# การยุบตัวของ “สสารประเภทโบซอน”

นายชัยพจน์ มุทาพร

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรดุษฎีบัณฑิต
สาขาวิชาฟิสิกส์
มหาวิทยาลัยเทคโนโลยีสุรนารี
ปีการศึกษา 2547

ISBN 974-533-410-3

# THE COLLAPSE OF "BOSONIC MATTER"

Mr. Chaiyapoj Muthaporn

A Thesis Submitted in Partial Fulfillment of the Requirements

for the Degree of Doctor of Philosophy in Physics

Suranaree University of Technology

Academic Year 2004

ISBN 974-533-410-3

THE COLLAPSE OF "BOSONIC MATTER"

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

Thesis Examining Committee

(Asst. Prof. Dr. Prapun Manyum)

Chairperson

(Prof. Dr. Edouard B. Manoukian)

Member (Thesis Advisor)

(Assoc. Prof. Dr. Prasart Suebka)

Member

(Assoc. Prof. Dr. Yupeng Yan)

Member

(Asst. Prof. Dr. Prasert Kengkan)

Member

(Assoc. Prof. Dr. Sarawut Sujitjorn)

Vice Rector for Academic Affairs

(Assoc. Prof. Dr. Prasart Suebka)

Dean of Institute of Science

ชัยพจน์ มุทาพร : การยุบตัวของ "สสารประเภทโบซอน" (THE COLLAPSE OF "BOSONIC MATTER") อาจารย์ที่ปรึกษา : ศาสตราจารย์ ดร.เอ็ดเวิร์ด มานูเกียน, 361 หน้า. ISBN 974-533-410-3

วิทยานิพนธ์ฉบับนี้ เป็นเรื่องเกี่ยวข้องกับการวิเคราะห์ทางคณิตศาสตร์ของเสถียรภาพของ "สสารประเภทโบซอน" ในก้อนสสารที่มีโบซอนประจุลบและโบซอนประจุบวกอันตรกิริยาแบบคูลอมบ์ โดยได้คำนวณหาขอบเขตบนสำหรับพลังงานสถานะพื้นอย่างแม่นตรง ผลลัพธ์ที่ได้ถูกแสดงในรูปฟังก์ชันของตัวเลขที่มีความสัมพันธ์กับจำนวนอนุภาคของสสารโบซอนในระบบดังกล่าว เราได้พิจารณาระบบขนาดใหญ่ขนาด $10^{23}$ อนุภาค และขนาดเล็กขนาด 8 อนุภาค ขอบเขตบนที่ได้แสดงถึงอเสถียรภาพของสสารดังกล่าว เราได้แสดงให้เห็นว่า อเสถียรภาพไม่เป็นลักษณะเกี่ยวข้องกับจำนวนมิติของอวกาศ และไม่เกี่ยวข้องกับจำนวนมิติของอวกาศที่คัดสรรโดยธรรมชาติ สาเหตุที่เราวิเคราะห์ความเกี่ยวข้องดังกล่าว เพราะเราอยากรู้ว่าถ้ามีการเปลี่ยนจำนวนมิติของอวกาศ จะมีการเปลี่ยนเฟสของสสารจากเฟส "ยุบตัว" ไปสู่เฟส "เสถียร" หรือจากเฟส "ยุบตัว" ไปสู่เฟสของการ "ระเบิด" อย่างใดอย่างหนึ่งหรือไม่ ซึ่งการวิเคราะห์ของเราได้ให้คำตอบคือ จะไม่มีเหตุการณ์ดังกล่าวเกิดขึ้น และนั่นแสดงให้เห็นว่าหากอนุภาคในสสารธรรมดาทั่วไปไม่มีการเชื่อมโยงของสปินและสถิติแล้ว โลกของเราจะไม่ปรากฏอยู่ดังเช่นทุกวันนี้ นอกจากนี้การประมาณค่าขอบเขตบนที่แม่นยำของเรายังได้แสดงถึงการปลดปล่อยพลังงานอย่างมหาศาล ซึ่งมากกว่าพลังงานของการระเบิดที่เมืองฮิโรชิมาและเมืองนางาซากิ ซึ่งสอดคล้องกับคำกล่าวที่มีชื่อเสียงของไดสันที่แสดงไว้ในวิทยานิพนธ์

สาขาวิชาฟิสิกส์ ลายมือชื่อนักศึกษา ____________

ปีการศึกษา 2547 ลายมือชื่ออาจารย์ที่ปรึกษา ____________

CHAIYAPOJ MUTHAPORN : THE COLLAPSE OF "BOSONIC MATTER". THESIS ADVISOR : PROF. EDOUARD B. MANOUKIAN, Ph.D. 361 PP. ISBN 974-533-410-3

STABILITY AND INSTABILITY OF MATTER/CLUSTER PHYSICS AND QUANTUM THEORY OF VERY LARGE MATTER

This thesis is involved with a mathematically rigorous analysis of the stability of "bosonic matter" in the bulk of negatively and positively charged bosons with Coulomb interactions. To do this we derive detailed upper bounds for the *exact* ground-state energy of such matter as functions of the number of the charged particles involved. We consider systems with arbitrary large number of particles as large as $10^{23}$ or more, and as low as 8 particles. The upper bounds derived imply the instability of such matter. We prove that instability is not a characteristic of the dimensionality of space and is not a mere property of the dimension of space chosen by nature. The analysis corresponding to this latter conclusion arose from our interest in finding out whether the change of the dimensionality of space would change such matter from an "implosive" to a "stable" or to an "explosive" one. Our analysis shows that this does not happen. It also shows as to what would happen to matter without the Spin and Statistics connection and that our world will cease to exist. Our precise estimates show that the release of energy from the collapse of two objects of relatively small $N$ would already release energy of several orders of magnitude larger than that of the Hiroshima and Nagasaki bombs in conformity with Dyson's famous statement quoted in the text.

School of Physics — Student's Signature C. Muthaporn

Academic Year 2004 — 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 wish to thank Suppiya Siranan and Siri Sirininlakul for their cooperation and discussion on this work, Nattapong Yongram and Seckson Sukkhasena for their great support. Thanks also go to Dr. Jessada Tanthanuch, Dr. Khanchai Khosonthongkee, Dr. Kanthima Thailert and Ayut Limphirat for their consistent help, especially in building up the SUT-thesis format in $\mathcal{AMS}$-LaTeX $2_\varepsilon$.

I would like to acknowledge with thanks for being granted a Royal Golden Jubilee Ph.D. Program (Grant No. PHD/0159/2543) by the Thailand Research Fund (TRF) for especially carrying out this project.

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

I would especially like to thank Nopmanee Supanam who always cheered me up whenever I got problems in the work and for the good relationship we are sharing.

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 my work, for his encouragement and for calling my contributions to the subject as "splendid".

Chaiyapoj Muthaporn

# CONTENTS


| | Page |
|---|---|
| ABSTRACT IN THAI | I |
| ABSTRACT IN ENGLISH | II |
| ACKNOWLEDGEMENTS | III |
| CONTENTS | IV |
| LIST OF TABLES | VI |
| LIST OF FIGURES | VII |
| **CHAPTERS** | |
| **I INTRODUCTION** | 1 |
| **II UPPER BOUNDS OF THE GROUND-STATE ENERGY OF BOSONIC SYSTEMS OF POSITIVE AND NEGATIVE CHARGES** | 8 |
| 2.1 Expectation Value of the Hamiltonian : Schwinger Functional Technique | 10 |
| 2.2 Basic Estimates | 76 |
| 2.3 Derivation of the Upper Bounds | 100 |
| **III IS 'BOSONIC MATTER' UNSTABLE IN $2D$?** | 132 |
| 3.1 Introduction and Orientation | 132 |
| 3.2 General Upper Bound Expression of $E_{N,N}$ | 133 |
| 3.3 Basic Estimates | 135 |
| 3.4 Derivation of Upper Bounds | 148 |
| **IV $N^{5/3}$ LAW FOR BOSONS FOR ARBITRARY LARGE $N$** | 174 |

# CONTENTS (Continued)


**Page**

4.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 174

4.2 Derivation of Upper Bounds . . . . . . . . . . . . . . . . . . . . . . . . 176

**V $N^2$ LAW FOR BOSONS IN $2D$ . . . . . . . . . . . . . . . . . . . . 247**

5.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 247

5.2 Derivation of Upper Bounds . . . . . . . . . . . . . . . . . . . . . . . . 248

**VI INSTABILITY OF "BOSONIC MATTER" IN ALL DIMENSIONS . . . . . . . . . . . . . . . . . . . . . . . . . . . 286**

6.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 286

6.2 Derivation of Upper Bounds . . . . . . . . . . . . . . . . . . . . . . . . 287

**VII CONCLUSION AND DISCUSSION . . . . . . . . . . . . . . 324**

REFERENCES . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 327

APPENDICES

APPENDIX A NUMBER OF DISTINCT STATES IN $3D$ . . . . . 340

APPENDIX B NUMBER OF DISTINCT STATES IN $2D$ . . . . . 344

APPENDIX C THE MANOUKIAN-SIRININLAKUL LOWER BOUND . . . . . . . . . . . . . . . . . . . . . . . . 346

APPENDIX D SOME BASIC INTEGRALS AND SUMS ENCOUNTERED IN THIS THESIS . . . . . . . . . . . . . . 351

APPENDIX E SOME TRIAL WAVEFUNCTIONS FOR THE BOSONIC SYSTEMS INVESTIGATED . . . . . . 356

CURRICULUM VITAE . . . . . . . . . . . . . . . . . . . . . . . . . . . 361

# LIST OF TABLES

**Table** **Page**

A.1 Number of distinct states for $6 \leqslant n^2 \leqslant 51$ . . . . . . . . . . . . . . . . . 340

A.2 Number of distinct states for $53 \leqslant n^2 \leqslant 101$ . . . . . . . . . . . . . . . 341

A.3 Number of distinct states for $9933 \leqslant n^2 \leqslant 9974$ . . . . . . . . . . . . . 342

A.4 Number of distinct states for $9976 \leqslant n^2 \leqslant 10000$ . . . . . . . . . . . . 343

B.1 Number of distinct states for $5 \leqslant n^2 \leqslant 58$ . . . . . . . . . . . . . . . . . 344

B.2 Number of distinct states for $61 \leqslant n^2 \leqslant 178$ . . . . . . . . . . . . . . . 345

E.1 Values of expectation value of $T$ of the kinetic energy for $0.43 \leqslant a \leqslant 0.58358$

# LIST OF FIGURES


**Figure** **Page**

2.1 The 1/8 sections of the sphere of radius $n$. . . . . . . . . . . . . . . . . 89

3.1 The first quadrant of a circle of radius $n$ . . . . . . . . . . . . . . . . . 137

4.1 The figure shows the regions (non-overlapping boxes) where particles are localized . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 188

4.2 The figure displays the vectors $\mathbf{L}_1, \ldots, \mathbf{L}_{N-k}$ . . . . . . . . . . . . . . . 189

5.1 The figure displays vectors $\mathbf{L}_1, \ldots, \mathbf{L}_4$ . . . . . . . . . . . . . . . . . . . . 251

E.1 Plot of $f_1(x)$ . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 356

E.2 Plot of $f_2(x)$ . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 357

E.3 Plot of $f_4(x)$ . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 358

E.4 Plot of $f_5(x)$ . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 359

E.5 Plot of $f_7(x)$ . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 360

# CHAPTER I

# INTRODUCTION

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 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 Sin-Itiro Tomonaga (1997), on the Story of Spin, Takeshi 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*". Elliot H. Lieb (1990), regarding "bosonic matter", i.e., matter for which the Pauli Exclusion Principle does not apply, 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); Iwanenko and Sokolow (1937); Fierz (1939); Pauli and Belinfante (1940); de Wet (1940); Pauli (1950); Wightman (1956); Schwinger (1958a, 1958b); Burgoyne (1958); Lüders and Zumino (1958); Jost (1960); Brown and Schwinger (1961).

