\sqrt{\widetilde{v}(\mathbf{k})}} \left(\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j} \right). \tag{A.12}$$

The Cauchy-Schwartz inequality

$$\left(\sum_{j=1}^{n} a_j b_j \right)^2 \leqslant \sum_{j=1}^{n} \left|a_j\right|^2 \sum_{j=1}^{n} \left|b_j\right|^2 \tag{A.13}$$

then implies that

$$\left(\sum_{j=1}^{k} A_j \phi\left(\mathbf{x}_j\right)\right)^2 = \left(\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \frac{\widetilde{\phi}(\mathbf{k})}{\sqrt{\widetilde{v}(\mathbf{k})}}\, \left(\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j}\right)\right)^2$$

$$\leqslant \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left|\frac{\widetilde{\phi}(\mathbf{k})}{\sqrt{\widetilde{v}(\mathbf{k})}}\right|^2 \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left|\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j}\right|^2. \quad \text{(A.14)}$$

Consider $\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left|\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j}\right|^2$ on left-hand side of (A.14), to obtain

$$\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left|\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j}\right|^2$$

$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left(\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j}\right) \cdot \left(\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j}\right)^*$$

$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left(\sum_{i=1}^{k} A_i \sqrt{\widetilde{v}(\mathbf{k})}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}_i}\right) \cdot \left(\sum_{j=1}^{k} A_j \sqrt{\widetilde{v}(\mathbf{k})}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}_j}\right)$$

$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \sum_{i=1}^{k} A_i \sum_{j=1}^{k} A_j\, \widetilde{v}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}_i-\mathbf{x}_j)}$$

$$= \sum_{i,j=1}^{k} A_i A_j \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{v}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}_i-\mathbf{x}_j)}$$

$$= \sum_{i,j=1}^{k} A_i A_j\, v(\mathbf{x}_i - \mathbf{x}_j) \quad \text{(A.15)}$$

where we recall that $A_1, \ldots, A_k\ (k \geq 2)$ are real and positive numbers, $\widetilde{v}(\mathbf{k}) \geq 0$ and

$$v(\mathbf{x}_i - \mathbf{x}_j) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{v}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}_i-\mathbf{x}_j)}. \quad \text{(A.16)}$$

Substitute (A.16) to the right-hand side of (A.14), to obtain

$$\left(\sum_{j=1}^{k} A_j \phi\left(\mathbf{x}_j\right)\right)^2 \leqslant \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} \sum_{i,j=1}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j). \tag{A.17}$$

We can rewrite (A.17) as

$$\frac{\left(\sum_{j=1}^{k} A_j \phi\left(\mathbf{x}_j\right)\right)^2}{\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}} \leqslant \sum_{i,j=1}^{k} A_i A_j \, v(\mathbf{x}_i - \mathbf{x}_j). \tag{A.18}$$

For any real number a, b such that $b > 0$, we have

$$\begin{aligned}
(a-b)^2 &\geqslant 0 \\
a^2 - 2ab + b^2 &\geqslant 0 \\
a^2 &\geqslant 2ab - b^2 \\
\frac{a^2}{2b} &\geqslant \frac{2ab}{2b} - \frac{b^2}{2b} \\
\frac{a^2}{2b} &\geqslant a - \frac{b}{2}.
\end{aligned} \tag{A.19}$$

Set

$$a = \sum_{j=1}^{k} A_j \phi\left(\mathbf{x}_j\right) \tag{A.20}$$

$$b = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} \tag{A.21}$$

and use the inequality in (A.19), to infer that

$$\frac{1}{2}\frac{\left(\sum_{j=1}^{k}A_j\phi\left(\mathbf{x}_j\right)\right)^2}{\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}} \geqslant \sum_{j=1}^{k}A_j\phi\left(\mathbf{x}_j\right) - \frac{1}{2}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}$$

$$\frac{1}{2}\sum_{i,j=1}^{k}A_iA_j\,v(\mathbf{x}_i-\mathbf{x}_j) \;\geqslant \sum_{j=1}^{k}A_j\phi\left(\mathbf{x}_j\right) - \frac{1}{2}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}. \qquad \text{(A.22)}$$

Consider the left-hand side of the inequality in (A.22), to obtain

$$\begin{aligned}\frac{1}{2}\sum_{i,j=1}^{k}A_iA_j\,v(\mathbf{x}_i-\mathbf{x}_j) &= \sum_{i<j}^{k}A_iA_j\,v(\mathbf{x}_i-\mathbf{x}_j) + \frac{1}{2}\sum_{i=j}^{k}A_iA_j\,v(\mathbf{x}_i-\mathbf{x}_j)\\ &= \sum_{i<j}^{k}A_iA_j\,v(\mathbf{x}_i-\mathbf{x}_j) + \frac{1}{2}\sum_{i=j}^{k}A_jA_j\,v(\mathbf{x}_j-\mathbf{x}_j)\\ &= \sum_{i<j}^{k}A_iA_j\,v(\mathbf{x}_i-\mathbf{x}_j) + \frac{1}{2}v(0)\sum_{j=1}^{k}A_j^2\end{aligned}$$

$$\sum_{i<j}^{k}A_iA_j\,v(\mathbf{x}_i-\mathbf{x}_j) = \frac{1}{2}\sum_{i,j=1}^{k}A_iA_j\,v(\mathbf{x}_i-\mathbf{x}_j) - \frac{1}{2}v(0)\sum_{j=1}^{k}A_j^2. \qquad \text{(A.23)}$$

Substitute (A.22) into (A.24), to obtain

$$\sum_{i<j}^{k}A_iA_j\,v(\mathbf{x}_i-\mathbf{x}_j) \geqslant \sum_{j=1}^{k}A_j\phi\left(\mathbf{x}_j\right) - \frac{1}{2}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} - \frac{1}{2}v(0)\sum_{j=1}^{k}A_j^2. \qquad \text{(A.24)}$$

Let $V(\mathbf{x})$ be real such that $V(\mathbf{x}) \geq v(\mathbf{x})$, and $\rho(\mathbf{x})$ real, and so far arbitrary,

$$\phi(\mathbf{x}) = \int \mathrm{d}^3\mathbf{x}'\;\rho(\mathbf{x}')\;V(\mathbf{x}'-\mathbf{x}). \qquad \text{(A.25)}$$

and

$$\phi(\mathbf{x}_j) = \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x} - \mathbf{x}_j). \tag{A.26}$$

Substitute (A.26) into (A.23), to obtain

$$\sum_{i<j}^{k} A_i A_j\, v(\mathbf{x}_i - \mathbf{x}_j) \geqslant \sum_{j=1}^{k} A_j \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x} - \mathbf{x}_j) - \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}$$
$$- \frac{1}{2} v(0) \sum_{j=1}^{k} A_j^2. \tag{A.27}$$

We obtain We may write

$$\widetilde{\phi}(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x} - \mathbf{x}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \tag{A.28}$$

and

$$\widetilde{\phi}^*(\mathbf{k}) = \int \mathrm{d}^3\mathbf{y}' \int \mathrm{d}^3\mathbf{y}\, \rho^*(\mathbf{y})\, V^*(\mathbf{y} - \mathbf{y}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}'}. \tag{A.29}$$

Since $\rho(\mathbf{x})$ and $V(\mathbf{x} - \mathbf{x}')$ are real function, i.e., $\rho(\mathbf{x}) = \rho^*(\mathbf{x})$ and $V(\mathbf{x} - \mathbf{x}') = V^*(\mathbf{x} - \mathbf{x}')$, we obtain from (A.28)

$$\widetilde{\phi}(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x} - \mathbf{x}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'}$$
$$= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V^*(\mathbf{x} - \mathbf{x}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'}. \tag{A.30}$$

With the following Fourier transforms

$$\rho(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{A.31}$$

$$\rho^*(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{A.32}$$

$$V(\mathbf{x}-\mathbf{x'}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{V}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x'})} \tag{A.33}$$

$$V^*(\mathbf{x}-\mathbf{x'}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{V}^*(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x'})} \tag{A.34}$$

substituted into (A.30), gives

$$\begin{aligned}
\widetilde{\phi}(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\, \widetilde{V}^*(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot(\mathbf{x}-\mathbf{x'})}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \\
&= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\, \widetilde{V}^*(\mathbf{k}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{x}}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}'} \\
&= \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) \int \mathrm{d}^3\mathbf{k}'\, \widetilde{V}^*(\mathbf{k}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{x}} \int \frac{\mathrm{d}^3\mathbf{x'}}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}'}.
\end{aligned} \tag{A.35}$$

To above end, we use an integral representation of the delta function in 3-dimensions:

$$\delta^3(\mathbf{k}-\mathbf{k}') = \frac{1}{(2\pi)^3} \int \mathrm{d}^3\mathbf{x}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \tag{A.36}$$

$$\delta^3(\mathbf{x}-\mathbf{x'}) = \frac{1}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k}\, \mathrm{e}^{\mathrm{i}(\mathbf{x}-\mathbf{x'})\cdot\mathbf{k}} \tag{A.37}$$

$$\int \mathrm{d}^3\mathbf{x}\, F(\mathbf{x})\, \delta^3(\mathbf{x}-\mathbf{x'}) = F(\mathbf{x'}). \tag{A.38}$$

Applying an integral representation of the delta function in 3-dimensions into (A.32), we obtain

$$\begin{aligned}
\widetilde{\phi}(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) \int \mathrm{d}^3\mathbf{k}'\, \widetilde{V}^*(\mathbf{k}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot\mathbf{x}}\, \delta^3(\mathbf{k}'-\mathbf{k}) \\
&= \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, \widetilde{V}^*(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}.
\end{aligned} \tag{A.39}$$

Substitute (A.31) and apply an integral representation of the delta function in 3-

dimensions into (A.39), to obtain

$$
\begin{aligned}
\widetilde{\phi}(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,\widetilde{V}^*(\mathbf{k})\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&= \int \mathrm{d}^3\mathbf{x} \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\,\widetilde{\rho}(\mathbf{k}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{x}}\,\widetilde{V}^*(\mathbf{k})\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&= \int \mathrm{d}^3\mathbf{k}'\,\widetilde{\rho}(\mathbf{k}')\,\widetilde{V}^*(\mathbf{k}) \int \frac{\mathrm{d}^3\mathbf{x}}{(2\pi)^3}\,\mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{x}} \\
&= \int \mathrm{d}^3\mathbf{k}'\,\widetilde{\rho}(\mathbf{k}')\,\widetilde{V}^*(\mathbf{k})\,\delta^3(\mathbf{k}'-\mathbf{k}) \\
&= \widetilde{\rho}(\mathbf{k})\,\widetilde{V}^*(\mathbf{k}).
\end{aligned} \tag{A.40}
$$