The question of why matter is stable has much interested physicists for years after the discovery by Rutherford that matter consists of positive and negative point particles interacting by Coulomb forces. This interest was particularly recorded historically in such debates between the experts in the thirties such as between Paul Ehrenfest (1959, 1931) and Wolfgang Pauli: "*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. 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 and stone are so bulky.*" These words were addressed by Ehrenfest to Pauli (Ehrenfest, 1931, 1959) as quoted by Freeman Dyson (1967), who did pioneering work on this problem, in 1967. It was known that an atom of a nuclear charge $Ze$ and $Z$ electrons of charge $-e$ could not have an energy state lower than $-Z^3\,\mathrm{Ry}$, where Ry is the Rydberg energy ($\mathrm{Ry} \equiv m_e e^4/2\hbar^2 = 13.605\,6923(12)$ eV), but this solution solved only the problem of stability for single atoms and did not tell physicists what happens with matter consisting of many large number of particles. The question was: Why is matter of such system stable? The importance of the Pauli exclusion principle (or as in the modern literature referred to the "Spin and Statistics Theorem") in the stability of matter and the prevention of its collapsing around us was clearly recognized quite early. The legendary Freeman Dyson writes (1967) in regard to the exclusion principle: "*We have been unable to find in literature of the 1920's and 1930's any more exact calculation of what would happen to matter if the exclusion principle were abolished.*"

Surprisingly, the first rigorous, non-speculative, study of what happens to matter in the absence of the exclusion principle came much later in 1967 by Dyson. The underlying mathematical analysis turned out to be exceedingly complicated and this perhaps explains the rather slow progress that has taken in tackling this very complex problem. Important earlier investigations to Dyson's work which have paved the way to his developments were due to Fermi (1927); Heisenberg (1927); Hartree (1928); Thomas (1927); Dirac (1930); Fock (1930); Slater (1930); Lenz (1932); Sommerfeld (1932); von Weizsäcker (1935); Sobolev (1938); Gombás (1949); Scott (1952); Sheldon (1955); Kompaneets and Pavlovskii (1956); Kirzhnits (1957); Birman (1961); Schwinger (1961); Teller (1962); Fisher (1964); Balàzs (1967). For later work, cf., Dyson and Lenard (1967); Lenard and Dyson (1968); Kato (1951, 1972); Rosen (1971); Stein (1971); Conlon (1984); Conlon, Lieb and Yau (1988); Helffer and Robert (1990); Hoffmann-Ostenhof and Hoffmann-Ostenhof (1977); Lieb (1976b, 1979, 1980, 1983, 1990); Lieb and Lebowitz (1972); Lieb and Simon (1974, 1977); Lieb and Thirring (1976); Perez, Malta and Coutinho (1988); Weidl (1996); Manoukian and Muthaporn (2002, 2003a, 2003b); Muthaporn and Manoukian (2004a, 2004b). The question raised by Dyson as to what happens to matter if the exclusion principle is abolished led to the investigation of the nature of "bosonic matter".

The Hamiltonian investigated in regard to "bosonic matter" is given by

$$H' = \sum_{i=1}^{2N} \frac{\mathbf{p}_i^2}{2m_i} \quad + \quad \sum_{i<j}^{2N} \frac{e^2 \varepsilon_i \varepsilon_j}{|\mathbf{x}_i - \mathbf{x}_j|} \tag{1.1}$$

for a neutral system consisting of $2N(N+N)$ bosonic spin 0 particles, where $\varepsilon_i$ and $\varepsilon_j$ equal to $\pm 1$. Dyson obtained an upper bound for the ground-state energy of the above Hamiltonian. By a very complicated analysis he derived the famous $N^{7/5}$ law for bosons. To investigate the nature of the so-called collapse or instability of "bosonic matter", the derivation of an *upper* bound for the ground-state energy is necessary. A lower bound, however, was also derived by Conlon, Lieb and Yau (1988) confirming the $N^{7/5}$ law by Dyson. The coefficient of the law turned out to be very small and this was as a result of fairly delicate estimates that were needed in obtaining it. Since his work, several papers have appeared on the stability problem rather than on the instability one, e.g., Lieb and Thirring (1975); Lieb (1990); Thirring (1983); Hundertmark, Laptev and Weidl (1999); Laptev and Weidl (1999). The instability problem, however, turned out to be much more difficult (Lieb, 1990, p.29). The reason is that the problem of instability yields a necessary condition on the fermionic property of the electron for stability, while the analysis involved with the stability problem demonstrates that the fermionic property of the electron satisfies the sufficiency condition for stability.

The purpose of this thesis is to carry out a quantitative and mathematically rigorous, non-speculative, analysis of "bosonic matter" in the bulk in regard to its exact ground-state energy, and investigate the nature of the instability problem of such matter by deriving new rigorous upper bounds for the ground-state energy. We consider bosonic systems with Hamiltonian in the form given in (1.1) describing the interaction of $N$ positive and $N$ negative charges treated dynamically. We also consider Hamiltonians of the form

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} - \sum_{j=1}^{N}\sum_{i=1}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{R}_j|} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{1.2}$$

for over all neutral systems, where the positively charges are fixed but have nevertheless a positive contribution to the ground-state energy by the presence of the positive last term in (1.2). Physically the Hamiltonian in (1.2) is expected to be more relevant (Lieb, 1979) to the instability problem of "bosonic matter". The reason for this is that in (1.2) we do not dwell on the fate of the dynamics of the so-called positive core which, undoubtedly, has a very complex dynamics at distances of nuclear dimensions. With the Hamiltonian in (1.2), one would be describing the collapse of "bosonic matter" down to the nuclear level beyond which some new physical insights may be needed. For "bosonic matter" the ground-state energy has a typical power law behaviour $N^\alpha$, where the power $\alpha > 1$. Such a power law implies instability of such a system, since the formation of such matter consisting of $(2N + 2N)$ particles will be fovourable over two separate systems brought into contact, each consisting of $(N + N)$ particles, and the energy released upon collapse, in the formation of the former systems, being proportional to $[(2N)^\alpha - 2(N)^\alpha]$, will be overwhelmingly large for realistically large $N$, e.g., $N \sim 10^{23}$ or larger. That is, the more matter you add the more negative the ground-state energy becomes in a non-linear manner. This is unlike fermionic matter which becomes more negative only linearly and remains stable.

Our rigorous bounds obtained allow us to estimate the exact ground-state energy of the systems considered and shows that the energy released upon the collapse of even relatively small $N$ will be much much more than that of the Hiroshima and Nagasaki bombs as well as of the Tsunami disaster off the west coast of northern Sumatra on December 26, 2004.

In this thesis, we are also particularly, interested in answering the question: Is the instability of "bosonic matter" characteristic of the dimensionality of space?. That is, is the collapse due to an accidental choice of nature to pick up the dimensionality of space we live in to be three, and also the very interesting related problem as to whether the change of the dimensionality of space will change such matter from an "implosive" to a "stable" or to an "explosive" phase. We establish rigorously that this does not happen and such systems are unstable in all dimensions. There have been, of course, much interest recently in physics in other dimensions than three. For example in investigating the role of the Spin and Statistics Theorem for $D \neq 3$ (e.g., Geyer, 1995; Bhaduri, Murthy and Srivastava, 1996; Semenoff and Wijewardhana, 1987; Forte, 1992) and investigations in $2D$ superconductivity. The interest in the physics of arbitrary dimensions has been also witnessed in string theories (e.g., Schwarz, 1985; Green, Schwarz and Witten, 1988). Another complication that arises in this type of analyses is that both signs of charges arise in this work which make the control of the positive part over the negative one in the Hamiltonian quite involved. As a matter of fact, when the couplings (charges) of bosons are considered to be of the same sign the analysis simplifies tremendously, cf., Hall (2000).

The outline of this Thesis is as follows. In Chapter II, we apply the powerful Schwinger functional technique (Schwinger, 1951a, 1951b, 1953, 1954, 1988; Manoukian, 1985, 1986) to evaluate the expectation value of the Hamiltonian in (1.1) with respect to a trial multi-particle wavefunction of the system. This simplifies the analysis in comparison to an analysis based on combinatorics which would be exceedingly tedious. Several Propositions and Lemmas are then proved to finally obtain our new upper bound of the exact ground-state energy for the Hamiltonian in (1.1). Our new bound, because of our sharp estimates, improves the classic bound of Dyson by a factor of 31. Chapter III extends the analyses carried out in Chapter II to $2D$ and we obtain a new law of $N^{3/2}$ for the ground-state energy of such matter. Surprisingly, several new propositions had to be established afresh for the $2D$ case to obtain our law. The analysis of Chapter IV is of central importance in this thesis is that we were able to derive an upper bound for the exact ground-state energy of the Hamiltonian (1.2) for *all* $N \geqslant 8$. This generalizes earlier work by Lieb (1979) who derived the upper bound for $N = 8,\ 64,\ 216,\ \ldots$ and so on, only, and his method, unfortunately, did not apply for all $N$. We had to group our particles in a very special way to derive our result. Initially we were trying to group them within spheres lying on the surfaces of consecutive spheres and the procedure was hopeless and we have soon realized that this is an *unsolved* problem in mathematics as announced in the Notices of the American Mathematical Society (Pfender and Ziegler, 2004; see also Croft, Falconer and Guy, 1991). In Chapter VI, we establish the instability of "bosonic matter" in *all* dimensions. The Final chapter deals with our conclusions and various comments are made on our work. Two appendices (Appendix A and Appendix B) are involved with some numerical work in classifying the states in this investigation. Appendix C deals with a recent lower bound derived for the exact ground-state energy. Several integrals and sums encountered in this work are given in Appendix D. Appendix E deals with some of the trial functions we have used in the process of deriving our results.

# CHAPTER II

# UPPER BOUNDS OF THE GROUND-STATE ENERGY OF BOSONIC SYSTEMS OF POSITIVE AND NEGATIVE CHARGES

This chapter deals with a mathematical rigorous derivation of several upper bounds of the ground-state energy $E_{N,N}$ of bosonic systems consisting of $N$ negatively charged and $N$ positively charged particles with Hamiltonians

$$H' = \sum_{i=1}^{2N} \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i<j}^{2N} \frac{e^2 \varepsilon_i \varepsilon_j}{|\mathbf{x}_i - \mathbf{x}_j|} \tag{2.1}$$

where $\varepsilon_i = \pm 1$. The process turns out to be quite involved and leads, in passing, to prove six Propositions and three Lemmas and many additional careful estimates. One of our basic upper bound of the ground-state energy for $N > 10^{15}$ for bosonic systems in the bulk obtained below is given by

$$E_{N,N} < -\frac{me^4}{2\,\hbar^2} \frac{N^{7/3}}{62\,\pi^4}. \tag{2.2}$$

Our new bound improves the classic bound of Dyson (1967) by a factor of 31. Here

$$m = \min_{1\leqslant i\leqslant N} \ m_i \tag{2.3}$$

i.e., it is the mass of the lightest particle involved in the sum in (2.1). Actually, $m$ may be taken to be *even smaller* than the smallest mass available in the system.

Since the kinetic energy operator is positive, we have for an arbitrary state $\Phi$, the bound $\langle \Phi \,|\mathbf{p}_i^2|\, \Phi \rangle \leqslant \left(\dfrac{m_i}{m}\right) \langle \Phi \,|\mathbf{p}_i^2|\, \Phi \rangle$, where $m$ is the smallest of the masses involved in equation (2.1) (or, it may be taken even smaller as mentioned above). It is sufficient for the purpose of obtaining an upper bound on the ground-state energy to consider instead the Hamiltonian in equation (2.4) given below. That is, we consider the more convenient Hamiltonian

$$H = \sum_{i=1}^{2N} \frac{p_i^2}{2m} \quad + \quad \sum_{i<j}^{2N} \frac{e^2 \varepsilon_i \varepsilon_j}{|\mathbf{x}_i - \mathbf{x}_j|}. \tag{2.4}$$

We denote the $2N$-particles trial wavefunction of the $2N$ particles by $\Psi_{2N}$. Since $\Psi_{2N}$ does not necessarily coincide with the ground-state wavefunction of $H$, it can be inferred that the quantity

$$\frac{\langle \Psi_{2N} | H | \Psi_{2N} \rangle}{\|\Psi_{2N}\|^2} \equiv H_{2N} \tag{2.5}$$

cannot be less than the ground-state energy $E_{2N,2N}$, i.e., that

$$E_{2N,2N} \leqslant H_{2N} \tag{2.6}$$

where $E_{N,N}$ denotes the ground-state energy $H'$ of $(N+N)$ particles and we obtain the expression of $H_{2N}$

$$H_{2N} = \beta_N \left[ \sum_{\alpha=1}^{k} T_\alpha - kT_0 + \frac{1}{3}(k-2) \sum_{\alpha=1}^{k} I_{0\alpha} \right] + 2N \left[ T_0 - \frac{1}{3} \sum_{\alpha=1}^{k} I_{0\alpha} \right] \tag{2.7}$$

where $\beta_N$ is the Dyson coefficient, $T_\alpha$, $T_0$ are the positive kinetic energy parts and $I_{0\alpha}$ is the interacting energy and $k$ is an arbitrary parameter, depending on the number of expansion coefficients of the relevant wavefunctions in terms of a complete set of functions and is optimally chosen. We are able to obtain a sharp estimate on $\beta_N$, and develop a method of counting the quantum states which is of central importance in establishing the upper bound on the ground-state energy.

We succeeded in deriving the inequality for $\dfrac{1}{3} \leqslant \beta_N \leqslant \dfrac{1}{2}$, $N \geqslant 2$, $k < 2N$.

By substituting $\beta_N$ in (2.7), we rewrite the expression in (2.6) as a useful bound

$$H_{2N} \leqslant \frac{1}{2} \sum_{\alpha=1}^{k} T_\alpha + \left(2N - \frac{k}{3}\right) T_0 + \frac{1}{3}\left[2N - (k-2)\frac{1}{2}\right] \left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right). \quad (2.8)$$

This provides a key estimate in our analyses to follow.

In Sect. 2.1, we carry out the expectation value of our Hamiltonian using Schwinger's elegant functional technique (Schwinger, 1951a, 1951b, 1953, 1954, 1988). This simplifies the rather tedious procedure that may be followed otherwise by using combinatoric methods. This section also deals with the construction of the trial multi-particle wavefunction to be used. The basic estimates and the various Propositions and Lemmas are proved in Sect. 2.2. In the final section, Sect. 2.3, several upper bounds for $E_{N,N}$ are derived including the one quoted in (2.2) above.

## 2.1 Expectation Value of the Hamiltonian : Schwinger Functional Technique

Since the kinetic energy operator is positive, we have for an arbitrary state $\Psi$, where $m$ is the smallest of the masses involved in equation (1.1) (or, it may be taken even smaller)

$$m \leqslant m_i. \quad (2.9)$$

Multiply (2.9) by 2, we obtain $2m \leqslant 2m_i$, then

$$\frac{1}{2m} \geqslant \frac{1}{2m_i}. \quad (2.10)$$

Since

$$\left\langle \Psi \middle| \mathbf{p}_i^2 \middle| \Psi \right\rangle \geqslant 0 \quad (2.11)$$

then, multiply (2.10) by (2.11), we obtain

$$\frac{1}{2m}\left\langle\Psi\left|\mathbf{p}_i^2\right|\Psi\right\rangle \geqslant \frac{1}{2m_i}\left\langle\Psi\left|\mathbf{p}_i^2\right|\Psi\right\rangle. \tag{2.12}$$

Therefore

$$\sum_{i=1}^{2N}\left\langle\Psi\left|\frac{\mathbf{p}_i^2}{2m}\right|\Psi\right\rangle+\sum_{i<j}^{2N}\left\langle\Psi\left|\frac{e^2\varepsilon_i\varepsilon_j}{|\mathbf{x}_i-\mathbf{x}_j|}\right|\Psi\right\rangle$$
$$\geqslant \sum_{i=1}^{2N}\left\langle\Psi\left|\frac{\mathbf{p}_i^2}{2m_i}\right|\Psi\right\rangle+\sum_{i<j}^{2N}\left\langle\Psi\left|\frac{e^2\varepsilon_i\varepsilon_j}{|\mathbf{x}_i-\mathbf{x}_j|}\right|\Psi\right\rangle. \tag{2.13}$$

Eq. (2.13) can be rewritten as

$$\langle\Psi|H|\Psi\rangle \geqslant \langle\Psi|H'|\Psi\rangle. \tag{2.14}$$

For any $\Psi_{2N}$ and by using (2.14), we obtain

$$H'_{2N} \equiv \frac{\langle\Psi_{2N}|H'|\Psi_{2N}\rangle}{\|\Psi_{2N}\|^2} \leqslant \frac{\langle\Psi_{2N}|H|\Psi_{2N}\rangle}{\|\Psi_{2N}\|^2} \equiv H_{2N} \tag{2.15}$$

where

$$H=\sum_{i=1}^{2N}\frac{\mathbf{p}_i^2}{2m}+\sum_{i<j}^{2N}\frac{e^2\varepsilon_i\varepsilon_j}{|\mathbf{x}_i-\mathbf{x}_j|}. \tag{2.16}$$

Let

$$\Psi_{2N}=\sum_{n=0}^{2N}\Phi_{n,2N-n} \tag{2.17}$$

where $\Phi_{N_+,N_-}$ is the state of $N_+$ positive and $N_-$ negative charges. Then

$$\langle\Psi_{2N}|H|\Psi_{2N}\rangle=\sum_{n=0}^{2N}\langle\Phi_{n,2N-n}|H|\Phi_{n,2N-n}\rangle \tag{2.18}$$

and

$$\|\Psi_{2N}\|^2=\sum_{n=0}^{2N}\|\Phi_{n,2N-n}\|^2. \tag{2.19}$$

Eq. (2.18) can be rewrite as

$$\langle \Psi_{2N} | H | \Psi_{2N} \rangle = \sum_{n=0}^{2N} \frac{\langle \Phi_{n,2N-n} | H | \Phi_{n,2N-n} \rangle}{\|\Phi_{n,2N-n}\|^2} \|\Phi_{n,2N-n}\|^2$$

$$= \sum_{n=0}^{2N} H_{n,2N-n} \|\Phi_{n,2N-n}\|^2 \tag{2.20}$$

where $H_{n,2N-n}$ is the expectation value of state $\Phi_{n,2N-n}$ and

$$H_{n,2N-n} \geqslant E_{n,2N-n} \tag{2.21}$$

where

$$E_{N_+,N_-} \equiv \text{ the ground-state energy of state } \Phi_{N_+,N_-}. \tag{2.22}$$

Then substitute (2.21) in (2.20), we obtain

$$\langle \Psi_{2N} | H | \Psi_{2N} \rangle \geqslant \sum_{n=0}^{2N} E_{n,2N-n} \|\Phi_{n,2N-n}\|^2 . \tag{2.23}$$

We put $k_+$ positive charges and $k_-$ negative charges separated at $\infty$ from the cloud of $N_+, N_-$ with zero kinetic energy. Let

$$k_+ = 2N - n, \tag{2.24}$$

$$k_- = n \tag{2.25}$$

then $k_+ + k_- = 2N$ and

$$E_{N_+ + k_+, N_- + k_-} \leqslant E_{N_+,N_-}. \tag{2.26}$$

Substitute (2.24) and (2.25) in (2.26), then

$$E_{N_+ + 2N - n, N_- + n} \leqslant E_{N_+,N_-}. \tag{2.27}$$

Let

$$N_+ = n, \tag{2.28}$$

$$N_- = 2N - n \tag{2.29}$$

substitute (2.28) and (2.29) in (2.27), then

$$E_{n,2N-n} \geqslant E_{2N,2N}. \tag{2.30}$$

Multiply (2.30) by $\sum_{n=0}^{2N} \|\Phi_{n,2N-n}\|^2$, then we obtain

$$\sum_{n=0}^{2N} E_{n,2N-n} \|\Phi_{n,2N-n}\|^2 \geqslant \sum_{n=0}^{2N} E_{2N,2N} \|\Phi_{n,2N-n}\|^2$$

$$= E_{2N,2N} \sum_{n=0}^{2N} \|\Phi_{n,2N-n}\|^2 . \tag{2.31}$$

Compare (2.31) with (2.23), then we obtain

$$\langle \Psi_{2N} | H | \Psi_{2N} \rangle \geqslant E_{2N,2N} \sum_{n=0}^{2N} \|\Phi_{n,2N-n}\|^2 . \tag{2.32}$$

Multiply (2.32) by $\|\Psi_{2N}\|^{-2}$ and from (2.15) and (2.19), we obtain

$$H_{2N} \geqslant \frac{E_{2N,2N} \sum_{n=0}^{2N} \|\Phi_{n,2N-n}\|^2}{\sum_{n=0}^{2N} \|\Phi_{n,2N-n}\|^2} \tag{2.33}$$

therefore

$$H_{2N} \geqslant E_{2N,2N} \tag{2.34}$$

where $E_{N,N}$ denotes the ground-state energy $H'$ of $2N(N+N)$ particles.

**Lemma 2.1.1**

$$\exp\left(\frac{a}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\exp\left(\frac{b}{2}x^2+cx\right)=\frac{\exp\left(cx+\frac{a}{2}c^2\right)}{\sqrt{1-ab}}\exp\left[\frac{b(ac+x)^2}{2(1-ab)}\right] \tag{2.35}$$

*where* $(ab)<1$.

We have the elementary integrals

$$\int_{-\infty}^{\infty}\mathrm{d}k\ \exp\left(-a'k^2\right)=\sqrt{\frac{\pi}{a'}}, \tag{2.36}$$

$$\int_{-\infty}^{\infty}\mathrm{d}k\ \exp\left[-a'(k+m)^2\right]=\sqrt{\frac{\pi}{a'}}, \tag{2.37}$$

$$\sqrt{\frac{a'}{\pi}}\int_{-\infty}^{\infty}\mathrm{d}k\ \exp\left[-a'(k+m)^2\right]=1. \tag{2.38}$$

Multiply (2.38) by $\exp\left(\frac{b}{2}x^2\right)$, then we obtain

$$\begin{aligned}\exp\left(\frac{b}{2}x^2\right)&=\sqrt{\frac{a'}{\pi}}\int_{-\infty}^{\infty}\mathrm{d}k\ \exp\left[-a'(k+m)^2\right]\exp\left(\frac{b}{2}x^2\right)\\&=\sqrt{\frac{a'}{\pi}}\int_{-\infty}^{\infty}\mathrm{d}k\ \exp\left[-a'(k+m)^2+\frac{b}{2}x^2\right]\\&=\sqrt{\frac{a'}{\pi}}\int_{-\infty}^{\infty}\mathrm{d}k\ \exp\left[-a'(k^2+2mk+m^2)+\frac{b}{2}x^2\right]\\&=\sqrt{\frac{a'}{\pi}}\int_{-\infty}^{\infty}\mathrm{d}k\ \exp\left(-a'k^2-2a'mk-a'm^2+\frac{b}{2}x^2\right).\end{aligned} \tag{2.39}$$