In the same way, to obtain $\widetilde{\phi}^*(\mathbf{k})$, we have

$$
\widetilde{\phi}^*(\mathbf{k}) = \widetilde{\rho}^*(\mathbf{k})\,\widetilde{V}(\mathbf{k}). \tag{A.41}
$$

Since $\left|\widetilde{\phi}(\mathbf{k})\right|^2 = \widetilde{\phi}^*(\mathbf{k})\,\widetilde{\phi}(\mathbf{k})$, we obtain from (A.40) and (A.41)

$$
\begin{aligned}
\left|\widetilde{\phi}(\mathbf{k})\right|^2 &= \widetilde{\phi}^*(\mathbf{k})\widetilde{\phi}(\mathbf{k}) \\
&= \widetilde{\rho}(\mathbf{k})\,\widetilde{V}^*(\mathbf{k})\,\widetilde{\rho}^*(\mathbf{k})\,\widetilde{V}(\mathbf{k}) \\
&= \widetilde{\rho}^*(\mathbf{k})\widetilde{\rho}(\mathbf{k})\,\widetilde{V}^*(\mathbf{k})\widetilde{V}(\mathbf{k}) \\
&= |\widetilde{\rho}(\mathbf{k})|^2 \left|\widetilde{V}(\mathbf{k})\right|^2.
\end{aligned} \tag{A.42}
$$

On the other hand for $\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}$(A.42)/$\widetilde{v}(\mathbf{k})$, we have

$$
\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\left|\widetilde{\phi}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,|\widetilde{\rho}(\mathbf{k})|^2\,\frac{\left|\widetilde{V}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} \tag{A.43}
$$

Since $V(\mathbf{y}) \geq v(\mathbf{y})$, so $V(\mathbf{y}-\mathbf{y'}) \geq v(\mathbf{y}-\mathbf{y'})$, replaced $V(\mathbf{y}-\mathbf{y'})$ with $v(\mathbf{y}-\mathbf{y'})$ in the right-hand side of (A.29). In analogy to $V(\mathbf{x})$ with $V(\mathbf{y}) \geq v(\mathbf{y})$, we may introduce

$$\begin{aligned}
\widetilde{\varphi}^*(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{y}' \int \mathrm{d}^3\mathbf{y}\, \rho^*(\mathbf{y})\, v^*(\mathbf{y}-\mathbf{y}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}'} \\
&= \int \mathrm{d}^3\mathbf{y}' \int \mathrm{d}^3\mathbf{y}\, \rho(\mathbf{y})\, v(\mathbf{y}-\mathbf{y}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}'} \\
&= \int \mathrm{d}^3\mathbf{y}' \int \mathrm{d}^3\mathbf{y}\, \rho(\mathbf{y}) \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\, \widetilde{v}(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot(\mathbf{y}-\mathbf{y}')}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}'} \\
&= \int \mathrm{d}^3\mathbf{y}\, \rho(\mathbf{y}) \int \mathrm{d}^3\mathbf{k}'\, \widetilde{v}(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{y}} \int \frac{\mathrm{d}\mathbf{y}'}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{y}'} \\
&= \int \mathrm{d}^3\mathbf{y}\, \rho(\mathbf{y}) \int \mathrm{d}^3\mathbf{k}'\, \widetilde{v}(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{y}}\, \delta^3(\mathbf{k}-\mathbf{k}') \\
&= \int \mathrm{d}^3\mathbf{y}\, \rho(\mathbf{y})\, \widetilde{v}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}}. \qquad \text{(A.44)}
\end{aligned}$$

Divide (A.44) by $\widetilde{v}(\mathbf{k})$, we obtain

$$\begin{aligned}
\frac{\widetilde{\varphi}^*(\mathbf{k})}{\widetilde{v}(\mathbf{k})} &= \int \mathrm{d}^3\mathbf{y}\, \rho(\mathbf{y})\, \frac{\widetilde{v}(\mathbf{k})}{\widetilde{v}(\mathbf{k})}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}} \\
&= \int \mathrm{d}^3\mathbf{y}\, \rho(\mathbf{y})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}}. \qquad \text{(A.45)}
\end{aligned}$$

Multiply (A.45) with $\widetilde{\varphi}(\mathbf{k})$, we obtain

$$\frac{\widetilde{\phi}(\mathbf{k})\widetilde{\varphi}^*(\mathbf{k})}{\widetilde{v}(\mathbf{k})} = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \int \mathrm{d}^3\mathbf{y}\, \rho(\mathbf{y})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}}. \qquad \text{(A.46)}$$

For $\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}$(A.46), we have

$$\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\widetilde{\phi}(\mathbf{k})\widetilde{\varphi}^*(\mathbf{k})}{\widetilde{v}(\mathbf{k})}$$

$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}')\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}'} \int \mathrm{d}^3\mathbf{y}\, \rho(\mathbf{y})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}}$$

$$= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}') \int \mathrm{d}^3\mathbf{y}\, \rho(\mathbf{y}) \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{y}-\mathbf{x}')}$$

$$= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}') \int \mathrm{d}^3\mathbf{y}\, \rho(\mathbf{y})\, \delta^3(\mathbf{y}-\mathbf{x}')$$

$$= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}')\, \rho(\mathbf{x}'). \qquad \text{(A.47)}$$

We rewrite as (A.47) as

$$\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{\widetilde{\phi}(\mathbf{k})\widetilde{\varphi}^*(\mathbf{k})}{\widetilde{v}(\mathbf{k})} = \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho^*(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}')\, \rho(\mathbf{x}')$$

$$= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho^*(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}') \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\, \widetilde{\rho}(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{x}'}$$

$$= \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho^*(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{V}(\mathbf{k}'')\, \mathrm{e}^{\mathrm{i}\mathbf{k}''\cdot(\mathbf{x}-\mathbf{x}')}$$

$$\times \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\, \widetilde{\rho}(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{x}'}$$

$$= \int \mathrm{d}^3\mathbf{x}\, \rho^*(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{V}(\mathbf{k}'')\, \mathrm{e}^{\mathrm{i}\mathbf{k}''\cdot\mathbf{x}} \int \mathrm{d}^3\mathbf{k}'\, \widetilde{\rho}(\mathbf{k}')$$

$$\times \int \frac{\mathrm{d}^3\mathbf{x}'}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{x}'}$$

$$= \int \mathrm{d}^3\mathbf{x}\, \rho^*(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{V}(\mathbf{k}'')\, \mathrm{e}^{\mathrm{i}\mathbf{k}''\cdot\mathbf{x}}$$

$$\times \int \mathrm{d}^3\mathbf{k}'\, \widetilde{\rho}(\mathbf{k}')\, \delta^3(\mathbf{k}'-\mathbf{k}'')$$

$$= \int \mathrm{d}^3\mathbf{x}\, \rho^*(\mathbf{x}) \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{V}(\mathbf{k}'')\, \mathrm{e}^{\mathrm{i}\mathbf{k}''\cdot\mathbf{x}}\, \widetilde{\rho}(\mathbf{k}'')$$

$$= \int \mathrm{d}^3\mathbf{x} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$$

$$
\begin{aligned}
&\times \int \frac{\mathrm{d}^3\mathbf{k}''}{(2\pi)^3}\, \widetilde{V}(\mathbf{k}'')\, \mathrm{e}^{\mathrm{i}\mathbf{k}''\cdot\mathbf{x}}\, \widetilde{\rho}(\mathbf{k}'') \\
&= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k}) \int \mathrm{d}^3\mathbf{k}''\, \widetilde{V}(\mathbf{k}'')\, \widetilde{\rho}(\mathbf{k}'') \\
&\times \int \frac{\mathrm{d}^3\mathbf{x}}{(2\pi)^3}\; \mathrm{e}^{\mathrm{i}(\mathbf{k}''-\mathbf{k})\cdot\mathbf{x}} \\
&= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k}) \int \mathrm{d}^3\mathbf{k}''\, \widetilde{V}(\mathbf{k}'')\, \widetilde{\rho}(\mathbf{k}'')\, \delta^3(\mathbf{k}''-\mathbf{k}) \\
&= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}^*(\mathbf{k})\, \widetilde{V}(\mathbf{k})\, \widetilde{\rho}(\mathbf{k}) \\
&= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\; |\widetilde{\rho}(\mathbf{k})|^2\; \widetilde{V}(\mathbf{k})
\end{aligned}
\tag{A.48}
$$

From (A.47) and (A.48), we have

$$
\int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}')\, \rho(\mathbf{x}') = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\; |\widetilde{\rho}(\mathbf{k})|^2\; \widetilde{V}(\mathbf{k}). \tag{A.49}
$$

Substitute (A.43) and (A.49) into (A.27), to obtain

$$
\begin{aligned}
\sum_{i<j}^{k} A_i A_j\, v(\mathbf{x}_i-\mathbf{x}_j) \geqslant & \sum_{j=1}^{k} A_j \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}_j) - \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\; |\widetilde{\rho}(\mathbf{k})|^2\; \frac{\left|\widetilde{V}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} \\
& + \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2\, \widetilde{V}(\mathbf{k}) \\
& - \frac{1}{2}\int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x}-\mathbf{x}')\, \rho(\mathbf{x}') \\
& - \frac{1}{2} v(0) \sum_{j=1}^{k} A_j^2.
\end{aligned}
\tag{A.50}
$$

Since $V(\mathbf{x}) \geq v(\mathbf{x}) \geq 0$, we have $\sum\limits_{i<j}^{k} A_i A_j V(\mathbf{x}_i-\mathbf{x}_j) \geq \sum\limits_{i<j}^{k} A_i A_j\, v(\mathbf{x}_i-\mathbf{x}_j)$, so that