We choose $a'=\frac{b}{2}$, $m=x$, then (2.39) becomes

$$\exp\left(\frac{b}{2}x^2\right)=\sqrt{\frac{b}{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}k\ \exp\left(-\frac{b}{2}k^2-bkx-\frac{b}{2}x^2+\frac{b}{2}x^2\right)$$

$$= \sqrt{\frac{b}{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k \; \exp\left(-\frac{b}{2}k^2 - bkx\right). \tag{2.40}$$

Multiply (2.40) by $\exp(cx)$, we obtain

$$\exp\left(\frac{b}{2}x^2 + cx\right) = \sqrt{\frac{b}{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k \; \exp\left(-\frac{b}{2}k^2 - bkx\right) \exp(cx)$$

$$= \sqrt{\frac{b}{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k \; \exp\left(-\frac{b}{2}k^2\right) \exp\big[(c - bk)x\big]. \tag{2.41}$$

Then, we operate $\exp\left(\frac{a}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)$ to (2.41), we obtain

$$\exp\left(\frac{a}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) \exp\left(\frac{b}{2}x^2 + cx\right)$$

$$= \sqrt{\frac{b}{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k \; \exp\left(-\frac{b}{2}k^2\right) \exp\left(\frac{a}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) \exp\big[(c - bk)x\big]$$

$$= \sqrt{\frac{b}{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k \; \exp\left(-\frac{b}{2}k^2\right) \exp\big[(c - bk)x\big] \exp\left[\frac{a}{2}(c - bk)^2\right]$$

$$= \sqrt{\frac{b}{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k \; \exp\left[-\frac{b}{2}k^2 + (c - bk)x + \frac{a}{2}(c - bk)^2\right]$$

$$\equiv \sqrt{\frac{b}{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k \; \exp[\,\cdot\,] \tag{2.42}$$

where

$$[\,\cdot\,] = -\frac{b}{2}k^2 + (c - bk)x + \frac{a}{2}(c - bk)^2$$

$$= -\frac{b}{2}k^2 + cx - bkx + \frac{a}{2}c^2 - abck + \frac{a}{2}b^2k^2$$

$$= \left(\frac{a}{2}b^2 - \frac{b}{2}\right)k^2 - (bx + abc)\,k + c\left(x + \frac{a}{2}c\right)$$

$$= \frac{b}{2}\left(ab-1\right)k^2 - b(x+ac)k + c\left(x+\frac{a}{2}c\right)$$

$$= -\left[\frac{b}{2}\left(1-ab\right)k^2 + b(x+ac)k - c\left(x+\frac{a}{2}c\right)\right]. \tag{2.43}$$

Let

$$\frac{b}{2}(1-ab)k^2 = q^2 \tag{2.44}$$

then

$$k = \frac{q}{\sqrt{\frac{b}{2}(1-ab)}} \tag{2.45}$$

and

$$\mathrm{d}k = \frac{\mathrm{d}q}{\sqrt{\frac{b}{2}(1-ab)}}. \tag{2.46}$$

We substitute $k$ from (2.45) in (2.43), we obtain

$$[\,\cdot\,] = -\left[q^2 + \frac{b(x+ac)}{\sqrt{\frac{b}{2}(1-ab)}}q - c\left(x+\frac{a}{2}c\right)\right]$$

$$= -\left\{\left[q + \left(\frac{b(x+ac)}{2\sqrt{\frac{b}{2}(1-ab)}}\right)\right]^2 - c\left(x+\frac{a}{2}c\right) - \left(\frac{b(x+ac)}{2\sqrt{\frac{b}{2}(1-ab)}}\right)^2\right\}$$

$$= -\left\{\left[q + \left(\frac{b(x+ac)}{2\sqrt{\frac{b}{2}(1-ab)}}\right)\right]^2 - c\left(x+\frac{a}{2}c\right) - \frac{b(x+ac)^2}{2(1-ab)}\right\}. \tag{2.47}$$

Substitute $[\,\cdot\,]$ from (2.47) in (2.42) and by using (2.46), we obtain

$$\exp\left(\frac{a}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\exp\left(\frac{b}{2}x^2 + cx\right)$$

$$= \sqrt{\frac{b}{2\pi}} \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{\sqrt{\frac{b}{2}(1-ab)}}$$

$$\times \exp\left\{-\left[\left(q + \frac{b(x+ac)}{2\sqrt{\frac{b}{2}(1-ab)}}\right)^2 - c\left(x + \frac{a}{2}c\right) - \frac{b(x+ac)^2}{2(1-ab)}\right]\right\}$$

$$= \sqrt{\frac{b}{2\pi}} \exp\left(cx + \frac{a}{2}c^2\right) \exp\left[\frac{b(x+ac)^2}{2(1-ab)}\right]$$

$$\times \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{\sqrt{\frac{b}{2}(1-ab)}} \exp\left[-\left(q + \frac{b(x+ac)}{2\sqrt{\frac{b}{2}(1-ab)}}\right)^2\right]. \tag{2.48}$$

Compare the integral in (2.48) with (2.37), we obtain

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}q}{\sqrt{\frac{b}{2}(1-ab)}} \exp\left[-\left(q + \frac{b(x+ac)}{2\sqrt{\frac{b}{2}(1-ab)}}\right)^2\right] = \frac{1}{\sqrt{\frac{b}{2}(1-ab)}}\sqrt{\pi}$$

$$= \sqrt{\frac{2\pi}{b(1-ab)}}. \tag{2.49}$$

Substitute (2.49) in (2.48), we obtain (2.35), that is

$$\exp\left(\frac{a}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right) \exp\left(\frac{b}{2}x^2 + cx\right)$$

$$= \sqrt{\frac{b}{2\pi}} \exp\left(cx + \frac{a}{2}c^2\right) \exp\left[\frac{b(ac+x)^2}{2(1-ab)}\right] \times \sqrt{\frac{2\pi}{b(1-ab)}}$$

$$= \frac{\exp\left(cx + \frac{a}{2}c^2\right)}{\sqrt{1-ab}} \exp\left[\frac{b(ac+x)^2}{2(1-ab)}\right]. \tag{2.50}$$

□

**Lemma 2.1.2**

$$\exp\left(\lambda\sum_\alpha \frac{\delta}{\delta S_\alpha}\frac{\delta}{\delta K_\alpha}\right)\exp\left(\sum_\alpha \frac{\lambda_\alpha}{2}K_\alpha^2\right)\exp\left(\sum_\alpha \frac{\lambda_\alpha}{2}S_\alpha^2\right)$$
$$=\left(\prod_\alpha \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\exp\left(\sum_\alpha \frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{1-\lambda^2\lambda_\alpha^2}\right)$$
$$\times\exp\left(\sum_\alpha \frac{\lambda_\alpha K_\alpha^2}{2(1-\lambda^2\lambda_\alpha^2)}\right)\exp\left(\sum_\alpha \frac{\lambda_\alpha S_\alpha^2}{2(1-\lambda^2\lambda_\alpha^2)}\right). \tag{2.51}$$

To obtain above expression, we have

$$\exp\left(a\frac{\mathrm{d}}{\mathrm{d}x}\right)f(x)=\exp\left(a\frac{\mathrm{d}}{\mathrm{d}x}\right)\int_{-\infty}^{\infty}\frac{\mathrm{d}k}{2\pi}\,\mathrm{e}^{\mathrm{i}kx}\tilde{f}(k)$$
$$=\int_{-\infty}^{\infty}\frac{\mathrm{d}k}{2\pi}\,\mathrm{e}^{\mathrm{i}ka}\,\mathrm{e}^{\mathrm{i}kx}\tilde{f}(k)$$
$$=f(a+x). \tag{2.52}$$

Consider

$$\exp\left(\lambda\sum_\alpha \frac{\delta}{\delta S_\alpha}\frac{\delta}{\delta K_\alpha}\right)\exp\left(\sum_\alpha \frac{\lambda_\alpha}{2}K_\alpha^2\right)\exp\left(\sum_\alpha \frac{\lambda_\alpha}{2}S_\alpha^2\right)$$
$$=\prod_\alpha\left[\exp\left(\lambda\frac{\delta}{\delta S_\alpha}\frac{\delta}{\delta K_\alpha}\right)\exp\left(\frac{\lambda_\alpha}{2}K_\alpha^2\right)\exp\left(\frac{\lambda_\alpha}{2}S_\alpha^2\right)\right]. \tag{2.53}$$

Consider the right-hand side of above equation and use (2.52) to obtain

$$\exp\left(\lambda\frac{\delta}{\delta S_\alpha}\frac{\delta}{\delta K_\alpha}\right)\exp\left(\frac{\lambda_\alpha}{2}K_\alpha^2\right)$$
$$=\exp\left[\frac{\lambda_\alpha}{2}\left(K_\alpha+\lambda\frac{\delta}{\delta S_\alpha}\right)^2\right]$$

$$= \exp\left(\frac{\lambda_\alpha}{2}K_\alpha^2\right)\exp\left(\lambda_\alpha\lambda K_\alpha\frac{\delta}{\delta S_\alpha}\right)\exp\left(\frac{\lambda_\alpha}{2}\lambda^2\frac{\delta^2}{\delta S_\alpha^2}\right). \tag{2.54}$$

Operate the operator from (2.54) to $\exp\left(\frac{\lambda_\alpha}{2}S_\alpha^2\right)$, we obtain

$$\exp\left(\lambda\frac{\delta}{\delta S_\alpha}\frac{\delta}{\delta K_\alpha}\right)\exp\left(\frac{\lambda_\alpha}{2}K_\alpha^2\right)\exp\left(\frac{\lambda_\alpha}{2}S_\alpha^2\right)$$
$$= \exp\left(\frac{\lambda_\alpha}{2}K_\alpha^2\right)\exp\left(\lambda_\alpha\lambda K_\alpha\frac{\delta}{\delta S_\alpha}\right)\exp\left(\frac{\lambda_\alpha}{2}\lambda^2\frac{\delta^2}{\delta S_\alpha^2}\right)\exp\left(\frac{\lambda_\alpha}{2}S_\alpha^2\right)$$
$$= \exp\left(\frac{\lambda_\alpha}{2}K_\alpha^2\right)\exp\left(\frac{\lambda_\alpha}{2}\lambda^2\frac{\delta^2}{\delta S_\alpha^2}\right)\exp\left(\lambda_\alpha\lambda K_\alpha\frac{\delta}{\delta S_\alpha}\right)\exp\left(\frac{\lambda_\alpha}{2}S_\alpha^2\right). \tag{2.55}$$

By using (2.52), we obtain

$$\exp\left(\lambda_\alpha\lambda K_\alpha\frac{\delta}{\delta S_\alpha}\right)\exp\left(\frac{\lambda_\alpha}{2}S_\alpha^2\right)$$
$$= \exp\left[\frac{\lambda_\alpha}{2}\left(S_\alpha + \lambda\lambda_\alpha K_\alpha\right)^2\right]$$
$$= \exp\left[\frac{\lambda_\alpha}{2}\left(S_\alpha^2 + 2\lambda\lambda_\alpha K_\alpha S_\alpha\right)\right]\exp\left(\frac{\lambda_\alpha}{2}\lambda^2\lambda_\alpha^2K_\alpha^2\right)$$
$$= \exp\left(\frac{\lambda_\alpha}{2}\lambda^2\lambda_\alpha^2K_\alpha^2\right)\exp\left[\frac{\lambda_\alpha}{2}\left(S_\alpha^2 + 2\lambda\lambda_\alpha K_\alpha S_\alpha\right)\right]. \tag{2.56}$$