(A.50) becomes

$$\sum_{i<j}^{k} A_i A_j V(\mathbf{x}_i - \mathbf{x}_j) \geqslant \sum_{j=1}^{k} A_j \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x} - \mathbf{x}_j) - \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2\, \frac{\left|\widetilde{V}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}$$

$$+ \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2\, \widetilde{V}(\mathbf{k})$$

$$- \frac{1}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x} - \mathbf{x}')\, \rho(\mathbf{x}')$$

$$- \frac{1}{2} v(0) \sum_{j=1}^{k} A_j^2$$

$$= \sum_{j=1}^{k} A_j \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x} - \mathbf{x}_j)$$

$$- \frac{1}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x} - \mathbf{x}')\, \rho(\mathbf{x}')$$

$$- \frac{1}{2} v(0) \sum_{j=1}^{k} A_j^2 - \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2\, \frac{\left|\widetilde{V}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})}$$

$$+ \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2\, \widetilde{V}(\mathbf{k})$$

$$\sum_{i<j}^{k} A_i A_j V(\mathbf{x}_i - \mathbf{x}_j) \geqslant \sum_{j=1}^{k} A_j \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x} - \mathbf{x}_j)$$

$$- \frac{1}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x})\, V(\mathbf{x} - \mathbf{x}')\, \rho(\mathbf{x}')$$

$$- \frac{1}{2} v(0) \sum_{j=1}^{k} A_j^2$$

$$- \frac{1}{2} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2 \left[\frac{\left|\widetilde{V}(\mathbf{k})\right|^2}{\widetilde{v}(\mathbf{k})} - \widetilde{V}(\mathbf{k}) \right] \qquad \text{(A.51)}$$

where, needless to say, $\int \mathrm{d}^3\mathbf{k} \mid \widetilde{\rho}(\mathbf{k})|^2 \ \widetilde{V}(\mathbf{k})$ is real. Let $v(\mathbf{x}) = e^2(1-\mathrm{e}^{-\lambda|\mathbf{x}|})/|\mathbf{x}|$, $\lambda > 0$, the Fourier transform of $v(\mathbf{x})$ is

$$\begin{aligned}
\widetilde{v}(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}\, v(\mathbf{x})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&= \int \mathrm{d}^3\mathbf{x}\, \frac{e^2(1-\mathrm{e}^{-\lambda|\mathbf{x}|})}{|\mathbf{x}|}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&= \int \mathrm{d}^3\mathbf{x}\, \frac{e^2(1-\mathrm{e}^{-\lambda x})}{x}\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|\cos\theta} \\
&= \int_0^\infty x^2 \mathrm{d}x \int_0^\pi \sin\theta\, \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi\, \frac{e^2(1-\mathrm{e}^{-\lambda x})}{x}\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|\cos\theta} \\
\widetilde{v}(\mathbf{k}) &= \int_0^\infty \mathrm{d}x\, x^2\, \frac{e^2(1-\mathrm{e}^{-\lambda x})}{x} \int_0^\pi \mathrm{d}\theta\, \sin\theta\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|\cos\theta} \int_0^{2\pi} \mathrm{d}\varphi. \qquad \text{(A.52)}
\end{aligned}$$

The φ integration gives

$$\int_0^{2\pi} \mathrm{d}\varphi = 2\pi. \qquad \text{(A.53)}$$

The θ integration is

$$\begin{aligned}
\int_0^\pi \sin\theta\, \mathrm{d}\theta\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|\cos\theta} &= -\int_1^{-1} \mathrm{d}u\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}|xu} \quad , \ u = \cos\theta \\
&= \int_{-1}^{1} \mathrm{d}u\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}|xu} \\
&= \frac{1}{i|\mathbf{k}||\mathbf{x}|}\left(\mathrm{e}^{\mathrm{i}|\mathbf{k}||\mathbf{x}|} - \mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|}\right). \qquad \text{(A.54)}
\end{aligned}$$

Substitute (A.53) and (A.54) into (A.52), to obtain

$$\begin{aligned}
\widetilde{v}(\mathbf{k}) &= 2\pi e^2 \int_0^\infty \mathrm{d}x\, x^2\, \frac{(1-\mathrm{e}^{-\lambda x})}{x}\, \frac{1}{i|\mathbf{k}||\mathbf{x}|}\left(\mathrm{e}^{\mathrm{i}|\mathbf{k}||\mathbf{x}|} - \mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{x}|}\right) \\
&= 2\pi e^2 \int_0^\infty \mathrm{d}x\, x^2\, \frac{(1-\mathrm{e}^{-\lambda x})}{x}\, \frac{1}{i|\mathbf{k}|x}\left(\mathrm{e}^{\mathrm{i}|\mathbf{k}|x} - \mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}\right)
\end{aligned}$$

$$=\frac{2\pi e^2}{i|\mathbf{k}|}\int_0^\infty \mathrm{d}x\,(1-\mathrm{e}^{-\lambda x})\left(\mathrm{e}^{\mathrm{i}|\mathbf{k}|x}-\mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}\right)$$

$$=\frac{2\pi e^2}{i|\mathbf{k}|}\left[\int_0^\infty \mathrm{d}x\;\left(\mathrm{e}^{\mathrm{i}|\mathbf{k}|x}-\mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}-\mathrm{e}^{(i|\mathbf{k}|-\lambda)x}+\mathrm{e}^{-(i|\mathbf{k}|+\lambda)x}\right)\right]$$

$$=\frac{2\pi e^2}{i|\mathbf{k}|}\left[\int_0^\infty \mathrm{d}x\,\mathrm{e}^{\mathrm{i}|\mathbf{k}|x}-\int_0^\infty \mathrm{d}x\,\mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}-\int_0^\infty \mathrm{d}x\,\mathrm{e}^{(i|\mathbf{k}|-\lambda)x}\right.$$

$$\left.+\int_0^\infty \mathrm{d}x\,\mathrm{e}^{-(i|\mathbf{k}|+\lambda)x}\right]$$

$$=\frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{\mathrm{e}^{\mathrm{i}|\mathbf{k}|x}}{i|\mathbf{k}|}\bigg|_0^\infty+\frac{\mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}}{i|\mathbf{k}|}\bigg|_0^\infty-\frac{\mathrm{e}^{(i|\mathbf{k}|-\lambda)x}}{i|\mathbf{k}|-\lambda}\bigg|_0^\infty-\frac{\mathrm{e}^{-(i|\mathbf{k}|+\lambda)x}}{i|\mathbf{k}|+\lambda}\bigg|_0^\infty\right]$$

$$=\frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{\mathrm{e}^\infty}{i|\mathbf{k}|}-\frac{1}{i|\mathbf{k}|}-\frac{1}{i|\mathbf{k}|}-\left(\frac{\mathrm{e}^\infty}{i|\mathbf{k}|-\lambda}-\frac{1}{i|\mathbf{k}|-\lambda}\right)+\left(\frac{1}{i|\mathbf{k}|+\lambda}\right)\right]$$

$$=\frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{\mathrm{e}^\infty}{i|\mathbf{k}|}-\frac{1}{i|\mathbf{k}|}-\frac{1}{i|\mathbf{k}|}-\frac{\mathrm{e}^\infty}{i|\mathbf{k}|+\lambda}+\frac{1}{i|\mathbf{k}|-\lambda}+\frac{1}{i|\mathbf{k}|+\lambda}\right]$$

$$=\frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{1}{i|\mathbf{k}|-\lambda}+\frac{1}{i|\mathbf{k}|+\lambda}-\frac{2}{i|\mathbf{k}|}\right]$$

$$=\frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{(i|\mathbf{k}|+\lambda)(i|\mathbf{k}|)+(i|\mathbf{k}|-\lambda)(i|\mathbf{k}|)-2(i|\mathbf{k}|+\lambda)(i|\mathbf{k}|-\lambda)}{(i|\mathbf{k}|-\lambda)(i|\mathbf{k}|+\lambda)(i|\mathbf{k}|)}\right]$$

$$=\frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{2\lambda^2}{(i|\mathbf{k}|^3-i|\mathbf{k}|\lambda^2)}\right]$$

$$=\frac{2\pi e^2}{i|\mathbf{k}|}\left[\frac{2\lambda^2}{(i|\mathbf{k}|^3-i|\mathbf{k}|\lambda^2)}\right]$$

$$\widetilde{v}(\mathbf{k})=\frac{4\pi\lambda^2 e^2}{|\mathbf{k}|^2(|\mathbf{k}|^2+\lambda^2)}. \tag{A.55}$$

We first introduce the Yukawa potential,

$$V_\lambda(\mathbf{x})=\frac{e^2\mathrm{e}^{-\lambda|\mathbf{x}|}}{|\mathbf{x}|}\;\;,\lambda>0 \tag{A.56}$$

and evaluate the Fourier transform. In the limit $\lambda\to 0$ we recover from (A.56) the

Coulomb potential. So that, to obtain the Fourier transform of the Coulomb potential, we may first find the Fourier transform of $V_\lambda(\mathbf{x})$. Let $\widetilde{v}_\lambda(\mathbf{k})$ denote the Fourier transform of the Yukawa potential ,$V_\lambda(\mathbf{x})$, given by

$$\begin{aligned}
\widetilde{v}_\lambda(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}\, v(\mathbf{x})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&= \int \mathrm{d}^3\mathbf{x}\, \frac{e^2 \mathrm{e}^{-\lambda|\mathbf{x}|}}{|\mathbf{x}|}\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \\
&= e^2 \int_0^\infty x^2 \mathrm{d}x \int_0^\pi \sin\theta\, \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi\, \frac{\mathrm{e}^{-\lambda x}}{x}\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}|x\cos\theta} \\
\widetilde{v}(\mathbf{k}) &= e^2 \int_0^\infty \mathrm{d}x\, x^2\, \frac{\mathrm{e}^{-\lambda x}}{x} \int_0^\pi \mathrm{d}\theta\, \sin\theta\, \mathrm{e}^{-\mathrm{i}|\mathbf{k}|x\cos\theta} \int_0^{2\pi} \mathrm{d}\varphi.
\end{aligned} \tag{A.57}$$