Substitute (2.56) in (2.55), we obtain

$$\exp\left(\lambda\frac{\delta}{\delta S_\alpha}\frac{\delta}{\delta K_\alpha}\right)\exp\left(\frac{\lambda_\alpha}{2}K_\alpha^2\right)\exp\left(\frac{\lambda_\alpha}{2}S_\alpha^2\right)$$
$$= \exp\left(\frac{\lambda_\alpha}{2}K_\alpha^2\right)\exp\left(\frac{\lambda_\alpha}{2}\lambda^2\lambda_\alpha^2K_\alpha^2\right)$$
$$\times \exp\left(\frac{\lambda_\alpha}{2}\lambda^2\frac{\delta^2}{\delta S_\alpha^2}\right)\exp\left[\frac{\lambda_\alpha}{2}\left(S_\alpha^2 + 2\lambda\lambda_\alpha K_\alpha S_\alpha\right)\right] \tag{2.57}$$

where

$$\exp\left(\frac{\lambda_\alpha}{2}K_\alpha^2\right)\exp\left(\frac{\lambda_\alpha}{2}\lambda^2\lambda_\alpha^2K_\alpha^2\right)=\exp\left[\frac{\lambda_\alpha K_\alpha^2}{2}\left(1+\lambda^2\lambda_\alpha^2\right)\right]. \tag{2.58}$$

Substitute (2.57) in (2.53), we obtain

$$\begin{aligned}
&\exp\left(\lambda\sum_\alpha\frac{\delta}{\delta S_\alpha}\frac{\delta}{\delta K_\alpha}\right)\exp\left(\sum_\alpha\frac{\lambda_\alpha}{2}K_\alpha^2\right)\exp\left(\sum_\alpha\frac{\lambda_\alpha}{2}S_\alpha^2\right)\\
&\quad=\prod_\alpha\left\{\exp\left[\frac{\lambda_\alpha K_\alpha^2}{2}\left(1+\lambda^2\lambda_\alpha^2\right)\right]\right.\\
&\qquad\left.\times\exp\left(\frac{\lambda_\alpha\lambda^2}{2}\frac{\delta^2}{\delta S_\alpha^2}\right)\exp\left(\frac{\lambda_\alpha}{2}S_\alpha^2+\lambda\lambda_\alpha^2K_\alpha S_\alpha\right)\right\}.
\end{aligned} \tag{2.59}$$

By using Lemma 2.1.1, we obtain

$$\begin{aligned}
&\exp\left(\frac{\lambda_\alpha\lambda^2}{2}\frac{\delta^2}{\delta S_\alpha^2}\right)\exp\left(\frac{\lambda_\alpha}{2}S_\alpha^2+\lambda\lambda_\alpha^2K_\alpha S_\alpha\right)\\
&\quad=\frac{\exp\left(\lambda\lambda_\alpha^2S_\alpha K_\alpha+\frac{\lambda^4\lambda_\alpha^5K_\alpha^2}{2}\right)}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\exp\left[\frac{\lambda_\alpha\left(\lambda^3\lambda_\alpha^3K_\alpha+S_\alpha\right)^2}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right].
\end{aligned} \tag{2.60}$$

Multiply (2.60) by $\exp\left[\frac{\lambda_\alpha K_\alpha^2}{2}\left(1+\lambda^2\lambda_\alpha^2\right)\right]$, we obtain

$$\begin{aligned}
&\exp\left[\frac{\lambda_\alpha K_\alpha^2}{2}\left(1+\lambda^2\lambda_\alpha^2\right)\right]\exp\left(\frac{\lambda_\alpha\lambda^2}{2}\frac{\delta^2}{\delta S_\alpha^2}\right)\exp\left(\frac{\lambda_\alpha}{2}S_\alpha^2+\lambda\lambda_\alpha^2K_\alpha S_\alpha\right)\\
&\quad=\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\exp\left[\frac{\lambda_\alpha K_\alpha^2\left(1+\lambda^2\lambda_\alpha^2\right)}{2}\right]\exp\left(\lambda\lambda_\alpha^2S_\alpha K_\alpha+\frac{\lambda^4\lambda_\alpha^5K_\alpha^2}{2}\right)\\
&\qquad\times\exp\left[\frac{\lambda_\alpha\left(\lambda^6\lambda_\alpha^6K_\alpha^2+S_\alpha^2+2\lambda^3\lambda_\alpha^3K_\alpha S_\alpha\right)}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right]\\
&\quad=\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\exp\left[\frac{\lambda_\alpha K_\alpha^2\left(1+\lambda^2\lambda_\alpha^2\right)}{2}+\frac{\lambda^4\lambda_\alpha^5K_\alpha^2}{2}\right]\exp\left(\lambda\lambda_\alpha^2S_\alpha K_\alpha\right)
\end{aligned}$$

$$\times \exp\left[\frac{\lambda^6\lambda_\alpha^7 K_\alpha^2 + \lambda_\alpha S_\alpha^2 + 2\lambda^3\lambda_\alpha^4 K_\alpha S_\alpha}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right]$$

$$= \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \exp\left[\frac{\lambda_\alpha K_\alpha^2\left(1+\lambda^2\lambda_\alpha^2+\lambda^4\lambda_\alpha^4\right)}{2}\right] \exp\left(\lambda\lambda_\alpha^2 S_\alpha K_\alpha\right)$$

$$\times \exp\left[\frac{\lambda^6\lambda_\alpha^7 K_\alpha^2 + \lambda_\alpha S_\alpha^2 + 2\lambda^3\lambda_\alpha^4 K_\alpha S_\alpha}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right]$$

$$= \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \exp\left[\frac{\lambda_\alpha K_\alpha^2\left(1+\lambda^2\lambda_\alpha^2+\lambda^4\lambda_\alpha^4\right)}{2} + \frac{\lambda^6\lambda_\alpha^7 K_\alpha^2}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right]$$

$$\times \exp\left[\lambda\lambda_\alpha^2 S_\alpha K_\alpha + \frac{\lambda^3\lambda_\alpha^4 K_\alpha S_\alpha}{\left(1-\lambda^2\lambda_\alpha^2\right)}\right] \exp\left[\frac{\lambda_\alpha S_\alpha^2}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right]. \tag{2.61}$$

Eq. (2.61) can be simplified as

$$\exp\left[\frac{\lambda_\alpha K_\alpha^2}{2}\left(1+\lambda^2\lambda_\alpha^2\right)\right] \exp\left(\frac{\lambda_\alpha\lambda^2}{2}\frac{\delta^2}{\delta S_\alpha^2}\right) \exp\left(\frac{\lambda_\alpha}{2}S_\alpha^2 + \lambda\lambda_\alpha^2 K_\alpha S_\alpha\right)$$

$$= \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \exp\left[\frac{K_\alpha^2\lambda_\alpha}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right]$$

$$\times \exp\left[\frac{\lambda_\alpha S_\alpha^2}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right] \exp\left[\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{\left(1-\lambda^2\lambda_\alpha^2\right)}\right]. \tag{2.62}$$

Substitute Eq. (2.62) in Eq. (2.59), we obtain Lemma 2.1.2

$$\exp\left(\lambda\sum_\alpha \frac{\delta}{\delta S_\alpha}\frac{\delta}{\delta K_\alpha}\right) \exp\left(\sum_\alpha \frac{\lambda_\alpha}{2}K_\alpha^2\right) \exp\left(\sum_\alpha \frac{\lambda_\alpha}{2}S_\alpha^2\right)$$

$$= \left(\prod_\alpha \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right) \exp\left[\sum_\alpha \frac{K_\alpha^2\lambda_\alpha}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right]$$

$$\times \exp\left[\sum_\alpha \frac{S_\alpha^2\lambda_\alpha}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right] \exp\left[\sum_\alpha \frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{\left(1-\lambda^2\lambda_\alpha^2\right)}\right]. \tag{2.63}$$

□

## The Trial Two-Particle States

Upon setting $z = z(\mathbf{x}, \varepsilon)$ and introducing trial two-particle states (Dyson, 1967)

$$G(z, z') = \sum_{\alpha=0}^{k} \lambda_\alpha c_\alpha(\varepsilon) c_\alpha(\varepsilon') \psi_\alpha(\mathbf{x}) \psi_\alpha(\mathbf{x}') \tag{2.64}$$

where $\Psi_0(\mathbf{x}), \ \ldots, \ \Psi_k(\mathbf{x})$ are mutually orthonormal and $k$ will be conveniently chosen, with coefficients in (2.64) chosen (Dyson, 1967) as given by

$$\lambda_\alpha = \begin{cases} 1, & \alpha = 0 \\ -\xi, \ \xi > 0, & \alpha = 1, \ldots, k \end{cases} \tag{2.65}$$

$$c_\alpha(\varepsilon) = \begin{cases} \dfrac{1}{\sqrt{2}}, & \alpha = 0 \\ \dfrac{\varepsilon}{\sqrt{2}}, & \alpha = 1, \ldots, k \end{cases} \tag{2.66}$$

where $\varepsilon = \pm 1$, then

$$|c_\alpha(\varepsilon)| = \frac{1}{\sqrt{2}}, \quad \alpha = 0, \ldots, k \tag{2.67}$$

and

$$\sum_{\varepsilon=\pm 1} |c_\alpha(\varepsilon)|^2 \equiv c_\alpha^2 = 1. \tag{2.68}$$

- Consider $\sum_{\varepsilon=\pm 1} \varepsilon c_\alpha(\varepsilon) c_\beta(\varepsilon)$, for $\alpha = 0$, $\beta = 0$ :

$$\begin{aligned} \sum_{\varepsilon=\pm 1} \varepsilon c_\alpha(\varepsilon) c_\beta(\varepsilon) &= \sum_{\varepsilon=\pm 1} \varepsilon \cdot \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} \\ &= \frac{1}{2} \sum_{\varepsilon=\pm 1} \varepsilon = 0. \end{aligned} \tag{2.69}$$

- Consider $\sum_{\varepsilon=\pm 1} \varepsilon c_\alpha(\varepsilon) c_\beta(\varepsilon)$, for $\alpha = 0$, $\beta \neq 0$ :

$$\begin{aligned}\sum_{\varepsilon=\pm 1} \varepsilon c_\alpha(\varepsilon) c_\beta(\varepsilon) &= \sum_{\varepsilon=\pm 1} \varepsilon \cdot \frac{1}{\sqrt{2}} \cdot \frac{\varepsilon}{\sqrt{2}} \\ &= \frac{1}{2} \sum_{\varepsilon=\pm 1} \varepsilon^2 = \frac{1}{2}(1+1) = 1. \end{aligned} \tag{2.70}$$

- Consider $\sum_{\varepsilon=\pm 1} \varepsilon c_\alpha(\varepsilon) c_\beta(\varepsilon)$, for $\alpha \neq 0$, $\beta = 0$ :

$$\begin{aligned}\sum_{\varepsilon=\pm 1} \varepsilon c_\alpha(\varepsilon) c_\beta(\varepsilon) &= \sum_{\varepsilon=\pm 1} \varepsilon \cdot \frac{\varepsilon}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} \\ &= \frac{1}{2}(1+1) = 1. \end{aligned} \tag{2.71}$$

- Consider $\sum_{\varepsilon=\pm 1} \varepsilon c_\alpha(\varepsilon) c_\beta(\varepsilon)$, for $\alpha \neq 0$, $\beta \neq 0$ :

$$\begin{aligned}\sum_{\varepsilon=\pm 1} \varepsilon c_\alpha(\varepsilon) c_\beta(\varepsilon) &= \sum_{\varepsilon=\pm 1} \varepsilon \cdot \frac{\varepsilon}{\sqrt{2}} \cdot \frac{\varepsilon}{\sqrt{2}} \\ &= \frac{1}{2} \sum_{\varepsilon=\pm 1} \varepsilon^3 = \frac{1}{2} \left[(-1)^3 + 1^3\right] = 0. \end{aligned} \tag{2.72}$$

Then, from (2.69)–(2.72), we obtain

$$\sum_{\varepsilon=\pm 1} \varepsilon c_\alpha(\varepsilon) c_\beta(\varepsilon) = \frac{1}{2} \sum_{\varepsilon=\pm 1} \varepsilon^{[1+\Theta(\alpha)+\Theta(\beta)]} \tag{2.73}$$

where the step function $\Theta(\alpha) = 1$, $\alpha > 0$ and $\Theta(\alpha) = 0$, $\alpha \leqslant 0$.

## $2N$-Particle Wavefunction

We can define a $2N$-particle wavefunction as follows

$$\Psi_{2N}(z_1,\ldots,z_{2N}) = \sum_{\pi} G(z(\pi_1),z(\pi_2))\cdots G(z(\pi_{2N-1}),z(\pi_{2N})) \tag{2.74}$$

Here, the sum is over all permutations $(\pi_1,\ldots,\pi_{2N})$ of $(1,\ldots,2N)$, and $\Psi_{2N}$ is not yet normalized and $G(z,z')$ symmetrize with respect to $z$. Since $\Psi_{2N}$ does not necessarily coincide with the ground-state wavefunction of $H$, then Eq. (2.34) will be obtained, i.e., $E_{2N,2N} \leqslant H_{2N}$.

To evaluate Eq. (2.34), one may define the generating functions (Dyson, 1967)

$$\mathcal{H}(\lambda^2) = \sum_{N\geqslant 0} \frac{(\lambda^2)^N}{(2N)!} \left\langle \Psi_{2N} \right| H \left| \Psi_{2N} \right\rangle , \tag{2.75}$$

$$\mathcal{N}(\lambda^2) = \sum_{N\geqslant 0} \frac{(\lambda^2)^N}{(2N)!} \left\| \Psi_{2N} \right\|^2 . \tag{2.76}$$

Hence from (2.15), (2.75) and (2.76), we find

$$H_{2N} = \frac{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{H}(\lambda^2)}{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)}. \tag{2.77}$$

To evaluate (2.77), we use the Schwinger Functional Technique.

## Schwinger Functional Technique

From Eq. (2.64), we have $\Psi_{2N}$ for $N = 1, 2$

$$\Psi_1(z_1,z_2) = G(z_1,z_2) \tag{2.78}$$

and

$$\Psi_4(z_1,\ldots,z_4) = G(z_1,z_2)G(z_3,z_4) + G(z_1,z_3)G(z_2,z_4) + G(z_1,z_4)G(z_2,z_3) \tag{2.79}$$

where $z = (\mathbf{x}, \varepsilon)$.

Let

$$F[K] = \exp\left[\frac{1}{2}\int (\mathrm{d}z)(\mathrm{d}z')\; K(z)G(z,z')K(z')\right]. \tag{2.80}$$

Then, $\Psi_{2N}$ can be obtained from

$$\begin{aligned}\Psi_{2N}(z_1,\ldots,z_{2N}) &= \frac{\delta}{\delta K(z_1)}\cdots\frac{\delta}{\delta K(z_{2N})}F[K]\bigg|_{K\to 0} \\ &\equiv \frac{\delta}{\delta K(z_1)}\cdots\frac{\delta}{\delta K(z_{2N})}F[K]_0. \end{aligned}\tag{2.81}$$

For arbitrary function $f(\mathbf{x})$, we have

$$\frac{\delta f(\mathbf{x})}{\delta f(\mathbf{x}')} = \delta(\mathbf{x}-\mathbf{x}'). \tag{2.82}$$

Then, we will show how to find $\Psi_{2N}$ for $N = 2$. By using (2.81) we have

$$\Psi_4(z_1,z_2,z_3,z_4) = \frac{\delta}{\delta K(z_1)}\cdots\frac{\delta}{\delta K(z_4)}F[K]_0. \tag{2.83}$$

Consider

$$\begin{aligned}\frac{\delta}{\delta K(z_4)}F[K] &= F[K]\frac{1}{2}\int(\mathrm{d}z)(\mathrm{d}z')\; G(z,z')\left[K(z)\frac{\delta K(z')}{\delta K(z_4)} + \frac{\delta K(z)}{\delta K(z_4)}K(z')\right] \\ &= \frac{1}{2}F[K]\int(\mathrm{d}z)(\mathrm{d}z')\; G(z,z')\left[K(z)\delta(z'-z_4) + \delta(z-z_4)K(z')\right] \\ &= \frac{1}{2}F[K]\left[\int(\mathrm{d}z)(\mathrm{d}z')\; G(z,z')K(z)\delta(z'-z_4)\right. \\ &\qquad \left. + \int(\mathrm{d}z)(\mathrm{d}z')\; G(z,z')\delta(z-z_4)K(z')\right] \\ &= \frac{1}{2}F[K]\left[\int(\mathrm{d}z)\; G(z,z_4)K(z) + \int(\mathrm{d}z')\; G(z_4,z')K(z')\right]\end{aligned}$$

$$= F[K] \int (\mathrm{d}z)\; G(z, z_4) K(z). \tag{2.84}$$

Multiply (2.84) by $\dfrac{\delta}{\delta K(z_3)}$, we obtain

$$\frac{\delta}{\delta K(z_3)} \frac{\delta}{\delta K(z_4)} F[K] = \frac{\delta}{\delta K(z_3)} \left( F[K] \int (\mathrm{d}z)\; G(z, z_4) K(z) \right)$$

$$= F[K] \int (\mathrm{d}z)\; G(z, z_4) \frac{\delta K(z)}{\delta K(z_3)} + \frac{\delta F[K]}{\delta K(z_3)} \int (\mathrm{d}z)\; G(z, z_4) K(z)$$

$$= F[K] \int (\mathrm{d}z)\; G(z, z_4) \delta(z - z_3)$$

$$+ F[K] \left( \int (\mathrm{d}z)\; G(z, z_3) K(z) \right) \left( \int (\mathrm{d}z)\; G(z, z_4) K(z) \right)$$

$$= F[K] G(z_3, z_4)$$

$$+ F[K] \left( \int (\mathrm{d}z)\; G(z, z_3) K(z) \right) \left( \int (\mathrm{d}z)\; G(z, z_4) K(z) \right) \tag{2.85}$$

then, multiply (2.85) by $\dfrac{\delta}{\delta K(z_2)}$, we obtain

$$\frac{\delta}{\delta K(z_2)} \frac{\delta}{\delta K(z_3)} \frac{\delta}{\delta K(z_4)} F[K]$$

$$= \frac{\delta}{\delta K(z_2)} \left[ F[K] G(z_3, z_4) + F[K] \left( \int (\mathrm{d}z)\; G(z, z_3) K(z) \right) \right.$$

$$\left. \times \left( \int (\mathrm{d}z)\; G(z, z_4) K(z) \right) \right]$$

$$= \frac{\delta}{\delta K(z_2)} F[K] G(z_3, z_4) + \frac{\delta}{\delta K(z_2)} \left[ F[K] \left( \int (\mathrm{d}z)\; G(z, z_3) K(z) \right) \right.$$

$$\left. \times \left( \int (\mathrm{d}z)\; G(z, z_4) K(z) \right) \right]$$

$$
\begin{aligned}
&= \left(\frac{\delta F[K]}{\delta K(z_2)}\right) G(z_3, z_4) \\
&\quad + \left(\frac{\delta F[K]}{\delta K(z_2)}\right) \left(\int (\mathrm{d}z)\ G(z, z_3) K(z)\right) \left(\int (\mathrm{d}z)\ G(z, z_4) K(z)\right) \\
&\quad + F[K] \left(\int (\mathrm{d}z)\ G(z, z_3) \frac{\delta K(z)}{\delta K(z_2)}\right) \left(\int (\mathrm{d}z)\ G(z, z_4) K(z)\right) \\
&\quad + F[k] \left(\int (\mathrm{d}z)\ G(z, z_3) K(z)\right) \left(\int (\mathrm{d}z)\ G(z, z_4) \frac{\delta K(z)}{\delta K(z_2)}\right) \\
&= F[K] \left(\int (\mathrm{d}z)\ G(z, z_2) K(z)\right) G(z_3, z_4) \\
&\quad + F[K] \left(\int (\mathrm{d}z)\ G(z, z_2) K(z)\right) \left(\int (\mathrm{d}z)\ G(z, z_3) K(z)\right) \\
&\qquad \times \left(\int (\mathrm{d}z)\ G(z, z_4) K(z)\right) \\
&\quad + F[K] \left(\int (\mathrm{d}z)\ G(z, z_3) \delta(z - z_3)\right) \left(\int (\mathrm{d}z)\ G(z, z_4) K(z)\right) \\
&\quad + F[K] \left(\int (\mathrm{d}z)\ G(z, z_3) K(z)\right) \left(\int (\mathrm{d}z)\ G(z, z_4) \delta(z - z_2)\right) \\
&= F[K] \left(\int (\mathrm{d}z)\ G(z, z_2) K(z)\right) G(z_3, z_4) \\
&\quad + F[K] \left(\int (\mathrm{d}z)\ G(z, z_2) K(z)\right) \left(\int (\mathrm{d}z)\ G(z, z_3) K(z)\right) \\
&\qquad \times \left(\int (\mathrm{d}z)\ G(z, z_4) K(z)\right) \\
&+ F[K] G(z_2, z_3) \left(\int (\mathrm{d}z)\ G(z, z_4) K(z)\right) \\
&+ F[K] \left(\int (\mathrm{d}z)\ G(z, z_3) K(z)\right) G(z_2, z_4).
\end{aligned} \tag{2.86}
$$

Multiply (2.86) by $\dfrac{\delta}{\delta K(z_1)}$, we obtain

$$
\begin{aligned}
&\frac{\delta}{\delta K(z_1)}\frac{\delta}{\delta K(z_2)}\frac{\delta}{\delta K(z_3)}\frac{\delta}{\delta K(z_4)}F[K] \\
&\qquad = \frac{\delta}{\delta K(z_1)}\left[F[K]\left(\int(\mathrm{d}z)\; G(z,z_2)K(z)\right)G(z_3,z_4)\right] \\
&\qquad\quad + \frac{\delta}{\delta K(z_1)}\left[F[K]\left(\int(\mathrm{d}z)\; G(z,z_2)K(z)\right)\left(\int(\mathrm{d}z)\; G(z,z_3)K(z)\right)\right. \\
&\qquad\qquad \left.\times\left(\int(\mathrm{d}z)\; G(z,z_4)K(z)\right)\right] \\
&\qquad\quad + \frac{\delta}{\delta K(z_1)}\left[F[K]G(z_2,z_3)\left(\int(\mathrm{d}z)\; G(z,z_4)K(z)\right)\right] \\
&\qquad\quad + \frac{\delta}{\delta K(z_1)}\left[F[K]\left(\int(\mathrm{d}z)\; G(z,z_3)K(z)\right)G(z_2,z_4)\right] \\
&\qquad = F[K]\left(\int(\mathrm{d}z)\; G(z,z_1)K(z)\right)\left(\int(\mathrm{d}z)\; G(z,z_2)K(z)\right)G(z_3,z_4) \\
&\qquad\quad + F[K]G(z_1,z_2)G(z_3,z_4) + F[K]\left(\int(\mathrm{d}z)\; G(z,z_1)K(z)\right) \\
&\qquad \times\left(\int(\mathrm{d}z)\; G(z,z_2)K(z)\right)\left(\int(\mathrm{d}z)\; G(z,z_3)K(z)\right)\left(\int(\mathrm{d}z)\; G(z,z_4)K(z)\right) \\
&\qquad + F[K]G(z_1,z_2)\left(\int(\mathrm{d}z)\; G(z,z_3)K(z)\right)\left(\int(\mathrm{d}z)\; G(z,z_4)K(z)\right) \\
&\qquad + F[K]\left(\int(\mathrm{d}z)\; G(z,z_2)K(z)\right)G(z_1,z_3)\left(\int(\mathrm{d}z)\; G(z,z_4)K(z)\right) \\
&\qquad + F[K]\left(\int(\mathrm{d}z)\; G(z,z_2)K(z)\right)\left(\int(\mathrm{d}z)\; G(z,z_3)K(z)\right)G(z_1,z_4) \\
&\qquad + F[K]\left(\int(\mathrm{d}z)\; G(z,z_1)K(z)\right)G(z_2,z_3)\left(\int(\mathrm{d}z)\; G(z,z_4)K(z)\right)
\end{aligned}
$$

$$+ F[K]G(z_2, z_3)G(z_1, z_4)$$

$$+ F[K]\left(\int(\mathrm{d}z)\ G(z, z_1)K(z)\right)\left(\int(\mathrm{d}z)\ G(z, z_3)K(z)\right)G(z_2, z_4)$$

$$+ F[K]G(z_1, z_3)G(z_2, z_4). \tag{2.87}$$

From (2.80), we have

$$\lim_{K\to 0} F[K] = \lim_{K\to 0} \exp\left[\frac{1}{2}\int(\mathrm{d}z)(\mathrm{d}z')\ K(z)G(z, z')K(z')\right] = 1 \tag{2.88}$$

and

$$\lim_{K\to 0}\int(\mathrm{d}z)\ G(z, z')K(z) = 0. \tag{2.89}$$

Then, by using (2.88) and (2.89), Eq. (2.87) becomes

$$\frac{\delta}{\delta K(z_1)}\cdots\frac{\delta}{\delta K(z_4)}F[K]_0$$

$$= G(z_1, z_2)G(z_3, z_4) + G(z_2, z_3)G(z_1, z_4) + G(z_1, z_3)G(z_2, z_4)$$

$$\equiv \Psi_4(z_1, \ldots, z_4). \tag{2.90}$$

The above derivation of $\Psi_2$ and $\Psi_4$ shows that $\Psi_{2N}$ can be derived by using (2.81).