Reference (A.53)-(A.54), applying to (A.57), we obtain

$$\begin{aligned}
\widetilde{v}_\lambda(\mathbf{k}) &= 2\pi e^2 \int_0^\infty \mathrm{d}x\, x^2\, \frac{\mathrm{e}^{-\lambda x}}{x} \frac{1}{\mathrm{i}|\mathbf{k}|x} \left(\mathrm{e}^{\mathrm{i}|\mathbf{k}|x} - \mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}\right) \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \int_0^\infty \mathrm{d}x\, \mathrm{e}^{-\lambda x} \left(\mathrm{e}^{\mathrm{i}|\mathbf{k}|x} - \mathrm{e}^{-\mathrm{i}|\mathbf{k}|x}\right) \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \int_0^\infty \mathrm{d}x\, \left(\mathrm{e}^{(-\lambda+\mathrm{i}|\mathbf{k}|)x} - \mathrm{e}^{-(\lambda+\mathrm{i}|\mathbf{k}|)x}\right) \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \lim_{a\to\infty} \left[\int_0^a \mathrm{d}x\, \left(\mathrm{e}^{(-\lambda+\mathrm{i}|\mathbf{k}|)x} - \mathrm{e}^{-(\lambda+\mathrm{i}|\mathbf{k}|)x}\right)\right] \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \lim_{a\to\infty} \left[\left.\frac{\mathrm{e}^{(-\lambda+\mathrm{i}|\mathbf{k}|)x}}{-\lambda+\mathrm{i}|\mathbf{k}|}\right|_0^a + \left.\frac{\mathrm{e}^{-(\lambda+\mathrm{i}|\mathbf{k}|)x}}{\lambda+\mathrm{i}|\mathbf{k}|}\right|_0^a\right] \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \lim_{a\to\infty} \left[\left.\frac{\mathrm{e}^{(-\lambda+\mathrm{i}|\mathbf{k}|)x}}{-\lambda+\mathrm{i}|\mathbf{k}|}\right|_0^a + \left.\frac{\mathrm{e}^{-(\lambda+\mathrm{i}|\mathbf{k}|)x}}{\lambda+\mathrm{i}|\mathbf{k}|}\right|_0^a\right] \\
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|} \lim_{a\to\infty} \left[\frac{\mathrm{e}^{(-\lambda+\mathrm{i}|\mathbf{k}|)a} - 1}{-\lambda+\mathrm{i}|\mathbf{k}|} + \frac{\mathrm{e}^{-(\lambda+\mathrm{i}|\mathbf{k}|)a} - 1}{\lambda+\mathrm{i}|\mathbf{k}|}\right]
\end{aligned}$$

$$
\begin{aligned}
&= \frac{2\pi e^2}{\mathrm{i}|\mathbf{k}|}\left[\frac{-2\mathrm{i}|\mathbf{k}|}{-|\mathbf{k}|^2-\lambda^2}\right] \\
&= \frac{4\pi e^2}{(|\mathbf{k}|^2+\lambda^2)}. \qquad \text{(A.58)}
\end{aligned}
$$

In fact, it was in response to the short range of nuclear forces that Yukawa introduced λ. For electromagnetism, where the range is infinite, λ becomes zero and $V_\lambda(\mathbf{x}) \to \frac{\mathrm{e}^{-\lambda|\mathbf{x}|}}{|\mathbf{x}|}$ reduces to $V_{\lambda\to 0}(\mathbf{x}) = \frac{1}{|\mathbf{x}|}$ the Coulomb potential. Thus, in reference to (A.55), the Fourier transform of the Coulomb potential in 3-dimensions is

$$
\begin{aligned}
\widetilde{V}_{\lambda\to 0}(\mathbf{k}) &= \lim_{\lambda\to 0}\frac{4\pi e^2}{(p^2+\lambda^2)} \\
&= \frac{4\pi e^2}{p^2}. \qquad \text{(A.59)}
\end{aligned}
$$

Consider $v(0)$ when $v(\mathbf{x}) = e^2(1-\mathrm{e}^{-\lambda|\mathbf{x}|})/|\mathbf{x}|$

$$
\begin{aligned}
v(0) &= \lim_{|\mathbf{x}|\to 0}\frac{e^2(1-\mathrm{e}^{-\lambda|\mathbf{x}|})}{|\mathbf{x}|} \\
&= e^2\lim_{|\mathbf{x}|\to 0}\left[\sum_{n=1}^{\infty}-\frac{(-\lambda|\mathbf{x}|)^n}{|\mathbf{x}|\,n!}\right] \\
&= e^2\lim_{|\mathbf{x}|\to 0}\left[\lambda-\frac{1}{2!}\lambda^2|\mathbf{x}|+\frac{1}{3!}\lambda^3|\mathbf{x}|^2-\frac{1}{4!}\lambda^4|\mathbf{x}|^3+\cdots-\cdots\right] \\
v(0) &= e^2\lambda. \qquad \text{(A.60)}
\end{aligned}
$$

Substitute (A.55), (A.59) and (A.60) into (A.51), to obtain the bound $(k \geq 2)$

$$
\begin{aligned}
\sum_{i<j}^{k}\frac{e^2A_iA_j}{|\mathbf{x}_i-\mathbf{x}_j|} \geqslant &\sum_{j=1}^{k}e^2A_j\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|}-\frac{1}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \\
&-\frac{e^2\lambda}{2}\sum_{j=1}^{k}A_j^2-\frac{1}{2}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,|\widetilde{\rho}(\mathbf{k})|^2\left[\frac{\left|\frac{4\pi e^2}{p^2}\right|^2}{\frac{4\pi\lambda^2e^2}{p^2(p^2+\lambda^2)}}-\frac{4\pi e^2}{p^2}\right]
\end{aligned}
$$

$$=\sum_{j=1}^{k} e^2 A_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} - \frac{1}{2}\int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

$$- \frac{e^2\lambda}{2}\sum_{j=1}^{k} A_j^2 - R(\mathbf{k}) \tag{A.61}$$

where

$$R(\mathbf{k}) =\frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2 \left[\frac{\left|\frac{4\pi e^2}{p^2}\right|^2}{\frac{4\pi\lambda^2 e^2}{p^2(p^2+\lambda^2)}} - \frac{4\pi e^2}{p^2} \right]$$

$$=\frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2 \left[\left|\frac{4\pi e^2}{p^2}\right|^2 \frac{p^2(p^2+\lambda^2)}{4\pi\lambda^2 e^2} - \frac{4\pi e^2}{p^2} \right]$$

$$=\frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2 \left[\left(\frac{4\pi e^2(p^2+\lambda^2)}{p^2\lambda^2}\right) - \frac{4\pi e^2}{p^2} \right]$$

$$=\frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2 \left[\left(\frac{4\pi e^2(p^2+\lambda^2)}{p^2\lambda^2}\right) - \frac{4\pi e^2}{p^2} \right]$$

$$=\frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2\, \frac{4\pi e^2}{\lambda^2}$$

$$=\frac{2\pi e^2}{\lambda^2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, |\widetilde{\rho}(\mathbf{k})|^2$$

$$=\frac{2\pi e^2}{\lambda^2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \widetilde{\rho}(\mathbf{k})\widetilde{\rho}^*(\mathbf{k})$$

$$=\frac{2\pi e^2}{\lambda^2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \cdot \int \mathrm{d}^3\mathbf{x}'\,\rho(\mathbf{x}')\,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}'}$$

$$=\frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x}) \int \mathrm{d}^3\mathbf{x}'\,\rho(\mathbf{x}') \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}'-\mathbf{x})}$$

$$=\frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x}) \int \mathrm{d}^3\mathbf{x}'\rho(\mathbf{x}')\,\delta^3(\mathbf{x}'-\mathbf{x})$$

$$R(\mathbf{k}) =\frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}). \tag{A.62}$$

Substitute this into (A.61), to derive the bound $(k \geq 2)$

$$\sum_{i<j}^{k} \frac{e^2 A_i A_j}{|\mathbf{x}_i - \mathbf{x}_j|} \geqslant \sum_{j=1}^{k} e^2 A_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} - \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

$$- \frac{e^2\lambda}{2} \sum_{j=1}^{k} A_j^2 - \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}). \quad \text{(A.63)}$$

In the Hamiltonian, it is then straightforward to use (A.63) twice, once for the repulsive potentials in (A.2), let $A_i, A_j = 1$ and $k \longrightarrow N$, to obtain

$$\sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \geqslant \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} - \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

$$- \frac{e^2\lambda}{2} \sum_{j=1}^{N} (1) - \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) \quad \text{(A.64)}$$

and then again for the repulsive potentials in (A.3), let $A_i = Z_i, A_j = Z_j$ and $\mathbf{x}_j \longrightarrow \mathbf{R}_j$ for $k \geq 2$, to obtain

$$\sum_{i<j}^{k} \frac{e^2 Z_i Z_j}{|\mathbf{R}_i - \mathbf{R}_j|} \geqslant \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|} - \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

$$- \frac{e^2\lambda}{2} \sum_{j=1}^{k} Z_j^2 - \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}). \quad \text{(A.65)}$$

Substitute (A.64) and (A.65) into (A.1), to obtain the Hamiltonian

$$H \geqslant \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} - \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

$$- \frac{e^2\lambda}{2} \sum_{j=1}^{N} (1) - \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) + \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|}$$

$$- \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} - \frac{e^2\lambda}{2} \sum_{j=1}^{k} Z_j^2 - \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})$$

$$-\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{e^2 Z_j}{|\mathbf{x}_i-\mathbf{R}_j|} \tag{A.66}$$

$\sum_{i=1}^{k} Z_i = N$, $k \geq 2$ and $\sum_{i=1}^{N}(1) = N$. Eq.(A.66) can be rewritten as

$$\begin{aligned}
H \geqslant & \sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m} + \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} - \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \\
& - \frac{e^2\lambda N}{2} - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}) + \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|} \\
& - \frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} - \frac{e^2\lambda}{2}\sum_{i=1}^{k} Z_i^2 - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}) \\
& - \sum_{i=1}^{N}\sum_{j=1}^{k}\frac{e^2 Z_j}{|\mathbf{x}_i-\mathbf{R}_j|} \\
= & \sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m} - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}) - \frac{2\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}) - \frac{e^2\lambda N}{2} - \frac{e^2\lambda}{2}\sum_{i=1}^{k} Z_i^2 \\
& + \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} + \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|} \\
& - e^2\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\;\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} - \sum_{i=1}^{N}\sum_{j=1}^{k}\frac{e^2 Z_j}{|\mathbf{x}_i-\mathbf{R}_j|} \\
= & \sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m} - \frac{4\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}) - \frac{e^2\lambda}{2}\left(N + \sum_{i=1}^{k} Z_i^2\right) \\
& + \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} + \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|} \\
& - e^2\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\;\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} - \sum_{i=1}^{N}\sum_{j=1}^{k}\frac{e^2 Z_j}{|\mathbf{x}_i-\mathbf{R}_j|}
\end{aligned}$$

$$\therefore \quad H \geqslant \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} - \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{e^2\lambda}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right)$$

$$\sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} + \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|}$$

$$- e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} - \sum_{i=1}^{N}\sum_{j=1}^{k} \frac{e^2 Z_j}{|\mathbf{x}_i - \mathbf{R}_j|}. \tag{A.67}$$

To obtain a lower bound for $\langle\psi| H |\psi\rangle$ with $k \geq 2$, we note that

$$\langle\psi| H |\psi\rangle \geqslant T - \langle\psi| \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) |\psi\rangle - \langle\psi| \frac{e^2\lambda}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right) |\psi\rangle$$

$$- \langle\psi| \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} |\psi\rangle + \langle\psi| \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|} |\psi\rangle$$

$$- \langle\psi| e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} |\psi\rangle - \langle\psi| \sum_{i=1}^{N}\sum_{j=1}^{k} \frac{e^2 Z_j}{|\mathbf{x}_i - \mathbf{R}_j|} |\psi\rangle \tag{A.68}$$

where

$$T = \langle\psi| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} |\psi\rangle\,. \tag{A.69}$$

For the bosonic case (of spin 0 for simplicity) in multi-particle systems, for example, we have for the particle density

$$\rho(\mathbf{x}) = N \int \mathrm{d}^3\mathbf{x}_2 ... \mathrm{d}^3\mathbf{x}_N \, |\psi(\mathbf{x}, \mathbf{x}_2, ..., \mathbf{x}_N)|^2 \tag{A.70}$$

where ψ is an N-boson symmetric normalized wavefunction.