We have

$$\int(\mathrm{d}z) = \sum_{\varepsilon=\pm 1}\int \mathrm{d}^3\mathbf{x}, \tag{2.91}$$

$$\int \mathrm{d}^3\mathbf{x}\ \psi_\alpha(\mathbf{x})\psi_\beta(\mathbf{x}) = \delta_{\alpha\beta}. \tag{2.92}$$

From (2.64) and by using (2.91), we obtain

$$
\begin{aligned}
&\int (\mathrm{d}z)(\mathrm{d}z')\; K(z)G(z,z')K(z') \\
&= \sum_{\varepsilon=\pm 1}\sum_{\varepsilon'=\pm 1}\int \mathrm{d}^3\mathbf{x}\int \mathrm{d}^3\mathbf{x}'\; K(z)\sum_{\alpha=0}^{k}\lambda_\alpha c_\alpha(\varepsilon)c_\alpha(\varepsilon')\psi_\alpha(\mathbf{x})\psi_\alpha(\mathbf{x}')K(z') \\
&= \sum_{\alpha=0}^{k}\lambda_\alpha\left[\left(\sum_{\varepsilon}\int \mathrm{d}^3\mathbf{x}\; c_\alpha(\varepsilon)K(z)\psi_\alpha(\mathbf{x})\right)\right. \\
&\qquad\qquad \left.\times\left(\sum_{\varepsilon'}\int \mathrm{d}^3\mathbf{x}'\; c_\alpha(\varepsilon')K(z')\psi_\alpha(\mathbf{x}')\right)\right] \\
&= \sum_{\alpha=0}^{k}\lambda_\alpha\left(\sum_{\varepsilon}c_\alpha(\varepsilon)\int \mathrm{d}^3\mathbf{x}\; K(z)\psi_\alpha(\mathbf{x})\right)^2 \\
&\equiv \sum_{\alpha=0}^{k}\lambda_\alpha K_\alpha^2
\end{aligned} \tag{2.93}
$$

where

$$K_\alpha = \sum_{\varepsilon=\pm 1}c_\alpha(\varepsilon)\int \mathrm{d}^3\mathbf{x}\; K(z)\psi_\alpha(\mathbf{x}). \tag{2.94}$$

Compare (2.93) with (2.80), then we obtain

$$F[K] = \exp\left(\frac{1}{2}\sum_{\alpha=0}^{k}\lambda_\alpha K_\alpha^2\right). \tag{2.95}$$

Let

$$\frac{\delta}{\delta K(z)} = \sum_{\alpha}\frac{\delta K_\alpha}{\delta K(z)}\frac{\delta}{\delta K_\alpha}. \tag{2.96}$$

From (2.94), we obtain

$$\frac{\delta K_\alpha}{\delta K(z)} = \frac{\delta}{\delta K(z)}\left(\sum_{\varepsilon'=\pm 1}c_\alpha(\varepsilon')\int \mathrm{d}^3\mathbf{x}'\; K(z')\psi_\alpha(\mathbf{x}')\right)$$

$$= \sum_{\varepsilon'=\pm 1} c_\alpha(\varepsilon') \int \mathrm{d}^3\mathbf{x'}\ \psi_\alpha(\mathbf{x'}) \frac{\delta K z'}{\delta K(z)}$$

$$= \sum_{\varepsilon'=\pm 1} c_\alpha(\varepsilon')\delta_{\epsilon,\epsilon'} \int \mathrm{d}^3\mathbf{x'}\ \psi_\alpha(\mathbf{x'})\delta(\mathbf{x}' - \mathbf{x})$$

$$= c_\alpha(\varepsilon)\psi_\alpha(\mathbf{x}). \tag{2.97}$$

Substitute (2.97) in (2.96), then we obtain

$$\frac{\delta}{\delta K(z)} = \sum_\alpha c_\alpha(\varepsilon)\psi_\alpha(\mathbf{x}) \frac{\delta}{\delta K_\alpha}. \tag{2.98}$$

By using (2.98), we consider

$$\int (\mathrm{d}z)\ \frac{\delta}{\delta K(z)} \frac{\delta}{\delta S(z)} = \sum_{\varepsilon=\pm 1} \int \mathrm{d}^3\mathbf{x}\ \sum_\alpha c_\alpha(\varepsilon)\psi_\alpha(\mathbf{x}) \frac{\delta}{\delta K_\alpha} \sum_\beta c_\beta(\varepsilon)\psi_\beta(\mathbf{x}) \frac{\delta}{\delta S_\beta}$$

$$= \sum_\varepsilon \sum_{\alpha,\beta} c_\alpha(\varepsilon)c_\beta(\varepsilon) \frac{\delta}{\delta K_\alpha} \frac{\delta}{\delta S_\beta} \int \mathrm{d}^3\mathbf{x}\ \psi_\alpha(\mathbf{x})\psi_\beta(\mathbf{x})$$

$$= \sum_\varepsilon \sum_{\alpha,\beta} c_\alpha(\varepsilon)c_\beta(\varepsilon) \frac{\delta}{\delta K_\alpha} \frac{\delta}{\delta S_\beta} \delta_{\alpha\beta}$$

$$= \sum_\varepsilon \sum_\alpha c_\alpha(\varepsilon)c_\alpha(\varepsilon) \frac{\delta}{\delta K_\alpha} \frac{\delta}{\delta S_\alpha}$$

$$= \sum_\alpha \left( \sum_\varepsilon |c_\alpha(\varepsilon)|^2 \right) \frac{\delta}{\delta K_\alpha} \frac{\delta}{\delta S_\alpha}$$

$$= \sum_\alpha c_\alpha^2 \frac{\delta}{\delta K_\alpha} \frac{\delta}{\delta S_\alpha}$$

$$= \sum_\alpha \frac{\delta}{\delta K_\alpha} \frac{\delta}{\delta S_\alpha} \tag{2.99}$$

where $c_\alpha^2 = 1$.

# A: Normalization of the Many-Particle Wavefunction

Consider $\|\Psi_{2N}\|^2$, from (2.81), we have

$$\begin{aligned}
\|\Psi_{2N}\|^2 &= \int(\mathrm{d}z_1)\cdots(\mathrm{d}z_{2N})\ \Psi^2_{2N}(z_1,\ldots,z_{2N}) \\
&= \int(\mathrm{d}z_1)\cdots(\mathrm{d}z_{2N})\ \frac{\delta}{\delta K(z_1)}\cdots\frac{\delta}{\delta K(z_{2N})}F[K]_0\frac{\delta}{\delta S(z_1)}\cdots\frac{\delta}{\delta S(z_{2N})}F[S]_0 \\
&= \int(\mathrm{d}z_1)\cdots(\mathrm{d}z_{2N})\left(\frac{\delta}{\delta K(z_1)}\frac{\delta}{\delta S(z_1)}\right)\cdots\left(\frac{\delta}{\delta K(z_{2N})}\frac{\delta}{\delta S(z_{2N})}\right)F[K]_0F[S]_0 \\
&= \left(\int(\mathrm{d}z)\ \frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)^{2N}F[K]_0F[S]_0. \qquad (2.100)
\end{aligned}$$

Multiply (2.100) by $\sum_{N=0}^{\infty}$ and $\frac{\lambda^{2N}}{(2N)!}$, we obtain

$$\begin{aligned}
\sum_{N=0}^{\infty}\frac{\lambda^{2N}}{(2N)!}\|\Psi_{2N}\|^2 &= \sum_{N=0}^{\infty}\left[\frac{1}{(2N)!}\left(\lambda\int(\mathrm{d}z)\ \frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)^{2N}\right]F[K]_0F[S]_0 \\
&\equiv \mathcal{N}(\lambda^2). \qquad (2.101)
\end{aligned}$$

Consider

$$\begin{aligned}
\sum_{N=0}^{\infty}\frac{X^{2N}}{(2N)!} &= \frac{X^0}{0!}+\frac{X^2}{2!}+\frac{X^4}{4!}+\cdots \\
&= \frac{1}{2}\left(\frac{X^0}{0!}+\frac{X^1}{1!}+\frac{X^2}{2!}+\cdots+\frac{X^0}{0!}-\frac{X^1}{1!}+\frac{X^2}{2!}-\cdots\right) \\
&= \frac{1}{2}\sum_{k=0}^{\infty}\left[\frac{(X)^k}{k!}+\frac{(-X)^k}{k!}\right] \\
&= \frac{1}{2}\left[\exp(X)+\exp(-X)\right]. \qquad (2.102)
\end{aligned}$$

Then, by comparing (2.102) with (2.101), we obtain

$$\mathcal{N}(\lambda^2) = \frac{1}{2}\left[\exp\left(\lambda\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)\right.$$

$$\left. + \exp\left(-\lambda\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)\right] F[K]_0 F[S]_0. \qquad (2.103)$$

Consider the 1st term in (2.103) without the coefficient $\frac{1}{2}$, by using (2.99) and (2.95), we obtain

$$\exp\left(\lambda\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right) F[K]F[S]$$

$$= \exp\left(\lambda\sum_{\alpha=0}^{k}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\alpha}\right)\exp\left(\frac{1}{2}\sum_{\alpha=0}^{k}\lambda_\alpha K_\alpha^2\right)\exp\left(\frac{1}{2}\sum_{\alpha=0}^{k}\lambda_\alpha S_\alpha^2\right) \qquad (2.104)$$

where $K \to 0$, $S \to 0$. From Lemma 2.1.2, we rewrite Eq. (2.104) as

$$\exp\left(\lambda\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right) F[K]F[S]$$

$$= \left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\exp\left[\sum_{\alpha=0}^{k}\frac{K_\alpha^2\lambda_\alpha}{2\,(1-\lambda^2\lambda_\alpha^2)}\right]$$

$$\times \exp\left[\sum_{\alpha=0}^{k}\frac{S_\alpha^2\lambda_\alpha}{2\,(1-\lambda^2\lambda_\alpha^2)}\right]\exp\left[\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right]. \qquad (2.105)$$