In reference to (A.63) and (2.133)-(2.144), we obtain the lower bound for the ground-state energy of N identical bosons (for $k = 1$)

$$\langle\psi|\, H \,|\psi\rangle \geqslant T - \frac{3e^2}{2}\pi^{1/3}N^{2/3}\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{1/3} - Ne^2\int d^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}|} \tag{A.71}$$

and in reference to (A.63)-(A.69), we obtain the lower bound for the ground-state energy of N identical bosons (for $k \geq 2$)

$$\begin{aligned}\langle\psi|\, H \,|\psi\rangle \geqslant & T - \langle\psi|\,\frac{4\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\,|\psi\rangle - \langle\psi|\,\frac{e^2\lambda}{2}\left(N+\sum_{i=1}^{k}Z_i^2\right)|\psi\rangle \\ & - \langle\psi|\sum_{j=1}^{N}e^2\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|}\,|\psi\rangle + \langle\psi|\sum_{j=1}^{k}e^2Z_j\int \mathrm{d}^3\mathbf{x}\,\frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|}\,|\psi\rangle \\ & - \langle\psi|\,e^2\int \mathrm{d}^3\mathbf{x}'\int \mathrm{d}^3\mathbf{x}\;\frac{\rho(\mathbf{x})\,\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\,|\psi\rangle \\ & - \langle\psi|\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{e^2Z_j}{|\mathbf{x}_i-\mathbf{R}_j|}\,|\psi\rangle\,.\end{aligned} \tag{A.72}$$

For the second term on the right-hand side of (A.72) we have, by using (A.70)

$$\begin{aligned}\langle\psi|\,\frac{4\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\,|\psi\rangle =& \frac{4\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\int \mathrm{d}^3\mathbf{x}_2 ...\mathrm{d}^3\mathbf{x}_N\,\psi^*(\mathbf{x},\mathbf{x}_2,...,\mathbf{x}_N) \\ & \times\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)\psi(\mathbf{x},\mathbf{x}_2,...,\mathbf{x}_N) \\ =& \frac{4\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\,\langle\psi|\psi\rangle \\ =& \frac{4\pi e^2}{\lambda^2}\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x}).\end{aligned} \tag{A.73}$$

For the third term on the right-hand side of (A.72) we have, by using (A.70),

$$\langle\psi|\,\frac{e^2\lambda}{2}\left(N+\sum_{i=1}^{k}Z_i^2\right)|\psi\rangle = \frac{e^2\lambda}{2}\left(N+\sum_{i=1}^{k}Z_i^2\right)\langle\psi|\psi\rangle$$

$$= \left(N + \sum_{i=1}^{k} Z_i^2 \right). \tag{A.74}$$

For the fourth term on the right-hand side of (A.72) we have, by using (A.70),

$$\langle\psi| \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} \, |\psi\rangle$$

$$= \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}', \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \; \psi^*(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|} \right) \; \psi(\mathbf{x}', \mathbf{x}_2, \ldots \mathbf{x}_N)$$

$$= \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}_j|}$$

$$\times \int \mathrm{d}^3\mathbf{x_2}, \ldots, \mathrm{d}^3\mathbf{x}_N \; |\psi(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2$$

$$= \frac{e^2}{N} \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x}) \, \rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} + \frac{e^2}{N} \int \mathrm{d}^3\mathbf{x_2} \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x}) \, \rho(\mathbf{x}_2)}{|\mathbf{x}-\mathbf{x}_2|}$$

$$+ \ldots + \frac{e^2}{N} \int \mathrm{d}^3\mathbf{x}_N \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x}) \, \rho(\mathbf{x}_N)}{|\mathbf{x}-\mathbf{x}_N|}$$

$$= e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x}) \, \rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}. \tag{A.75}$$

For the fifth term on the right-hand side of (A.72) we have, by using (A.70),

$$\langle\psi| \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|} \, |\psi\rangle$$

$$= \sum_{j=1}^{N} e^2 \int \mathrm{d}^3\mathbf{x}', \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \; \psi^*(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x} \, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|} \right) \; \psi(\mathbf{x}', \mathbf{x}_2, \ldots \mathbf{x}_N)$$

$$= \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|}$$

$$\times \int \mathrm{d}^3\mathbf{x}', \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \; |\psi(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2$$

$$= \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|}. \tag{A.76}$$

For the sixth term on the right-hand side of (A.72) we have, by using (A.70),

$$\langle\psi|\, e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\; \frac{\rho(\mathbf{x})\;\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}\,|\psi\rangle$$

$$= \int \mathrm{d}^3\mathbf{x}'', \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \; \psi^*(\mathbf{x}'', \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \right) \psi(\mathbf{x}'', \mathbf{x}_2, \ldots \mathbf{x}_N)$$

$$= e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})\;\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

$$\times \int \mathrm{d}^3\mathbf{x}'', \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \, |\psi(\mathbf{x}'', \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2$$

$$= e^2 \int \mathrm{d}^3\mathbf{x}' \int \mathrm{d}^3\mathbf{x}\; \frac{\rho(\mathbf{x})\;\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}. \tag{A.77}$$

For the seventh term on the right-hand side of (A.72) we have, by using (A.70),

$$\langle\psi| \sum_{i=1}^{N} \sum_{j=1}^{k} \frac{e^2 Z_j}{|\mathbf{x}_i - \mathbf{R}_j|}\,|\psi\rangle$$

$$= \int \mathrm{d}^3\mathbf{x}, \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \; \psi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\sum_{i=1}^{N} \sum_{j=1}^{k} \frac{e^2 Z_j}{|\mathbf{x}_i - \mathbf{R}_j|} \right) \psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$= \sum_{j=1}^{k} \sum_{i=1}^{N} \int \mathrm{d}^3\mathbf{x}, \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \, \psi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$\times \left(\frac{e^2 Z_j}{|\mathbf{x}_i - \mathbf{R}_j|} \right) \psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$$= \sum_{j=1}^{k} \sum_{j=1}^{N} \int \mathrm{d}^3\mathbf{x} \frac{e^2 Z_j}{|\mathbf{x}_i - \mathbf{R}_j|} \int \mathrm{d}^3\mathbf{x}_2, \ldots, \mathrm{d}^3\mathbf{x}_N \, |\psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2$$

$$= \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x} \frac{e^2 Z_j}{|\mathbf{x} - \mathbf{R}_j|} \, \frac{\rho(\mathbf{x})}{N} + \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x}_2 \frac{e^2 Z_j}{|\mathbf{x}_2 - \mathbf{R}_j|} \, \frac{\rho(\mathbf{x}_2)}{N}$$

$$+ \ldots + \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x}_N \frac{e^2 Z_j}{|\mathbf{x}_N - \mathbf{R}_j|} \, \frac{\rho(\mathbf{x}_N)}{N}$$

$$= \sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^3\mathbf{x} \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{R}_j|}. \tag{A.78}$$

Substitute (A.73), (A.74), (A.75), (A.76), (A.77) and (A.78) into (A.72), to obtain the bound (for $k \geq 2$)

$$\langle\psi| \, H \, |\psi\rangle \geqslant T - \langle\psi| \, \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x} \, \rho^2(\mathbf{x}) \, |\psi\rangle - \langle\psi| \, \frac{e^2 \lambda}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right) |\psi\rangle \, . \tag{A.79}$$

Optimizing (A.79) over λ, gives

$$0 = \frac{\mathrm{d}}{\mathrm{d}\lambda} \langle\psi|H|\psi\rangle$$

$$= \frac{\mathrm{d}}{\mathrm{d}\lambda} T - \frac{\mathrm{d}}{\mathrm{d}\lambda} \left(\frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x} \, \rho^2(\mathbf{x}) \right) - \frac{\mathrm{d}}{\mathrm{d}\lambda} \left(\frac{\lambda e^2}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right) \right)$$

$$= 0 + \frac{8\pi e^2}{\lambda^3} \int \mathrm{d}^3\mathbf{x} \, \rho^2(\mathbf{x}) - \frac{e^2}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right)$$

$$\lambda^3 = \frac{16\pi \int \mathrm{d}^3\mathbf{x} \, \rho^2(\mathbf{x})}{\left(N + \sum_{i=1}^{k} Z_i^2 \right)}$$

$$\lambda = \left(\frac{16\pi \int \mathrm{d}^3\mathbf{x}\ \rho^2(\mathbf{x})}{\left(N + \sum\limits_{i=1}^{k} Z_i^2 \right)} \right)^{1/3} \tag{A.80}$$

Substitute (A.80) into (A.79), gives the remarkably simple bound $(k \geq 2)$

$$\begin{aligned}
\langle \psi | H | \psi \rangle \ &\geqslant T - \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\ \rho^2(\mathbf{x}) - \frac{\lambda e^2}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right) \\
&= T - 4\pi e^2 \int \mathrm{d}^3\mathbf{x}\ \rho^2(\mathbf{x}) \left(\frac{\left(N + \sum\limits_{i=1}^{k} Z_i^2 \right)}{16\pi \int \mathrm{d}^3\mathbf{x}\ \rho^2(\mathbf{x})} \right)^{2/3} \\
&\quad - \frac{e^2}{2} \left(N + \sum_{i=1}^{k} Z_i^2 \right) \left(\frac{16\pi \int \mathrm{d}^3\mathbf{x}\ \rho^2(\mathbf{x})}{\left(N + \sum\limits_{i=1}^{k} Z_i^2 \right)} \right)^{1/3} \\
&= T - \left(\frac{\pi^{1/3} e^2}{2^{2/3}} + 2^{1/3}\pi^{1/3} e^2 \right) \left(N + \sum_{i=1}^{k} Z_i^2 \right)^{2/3} \left(\int \mathrm{d}^3\mathbf{x}\ \rho^2(\mathbf{x}) \right)^{1/3} \\
&= T - \frac{3e^2}{2^{2/3}}\ \pi^{1/3} \left(N + \sum_{i=1}^{k} Z_i^2 \right)^{2/3} \left(\int \mathrm{d}^3\mathbf{x}\ \rho^2(\mathbf{x}) \right)^{1/3}
\end{aligned}$$

$$\therefore \quad \langle \psi | H | \psi \rangle \ \geqslant T - \frac{3e^2}{2^{2/3}}\ \pi^{1/3} \left(N + \sum_{i=1}^{k} Z_i^2 \right)^{2/3} \left(\int \mathrm{d}^3\mathbf{x}\ \rho^2(\mathbf{x}) \right)^{1/3} . \tag{A.81}$$

To the above end (for $k \geq 2$), we may use the Schwinger inequality,

$$N_{-\xi}\left(H_0 - v(\mathbf{x}) \right) \leqslant \left(\frac{m}{2\pi\hbar^2} \right)^2 \int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^3\mathbf{x'}\ v(\mathbf{x})\ v(\mathbf{x'}) \frac{\mathrm{e}^{-2|\mathbf{x}-\mathbf{x'}|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}-\mathbf{x'}|^2} \tag{A.82}$$

and by referring (2.26), we obtain

$$N_{-\xi}\left(H_0 - v(\mathbf{x}) \right) \leqslant \left(\frac{m}{2\pi\hbar^2} \right)^2 \left(\frac{4\pi\hbar}{\sqrt{8m\xi}} \right) \left(\int \mathrm{d}^3\mathbf{x}\ (v(\mathbf{x}))^2 \right)$$

$$= \left(\frac{m}{2\hbar^2}\right)^{3/2} \frac{1}{\pi\sqrt{\xi}} \int \mathrm{d}^3\mathbf{x} \ (v(\mathbf{x}))^2$$

$$\therefore \quad N_{-\xi}\left(H_0 - v(\mathbf{x})\right) \leqslant \left(\frac{m}{2\hbar^2}\right)^{3/2} \frac{1}{\pi\sqrt{\xi}} \int \mathrm{d}^3\mathbf{x} \ (v(\mathbf{x}))^2 \tag{A.83}$$

where $v(\mathbf{x}) \geq 0$.

From (A.83), for $N_{-\xi}\left(H_0 - v(\mathbf{x})\right) < 1$ we may choose ξ such that

$$\xi = \left(\frac{m}{2\hbar^2}\right)^3 \frac{1+\delta}{\pi^2} \left(\int \mathrm{d}^3\mathbf{x} \ (v(\mathbf{x}))^2\right)^2, \quad \delta > 0 \tag{A.84}$$

or

$$-\xi = -\left(\frac{m}{2\hbar^2}\right)^3 \frac{(1+\delta)}{\pi^2} \left(\int \mathrm{d}^3\mathbf{x} \, (v(\mathbf{x}))^2\right)^2 \tag{A.85}$$

so that $N_{-\xi}(\mathbf{p}^2/2m - v(\mathbf{x})) < 1$, which implies that $N_{-\xi}(\mathbf{p}^2/2m - v(\mathbf{x})) = 0$, and the right-hand side of (A.85) provides a lower bound to the spectrum of $[\mathbf{p}^2/2m - v(\mathbf{x})]$ since its spectrum would then be empty for energies $-\xi$. That is, (A.85) gives the following lower bound for the ground-state energy of the Hamiltonian,

$$-\left(\frac{m}{2\hbar^2}\right)^3 \frac{(1+\delta)}{\pi^2} \left(\int \mathrm{d}^3\mathbf{x} \, (v(\mathbf{x}))^2\right)^2. \tag{A.86}$$

Accordingly, with the positive function (2.42)

$$v(\mathbf{x}) = \frac{4}{3} \frac{\rho(\mathbf{x})}{\int \mathrm{d}^3\mathbf{x} \, \rho^2(\mathbf{x})} \, T \tag{A.87}$$

where

$$T = \left\langle \psi \left| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \right| \psi \right\rangle \tag{A.88}$$

then it is easily verified that

$$\left\langle \psi \left| \sum_{i=1}^{N} v(\mathbf{x}_i) \right| \psi \right\rangle = -\frac{4}{3} T \tag{A.89}$$

where $\sum_{i=1}^{N} v(\mathbf{x}_i) = v(\mathbf{x})$ and $v(\mathbf{x})$ is not the potential energy for any Hamiltonian. It is just introduced in order to be able to obtain the expectation value of the kinetic energy T (for N identical bosons) in three dimensions.

From (A.88) and (A.89), we obtain

$$\left\langle \psi \left| \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i) \right] \right| \psi \right\rangle = -\frac{1}{3} T. \tag{A.90}$$

To obtain a lower bound to the lower of the spectrum of the “Hamiltonian” in (A.90), we can put N bosons in the same state without Pauli’s exclusion principle (put all of the N bosons at the bottom of the spectrum of $[\mathbf{p}^2/2m - v(\mathbf{x})]$). That is, the Hamiltonian (A.90) is bounded below by N times the ground-state energy in (A.86). This is for N identical bosons we have

$$\left\langle \psi \left| \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i) \right] \right| \psi \right\rangle \geqslant -N\xi$$

$$\therefore \quad \left\langle \psi \left| \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i) \right] \right| \psi \right\rangle \geqslant -N \left(\frac{m}{2\hbar^2} \right)^3 \frac{(1+\delta)}{\pi^2} \left(\int \mathrm{d}^3\mathbf{x}\, (v(\mathbf{x}))^2 \right)^2 . \tag{A.91}$$

Substitution (A.90) into (A.91) and using the normalization condition $\int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) = N$, we obtain for the expectation value of the kinetic energy T (for N identical bosons)

$$-\frac{1}{3} T \geqslant -N \left(\frac{m}{2\hbar^2} \right)^3 \frac{(1+\delta)}{\pi^2} \left(\int \mathrm{d}^3\mathbf{x}\, (v(\mathbf{x}))^2 \right)^2$$

$$= -N \left(\frac{m}{2\hbar^2} \right)^3 \frac{(1+\delta)}{\pi^2} \left(\frac{4}{3} \right)^4 T^4 \frac{1}{\left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) \right)^2}$$

$$
\begin{aligned}
T \geqslant & \frac{1}{N^{1/3}}\frac{3}{4^{4/3}}\frac{4\pi^{2/3}}{(1+\delta)^{1/3}}\left(\frac{\hbar^2}{2m}\right)\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3} \\
= & \frac{1}{N^{1/3}}\frac{3}{(1+\delta)^{1/3}}\left(\frac{\pi}{2}\right)^{2/3}\left(\frac{\hbar^2}{2m}\right)\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3} \\
\therefore \quad T \geqslant & \frac{1}{N^{1/3}}\frac{3}{(1+\varepsilon)}\left(\frac{\pi}{2}\right)^{2/3}\left(\frac{\hbar^2}{2m}\right)\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3}
\end{aligned}
\tag{A.92}
$$

for any $\varepsilon > 0$, where we have set $(1+\delta)^{1/3} \equiv 1+\varepsilon$.

Substitute (A.92) into (A.81), to obtain

$$
\begin{aligned}
\langle\psi|H|\psi\rangle \geqslant & \frac{3\hbar^2}{2mN^{1/3}}\left(\frac{\pi}{2}\right)^{2/3}\frac{1}{1+\varepsilon}\left(\int d^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3} \\
& -\frac{3e^2}{2^{2/3}}\,\pi^{1/3}\left(N+\sum_{i=1}^{k}Z_i^2\right)^{2/3}\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{1/3}
\end{aligned}
\tag{A.93}
$$

Upon setting $[\int d^3\mathbf{x}\,\rho^2(\mathbf{x})]^{1/3} = A$, $3\hbar^2(\pi/2)^{2/3}/2m(1+\varepsilon) = c$, (A.93) leads to $(k \geq 2)$

$$
\begin{aligned}
\langle\psi|H|\psi\rangle \geqslant & \frac{c}{N^{1/3}}A^2 - \frac{3}{2^{2/3}}e^2\pi^{1/3}\left(N+\sum_{i=1}^{k}Z_i^2\right)^{2/3} A \\
= & \frac{c}{N^{1/3}}\left[A - \frac{3e^2\pi^{1/3}N^{1/3}}{2^{5/3}c}\left(N+\sum_{i=1}^{k}Z_i^2\right)^{2/3}\right]^2 \\
& - \frac{9}{8}\frac{e^4}{2^{1/3}}\frac{\pi^{2/3}}{c}N^{1/3}\left(N+\sum_{i=1}^{k}Z_i^2\right)^{4/3} \\
> & -\frac{9}{8}\frac{e^4}{2^{1/3}}\frac{\pi^{2/3}}{c}N^{1/3}\left(N+\sum_{i=1}^{k}Z_i^2\right)^{4/3} \\
= & -1.89\left(\frac{me^4}{2\hbar^2}\right)N^{1/3}\left(N+\sum_{i=1}^{k}Z_i^2\right)^{4/3}
\end{aligned}
$$

$$= -\, c_B N^{1/3}\left(N+\sum_{i=1}^{k} Z_i^2\right)^{4/3}, \quad c_B = -1.89\left(\frac{me^4}{2\hbar^2}\right)$$

$$\langle\psi|H|\psi\rangle > -c_B N^{1/3}\left(N+\sum_{i=1}^{k} Z_i^2\right)^{4/3} \tag{A.94}$$

where we have taken ε arbitrarily small.

From (A.94), for $Z_1 = \ldots = Z_N = 1$, we have

$$\langle\psi|H|\psi\rangle\; > -c_B N^{1/3}\left(N+\sum_{i=1}^{k} Z_i\right)^{4/3}, \quad \sum_{i=1}^{k} Z_i^2 = \sum_{i=1}^{k} Z_i$$

$$= -\, c_B N^{1/3}\,(N+N)^{4/3} \quad , \quad \sum_{i=1}^{k} Z_i = N$$

$$= -\, 2c_B N^{5/3}$$

$$\langle\psi|H|\psi\rangle\; > -2c_B N^{5/3}, \tag{A.95}$$

and for $Z_1 = \ldots = Z_q = N/q$, $Z_{q+1} = ... = Z_k = 0$, we have

$$\langle\psi|H|\psi\rangle\; > -c_B N^{1/3}\left(N+\sum_{i=1}^{q}\left(\frac{N}{q}\right)^2 + \sum_{i=q+1}^{k}(0)^2\right)^{4/3},$$

$$= -\, c_B\; N^{1/3}\left(N+q\left(\frac{N}{q}\right)^2\right)^{4/3},$$

$$= -\, c_B\; N^{1/3}\left(\frac{N^{8/3}}{q^{4/3}}\right)\left(\frac{N}{(N^2/q)}+1\right)^{4/3},$$

$$= -\, c_B\;\frac{N^3}{q^{4/3}}$$

$$\langle\psi|H|\psi\rangle\; > -c_B\;\frac{N^3}{q^{4/3}}\,, \quad \text{when} \quad N \ll \frac{N^2}{q} \tag{A.96}$$

It is interesting to note that even if $Z_1 = ... = Z_N = 1$ in (A.4), the coefficient of $N^{5/3}$ in (A.4) is of the order 8.71, and the new estimate in (A.94) improves this numerical estimate by, a factor of about two (from (A.95)). For $Z_1 = ... = Z_q = N/q$, $Z_{q+1} = ... = Z_k = 0$, $2 \leqslant q \ll N$, i.e., $N \ll N^2/q$, the N dependence of the right-hand side of (A.94) is $N^3/q^{4/3}$ (from (A.96)), coinciding with that obtained from (A.4). Such N dependences alone with $N^{5/3}$ for $Z_1 = ... = Z_N = 1$ and $N^3/q^{4/3}$ for the case just discussed imply *physically* that for no arrangements of the positive charges corresponding to light or heavy nuclei, bosonic matter may be stable.

Finally we note that our new estimates (obtained by somewhat simple methods) and the other well known ones in (A.4) for the bosonic case are comparable leading to the $N^{5/3}$ law and, as expected, two different methods of estimation lead, in general, to different multiplicative numerical factors to $N^{5/3}$ with some improvement in our case. The lower bound for the ground-state energy arises as a competition between the kinetic energy and the interaction parts in (A.1) contributing, respectively, with positive and negative signs. A lower bound correspounding to the repulsive part of the potential in (A.63) based on the so-called ”no-binding theorem”, based on the $5/3$ power of ρ, is expected to be a better one than the one given in (A.63) based only on positivity arguments and hence the former will contribute more optimally to the lower bound of the ground-state energy being sought. Also the extra $N^{1/3}$ multiplicative factor arising in the second term on the right-hand side of (A.92) may presumably be accounted for by an application of Hölder's inequality ,$\left|\int \mathrm{d}x\ f(x)g(x)\right| \leqslant \left\{\int \mathrm{d}x\ |f(x)|^p\right\}^{1/p} \left\{\int \mathrm{d}x\ |g(x)|^q\right\}^{1/q}$, relating our integral of ρ^2 and the familiar one of the integral of $\rho^{5/3}$ of the density ρ. In this case, it reads

$$\int \mathrm{d}^3\mathbf{x}\ \rho^{5/3}(\mathbf{x}) \leqslant \left(\int \mathrm{d}^3\mathbf{x}\ \rho^2(\mathbf{x})\right)^{2/3} \left(\int \mathrm{d}^3\mathbf{x}\ \rho(\mathbf{x})\right)^{1/3} \tag{A.97}$$

or

$$\left(\int \mathrm{d}^3\mathbf{x}\ \rho^2(\mathbf{x})\right)^{2/3} \geq \frac{1}{N^{1/3}} \int \mathrm{d}^3\mathbf{x}\ \rho^{5/3}(\mathbf{x}) \tag{A.98}$$

which upon comparison with the known method, using the $5/3$ power of the density, would provide a weaker contribution to (a lower bound to) the kinetic energy in an estimation of the ground-state energy.

APPENDIX B

COLLAPSING STAGE OF "BOSONIC MATTER"

The astonishment as to why matter occupies so large a volume and its connection to the Pauli exclusion principle was clearly expressed in words addressed by Ehrenfest to Pauli in 1931 on the occasion of the Lorentz medal (cf., (Dyson, 1967)) to this effect as discussed eariler. In regard to this, it was show in chapter 5 that for a non-vanishing probability of having electrons in matter, with Coulomb interactions, within a sphere of radius R, the latter necessarily grows not any slower than $N^{1/3}$ for large N, where N denotes the number of electrons. This conclusion is based on a derived inequality (Manoukian and Sirininlakul, 2005) relating the probability for the electrons to lie within such a sphere, the volume v_R of the latter and the number N of electrons:

$$\text{Prob}\left[|\mathbf{x}_1| \leq R, \ldots, |\mathbf{x}_N| \leq R\right] \left(\frac{N}{v_R}\right)^{2/5} < \left(\frac{1}{a_0^3}\right)^{2/5} 1.846 \left[1 + Z^{2/3}\right]^{6/5} \qquad \text{(B.1)}$$

where $a_0 = \hbar^2/me^2$ is the Bohr radius, and $Z|e|$ corresponds to the nucleus in matter carrying the largest positive charge. The above statement follows by noting from (B.1) that for a non-vanishing probability of having the electrons within the sphere, the corresponding volume v_R grows not any slower than the first power of N for $N \to \infty$, since otherwise the left-hand side of (B.1) would go to infinity and would be in contradiction with the finite upper bound on its right-hand side. We also note that N/v_R gives an average density, and one may also infer from (B.1) that the infinite density limit $N/v_R \to \infty$ does not occur, as the probability on the left-hand side of (B.1) necessarily goes to zero in such a limit.

The Hamiltonian in question is taken to be the N-electron one in (1.1) where $\mathbf{x}_i$, $\mathbf{R}_j$ correspond, respectively, to positions of electrons and nuclei. We have also considered neutral matter $\sum_{i=1}^{k} Z_i = N$.

What conclusion can be drawn about matter if the Pauli exclusion principle is not invoked? - that is regarding “ bosonic matter” (Dyson, 1967; Lieb, 1967; Manoukian and Muthaporn, 2003). Here we recall the drastic difference between matter (with the exclusion principle) and “bosonic matter” is that the ground-state energy E_N for the former $-E_N \sim N$ (Dyson and Lenard, 1968; Lieb and Thirring, 1975), while for the latter (Dyson, 1967; Lieb, 1967; Manoukian and Muthaporn, 2002, 2003) $-E_N \sim N^\alpha$ with $\alpha > 1$. And such a power law behavior with $\alpha > 1$ implies instability as the formation of a single system consisting of $(2N + 2N)$ particles is favored over two separate systems brought together each consisting of $(N + N)$ particles, and the energy released upon the collapse of the two systems into one, being proportional to $[(2N)^\alpha - 2\,(N)^\alpha]$ will be overwhelmingly large for realistic large N, e.g., $N \sim 10^{23}$. In regard to such a collapse Dyson states (Dyson, 1967): “[Bosonic] matter in bulk would collapse into a condensed high-density phase. The assembly of any two macroscopic objects would release energy comparable to that of an atomic bomb. . . . Matter without the exclusion principle is unstable”.

We prove rigorously that if deflation does occur for “bosonic matter”, upon collapse, as more and more such matter is put together, then for a non-vanishing probability of having the negatively charged particles within a sphere of radius R, the latter *necessarily* cannot decrease faster than $N^{-1/3}$ for large N. To this end, we define the particle density of N (spin 0) bosons:

$$\rho(\mathbf{x}) = \int \mathrm{d}^3\mathbf{x}_2 \ldots \mathrm{d}^3\mathbf{x}_N \left|\phi\left(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N\right)\right|^2 \tag{B.2}$$

and $\int \mathrm{d}^3\mathbf{x}\, \rho(\mathbf{x}) = N$, ϕ denotes a normalized state giving a strictly negative expectation value of the Hamiltonian, i.e.,

$$-\epsilon_N[m] \leq \langle\phi|\, H \,|\phi\rangle < 0 \tag{B.3}$$

where $-\epsilon_N[m] = E_N < 0$ is the ground-state energy emphasizing its dependence on m.

To establish the statement made above, we need (Manoukian and Sirininlakul, 2005) upper and lower bounds to the expectation value of the kinetic energy operator

$$T \equiv \left\langle \phi \left| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \right| \phi \right\rangle . \tag{B.4}$$

To the above end, we rewrite $|\phi\rangle = |\phi(m)\rangle$, emphasizing its dependence on the mass m. Since $|\phi(m/2)\rangle$ cannot lead for $\langle\phi(m/2)|H|\phi(m/2)\rangle$ a numerical value lower than $-\epsilon_N[m]$, we have $-\epsilon_N[m] \leq \langle\phi(m/2)|H|\phi(m/2)\rangle$. Accordingly, if we denote the interaction part in (1.1) by V, we have

$$-\epsilon_N[2m] \leq \left\langle \phi(m) \left| \frac{T}{2} + V \right| \phi(m) \right\rangle \tag{B.5}$$

and hence we have from the extreme right-hand side of the inequality (B.3)

$$T \leq 2\, \epsilon_N[2m]. \tag{B.6}$$

A lower bound for T was derived in (Manoukian and Sirininlakul, 2004). The basic idea in that derivation is to consider an effective interaction of the form $g(\mathbf{x}) = 4\rho(\mathbf{x})/(3\int \mathrm{d}^3\mathbf{x}\ \rho^2(\mathbf{x}))$, coupled with the way of counting the number of eigenvalues, in the manner of Schwinger (Schwinger, 1961), of the effective Hamiltonian $\sum\limits_{i=1}^{N} [\mathbf{p}_i^2/2m - g(\mathbf{x}_i)]$. This gives the lower bound (Manoukian and Sirininlakul, 2004)

$$\frac{3\hbar^2}{2mN^{1/3}} \left(\frac{\pi}{2}\right)^{2/3} \frac{1}{1+\varepsilon} \left(\int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^{2/3} \leq T \tag{B.7}$$

for any $\varepsilon > 0$ which may be taken as small as we please.

The lower bound expression obtained in (Manoukian and Sirininlakul, 2004) for

$-\epsilon_N[m]$ may be now used to derive from (B.6) and (B.7) the basic relations

$$\frac{3\hbar^2}{2mN^{1/3}}\left(\frac{\pi}{2}\right)^{2/3}\frac{1}{1+\varepsilon}\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3} \leq T < 3.78\left(\frac{me^4}{\hbar^2}\right)N^{5/3}\left[1+\sum_{i=1}^{k}\frac{Z_i^2}{N}\right]^{4/3}. \tag{B.8}$$

For the probability of the N negatively charged particles to lie within a sphere of radius R, we have

$$\begin{aligned}\text{Prob}\left[|\mathbf{x}_1| \leq R, \ldots, |\mathbf{x}_N| \leq R\right] \leq \text{Prob}\left[|\mathbf{x}_1| \leq R\right] \\ = \frac{1}{N}\int \mathrm{d}^3\mathbf{x}\,\rho(\mathbf{x})\mathcal{X}_R(\mathbf{x}) \\ \leq \frac{1}{N}\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{1/2}(v_R)^{1/2}\end{aligned} \tag{B.9}$$

where $\mathcal{X}_R(\mathbf{x}) = 1$ if $|\mathbf{x}| \leq R$, and $= 0$ otherwise. In writing the last inequality in (B.9) we have used the Cauchy-Schwarz inequality and that $(\mathcal{X}_R(\mathbf{x}))^2 = (\mathcal{X}_R(\mathbf{x}))\,, v_R = 4\pi R^3/3$.

From (B.8), (B.9), we then have the explicit inequality

$$\text{Prob}\left[|\mathbf{x}_1| \leq R, \ldots, |\mathbf{x}_N| \leq R\right]\frac{1}{(v_R N)^{1/2}} < \left(\frac{1}{a_0^3}\right)^{1/2} 1.61\left[1+Z\right]. \tag{B.10}$$

From this inequality we may infer the inescapable fact that if deflation of “bosonic matter” occurs, upon collapse, then for a non-vanishing probability of having the N negatively charged particles within a sphere of radius R, the corresponding volume, necessarily, cannot shrink faster than $1/N$ for $N \to \infty$, since otherwise the left-hand side of (B.10) would go to infinity and would be in contradiction with the finite upper bound on its right-hand side, thus establishing the above stated result. We note that the inequality in (B.10) is sufficient to reach such a conclusion but cannot establish the actual deflation of such matter. Methods similar to the ones developed above have been used to study the localizability and stability of other quantum mechanical systems as well (Manoukian, 2006).

APPENDIX C

FUNDAMENTAL POISSON EQUATION IN $2D$

We verify the Poisson's equation in $2D$

$$\boldsymbol{\nabla}^2 2\ln\frac{|\mathbf{x}-\mathbf{x}'|}{A} = 4\pi\delta^2(\mathbf{x}-\mathbf{x}'). \tag{C.1}$$

where A is an arbitrary scaling constant.

Let

$$\begin{aligned} f(\mathbf{x}-\mathbf{x}') =& 2\ln\frac{|\mathbf{x}-\mathbf{x}'|}{A} \\ =& 2\ln\frac{r}{A} \quad , \; r = |\mathbf{x}-\mathbf{x}'|. \end{aligned} \tag{C.2}$$

Applying the divergence theorem over a circular region A with boundary S , we obtain

$$\begin{aligned} \int_A \mathrm{d}^2\mathbf{x}\, \nabla^2 f(\mathbf{x}-\mathbf{x}') =& \int_A \mathrm{d}^2\mathbf{x}\, \nabla\cdot\nabla f(\mathbf{x}-\mathbf{x}') \\ =& \int_S \mathrm{d}S\; \mathbf{n}\cdot\nabla f(\mathbf{x}-\mathbf{x}') \end{aligned} \tag{C.3}$$

where $\mathbf{n}$ is a unit vector perpendicular to an element $\mathrm{d}\mathbf{S}$ of the boundary S.

Consider a small circle of radius R giving

$$\begin{aligned} \mathbf{n}\cdot\nabla f(\mathbf{x}-\mathbf{x}') =& \frac{\partial}{\partial r}\left(2\ln\frac{r}{A}\right) \\ =& \frac{2}{r} \end{aligned} \tag{C.4}$$

and

$$\int_S \mathrm{d}S\ \mathbf{n} \cdot \nabla f(\mathbf{x} - \mathbf{x}') = \int_0^{2\pi R} \mathrm{d}S\ \left(\frac{2}{r}\right)$$
$$= \frac{2(2\pi R)}{R}$$
$$= 4\pi. \tag{C.5}$$

By using the Dirac delta function in $2D$ is defined, in particular, by

$$\int_A \mathrm{d}^2\mathbf{x}\, \delta^2(\mathbf{x} - \mathbf{x}') = 1 \tag{C.6}$$

for $\mathbf{x}'$ within the region enclosed by A, we obtain from (C.3)

$$\int_A \mathrm{d}^2\mathbf{x}\, \nabla \cdot \nabla f(\mathbf{x} - \mathbf{x}') = 4\pi \int_A \mathrm{d}^2\mathbf{x}\, \delta^2(\mathbf{x} - \mathbf{x}'). \tag{C.7}$$

leading to

$$\nabla^2 f(\mathbf{x} - \mathbf{x}') = \nabla^2\, 2 \ln \frac{|\mathbf{x} - \mathbf{x}'|}{A} = 4\pi\, \delta^2(\mathbf{x} - \mathbf{x}') \tag{C.8}$$

APPENDIX D

FUNDAMENTAL POISSON EQUATION IN $3D$

We verify the Poisson's equation in $3D$

$$\boldsymbol{\nabla}^2 \frac{1}{|\mathbf{x}-\mathbf{x}'|} = -4\pi\delta^3(\mathbf{x}-\mathbf{x}'). \tag{D.1}$$

Let

$$\begin{aligned} g(\mathbf{x}-\mathbf{x}') =& \frac{1}{|\mathbf{x}-\mathbf{x}'|} \\ =& \frac{1}{r} \quad , \; r = |\mathbf{x}-\mathbf{x}'| \end{aligned} \tag{D.2}$$

Applying the divergence theorem over a spherical region V with boundary A, we have

$$\begin{aligned} \int_V \mathrm{d}^3\mathbf{x}\, \nabla^2 g(\mathbf{x}-\mathbf{x}') &= \int_V \mathrm{d}^3\mathbf{x}\, \nabla \cdot \nabla g(\mathbf{x}-\mathbf{x}') \\ &= \int_A \mathrm{d}A \; \mathbf{n} \cdot \nabla g(\mathbf{x}-\mathbf{x}') \end{aligned} \tag{D.3}$$

where $\mathbf{n}$ is a unit vector perpendicular to the surface element $\mathrm{d}\mathbf{A}$.

Consider a small sphere of radius R giving

$$\begin{aligned} \mathbf{n} \cdot \nabla g(\mathbf{x}-\mathbf{x}') =& \frac{\partial}{\partial r}\left(\frac{1}{r}\right) \\ =& -\frac{1}{r^2} \end{aligned} \tag{D.4}$$

and

$$\int_A \mathrm{d}A\ \mathbf{n} \cdot \nabla g(\mathbf{x} - \mathbf{x}') = -\int_0^{4\pi R^2} \mathrm{d}A\ \left(\frac{1}{r^2}\right)$$

$$= -\ \frac{4\pi R^2}{R^2}$$

$$= -\ 4\pi \tag{D.5}$$

By using the Dirac delta function in $3D$ is defined, in particular, by

$$\int_V \mathrm{d}^3\mathbf{x}\,\delta^3(\mathbf{x} - \mathbf{x}') = 1 \tag{D.6}$$

for $\mathbf{x}'$ in the region enclosed by V, we obtain from (D.3)

$$\int_V \mathrm{d}^3\mathbf{x}\,\nabla \cdot \nabla g(\mathbf{x} - \mathbf{x}') = 4\pi \int_V \mathrm{d}^3\mathbf{x}\,\delta^3(\mathbf{x} - \mathbf{x}') \tag{D.7}$$

leading to

$$\nabla^3 g(\mathbf{x} - \mathbf{x}') = \nabla^2\,\frac{1}{|\mathbf{x} - \mathbf{x}'|} = -4\pi\,\delta^3(\mathbf{x} - \mathbf{x}') \tag{D.8}$$

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1. Manoukian, E. B. and Sirininlakul, S. (2006). Stability of Matter in $2D$. **Reports on Mathematical Physics.** 57(x): xx-xx (accepted).
2. Manoukian, E. B., Muthaporn, C. and Sirininlakul, S. (2006). Collapsing Stage of "Bosonic Matter". **Physics Letters A.** 352(6): 488-490.
3. Manoukian, E. B. and Sirininlakul, S. (2005). High-Density Limit and Inflation of Matter. **Physical Review Letters.** 95: 190402-1.
4. Manoukian, E. B. and Sirininlakul, S. (2004). Rigorous Lower Bounds for the Ground-State Energy of Matter. **Physics Letters A.** 332 (1–2): 54–59. Errata: **Physics Letters A.** 337 (4–6): 496.
5. Trivijitkasem, S., Suthiopad, M. and Sirininlakul, S. (1999). Thermal and Physical Properties of Recycled-Plastic Film. **Kasetsart J. (Nat. Sci.)** 33(1): 111-125.

CONFERENCE: (Poster Session)

1. Sirininlakul, S. and Trivijitkasem, S. (1999). High Critical Magnetic Field, H_{c2}, of (Bi,Pb)-2223 Superconductor. **25th. STT.** A-126: 340-341.

2. Sirininlakul, S., Trivijitkasem, S. and Prunglag, N. (1998). First Harmonic AC Susceptibility of High T_c $(\mathtt{Bi}_{1-x}\mathtt{Pb}_x)_2\mathtt{Sr}_2\mathtt{Ca}_2\mathtt{Cu}_3\mathtt{O}_{10-\delta}$ Superconductor System $(x = 0, 0.1, 0.2, \ldots, 0.5)$. **36th KU Annual Conference**. Science Section : 1-7.

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