From (2.94), we obtain

$$\lim_{K\to 0} K_\alpha = 0 \qquad (2.106a)$$

$$\lim_{S\to 0} S_\alpha = 0 \qquad (2.106b)$$

then Eq. (2.105) becomes

$$\exp\left(\lambda\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)F[K]_0F[S]_0=\prod_{\alpha=0}^{k}\left(\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right). \tag{2.107}$$

Consider the $2^{\mathrm{nd}}$ term in (2.103) without $\dfrac{1}{2}$ :

$$\exp\left(-\lambda\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)F[K]F[S]$$

$$=\exp\left(-\lambda\sum_{\alpha=0}^{k}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\alpha}\right)\exp\left(\frac{1}{2}\sum_{\alpha=0}^{k}\lambda_\alpha K_\alpha^2\right)\exp\left(\frac{1}{2}\sum_{\alpha=0}^{k}\lambda_\alpha S_\alpha^2\right) \tag{2.108}$$

where $K\to 0$, $S\to 0$. From Lemma 2.1.2, Eq. (2.108) becomes

$$\exp\left(-\lambda\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)F[K]F[S]$$

$$=\left[\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-(-\lambda)^2\lambda_\alpha^2}}\right]\exp\left[\sum_{\alpha=0}^{k}\frac{K_\alpha^2\lambda_\alpha}{2\left(1-(-\lambda)^2\lambda_\alpha^2\right)}\right]$$

$$\times\exp\left[\sum_{\alpha=0}^{k}\frac{S_\alpha^2\lambda_\alpha}{2\left(1-(-\lambda)^2\lambda_\alpha^2\right)}\right]\exp\left[\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2(-\lambda)S_\alpha K_\alpha}{\left(1-(-\lambda)^2\lambda_\alpha^2\right)}\right]. \tag{2.109}$$

From (2.106), we obtain

$$\exp\left(-\lambda\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)F[K]_0F[S]_0=\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}. \tag{2.110}$$

Then from (2.107) and (2.110), we obtain (2.103) as below

$$\mathcal{N}(\lambda^2)=\frac{1}{2}\left[\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}+\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right]$$

$$=\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}. \tag{2.111}$$

## B: The Potential Energy

Consider the interaction term $\left\langle \Psi_{2N} \middle| \sum_{i<j} V(z_i, z_j) \middle| \Psi_{2N} \right\rangle$, where

$$\sum_{i<j} V(z_i, z_j) = \sum_{i<j} \frac{e^2 \varepsilon_i \varepsilon_j}{|\mathbf{x}_i - \mathbf{x}_j|}. \tag{2.112}$$

Then, we have

$$\begin{aligned}
\left\langle \Psi_{2N} \middle| \sum_{i<j} V(z_i, z_j) \middle| \Psi_{2N} \right\rangle &= \int (\mathrm{d}z_1) \cdots (\mathrm{d}z_{2N}) \sum_{i<j} V(z_i, z_j) \Psi_{2N}^2(z_1, \ldots, z_{2N}) \\
&= \int (\mathrm{d}z_1) \cdots (\mathrm{d}z_{2N}) \frac{\delta}{\delta K(z_1)} \cdots \frac{\delta}{\delta K(z_{2N})} F[K]_0 \\
&\quad \times \frac{\delta}{\delta S(z_1)} \cdots \frac{\delta}{\delta S(z_{2N})} F[S]_0 \sum_{i<j} V(z_i, z_j). \qquad (2.113)
\end{aligned}$$

Consider the elements $a_{ij}$ of arbitrary matrix $A$ of $(2N \times 2N)$:

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1(2N)} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2(2N)} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{(2N)1} & a_{(2N)2} & a_{(2N)3} & \cdots & a_{(2N)(2N)} \end{pmatrix}. \tag{2.114}$$

From above definition, it is obviously shown that number of elements of $A$ is $(2N)^2$. Number of diagonal elements; $n(i=j)$; is $(2N)$ and number of $(i<j)$ elements; $n(i<j)$; is equal to number of $(i>j)$ elements; $n(i>j)$.

$$\begin{aligned}
(2N)^2 &= n(i<j) + n(i>j) + n(i=j) \\
&= 2n(i<j) + (2N) \qquad (2.115)
\end{aligned}$$

then number of elements where $i < j$ is

$$n(i<j) = \frac{(2N)^2 - 2N}{2} = N(2N-1). \tag{2.116}$$

By using (2.116), we can rewrite (2.113) as below

$$\left\langle \Psi_{2N} \left| \sum_{i<j} V(z_i, z_j) \right| \Psi_{2N} \right\rangle$$

$$= \int (\mathrm{d}z_1) \cdots (\mathrm{d}z_{2N}) \, \frac{\delta}{\delta K(z_1)} \frac{\delta}{\delta S(z_1)} \cdots \frac{\delta}{\delta K(z_{2N})} \frac{\delta}{\delta S(z_{2N})}$$

$$\times \sum_{i<j} V(z_i, z_j) F[K]_0 F[S]_0$$

$$= N(2N-1) \int (\mathrm{d}z)(\mathrm{d}z') \, \frac{\delta}{\delta K(z)} \frac{\delta}{\delta S(z)} V(z, z') \frac{\delta}{\delta K(z')} \frac{\delta}{\delta S(z')}$$

$$\times \left( \int (\mathrm{d}z) \, \frac{\delta}{\delta K(z)} \frac{\delta}{\delta S(z)} \right)^{2N-2} F[K]_0 F[S]_0. \tag{2.117}$$

Multiply (2.117) by $\sum_{N=0}^{\infty} \frac{\lambda^{2N}}{(2N)!} \Theta(N-1)$, where $\Theta(N-1)$ is the unit step function, we obtain

$$\sum_{N=0}^{\infty} \frac{\lambda^{2N}}{(2N)!} \left\langle \Psi_{2N} \left| \sum_{i<j} V(z_i, z_j) \right| \Psi_{2N} \right\rangle \Theta(N-1)$$

$$= \int (\mathrm{d}z)(\mathrm{d}z') \, \frac{\delta}{\delta K(z)} \frac{\delta}{\delta S(z)} V(z, z') \frac{\delta}{\delta K(z')} \frac{\delta}{\delta S(z')}$$

$$\times \sum_{N=0}^{\infty} \frac{N(2N-1)\lambda^{2N}}{(2N)!} \left( \int (\mathrm{d}z) \, \frac{\delta}{\delta K(z)} \frac{\delta}{\delta S(z)} \right)^{2N-2}$$

$$\Theta(N-1) F[K]_0 F[S]_0$$

$$\equiv \mathcal{V}(\lambda^2). \tag{2.118}$$

Let

$$u=\sum_{N=0}^{\infty}\frac{N(2N-1)\lambda^{2N}}{(2N)!}\left(\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)^{2N-2}\Theta(N-1) \tag{2.119}$$

and

$$m=N-1, \tag{2.120}$$

$$N=m+1. \tag{2.121}$$

Substitute (2.120) and (2.121) in (2.119), then we obtain

$$\begin{aligned}u&=\sum_{m=0}^{\infty}N(2N-1)\frac{\lambda^{2(m+1)}}{(2N)(2N-1)(2N-2)!}\left(\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)^{2m}\\&=\sum_{m=0}^{\infty}N(2N-1)\frac{\lambda^{2m}\lambda^{2}}{(2N)(2N-1)(2m)!}\left(\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)^{2m}\\&=\frac{\lambda^2}{2}\sum_{m=0}^{\infty}\frac{1}{(2m)!}\left(\lambda\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)^{2m}.\end{aligned} \tag{2.122}$$

Compare (2.122) with (2.102), then we obtain

$$u=\frac{\lambda^2}{2}\cdot\frac{1}{2}\left[\exp\left(\lambda\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)+\exp\left(-\lambda\int(\mathrm{d}z)\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)\right]. \tag{2.123}$$

Substitute $u$ from (2.123) in (2.118), we obtain

$$\begin{aligned}\mathcal{V}(\lambda^2)&=\frac{\lambda^2}{2}\int(\mathrm{d}z)(\mathrm{d}z')\,\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}V(z,z')\frac{\delta}{\delta K(z')}\frac{\delta}{\delta S(z')}\\&\times\frac{1}{2}\left[\exp\left(\lambda\int(\mathrm{d}z)\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)+\exp\left(-\lambda\int(\mathrm{d}z)\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)\right]F[K]_0F[S]_0.\end{aligned} \tag{2.124}$$

From (2.105) and (2.109), Eq. (2.124) becomes

$$
\begin{aligned}
\mathcal{V}(\lambda^2) = {} & \frac{\lambda^2}{2}\int (\mathrm{d}z)(\mathrm{d}z')\ \frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}V(z,z')\frac{\delta}{\delta K(z')}\frac{\delta}{\delta S(z')} \\
& \times \frac{1}{2}\left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\exp\left(\sum_{\alpha=0}^{k}\frac{K_\alpha^2\lambda_\alpha}{2\,(1-\lambda^2\lambda_\alpha^2)}\right)\exp\left(\sum_{\alpha=0}^{k}\frac{S_\alpha^2\lambda_\alpha}{2\,(1-\lambda^2\lambda_\alpha^2)}\right) \\
& \times \left[\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)+\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2(-\lambda)S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)\right] \\
= {} & \frac{\lambda^2}{2}\int (\mathrm{d}z)(\mathrm{d}z')\ \frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}V(z,z')\frac{\delta}{\delta K(z')}\frac{\delta}{\delta S(z')} \\
& \quad \times \frac{1}{2}\left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\exp\left(\sum_{\alpha=0}^{k}\frac{K_\alpha^2\lambda_\alpha+S_\alpha^2\lambda_\alpha}{2\,(1-\lambda^2\lambda_\alpha^2)}\right) \\
& \quad \times \left[\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)+\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2(-\lambda)S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)\right]
\end{aligned}
\tag{2.125}
$$

where $K_\alpha, S_\alpha \to 0$.

Consider the integral in (2.125), by using (2.91) and (2.98), we obtain

$$
\begin{aligned}
& \int (\mathrm{d}z)(\mathrm{d}z')\ \frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}V(z,z')\frac{\delta}{\delta K(z')}\frac{\delta}{\delta S(z')} \\
& \qquad = \sum_{\varepsilon=\pm1}\int \mathrm{d}^3\mathbf{x}\sum_{\varepsilon'=\pm1}\int \mathrm{d}^3\mathbf{x'}\sum_{\alpha=0}^{k}c_\alpha(\varepsilon)\psi_\alpha(\mathbf{x})\frac{\delta}{\delta K_\alpha}\sum_{\beta=0}^{k}c_\beta(\varepsilon)\psi_\beta(\mathbf{x})\frac{\delta}{\delta S_\beta} \\
& \qquad\quad \times V(\mathbf{x},\varepsilon,\mathbf{x}',\varepsilon')\sum_{\alpha'=0}^{k}c_{\alpha'}(\varepsilon')\psi_{\alpha'}(\mathbf{x}')\frac{\delta}{\delta K_{\alpha'}}\sum_{\beta'=0}^{k}c_{\beta'}(\varepsilon')\psi_{\beta'}(\mathbf{x}')\frac{\delta}{\delta S_{\beta'}} \\
& \qquad = \sum_{\varepsilon,\varepsilon'}\sum_{\substack{\alpha,\beta\\ \alpha',\beta'}}c_\alpha(\varepsilon)c_\beta(\varepsilon)c_{\alpha'}(\varepsilon')c_{\beta'}(\varepsilon')\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}}
\end{aligned}
$$

$$\times \int d^3\mathbf{x}\, d^3\mathbf{x}'\ \psi_\alpha(\mathbf{x})\psi_\beta(\mathbf{x})V(\mathbf{x},\varepsilon,\mathbf{x}',\varepsilon')\psi_{\alpha'}(\mathbf{x}')\psi_{\beta'}(\mathbf{x}') \tag{2.126}$$

where

$$V(\mathbf{x},\varepsilon,\mathbf{x}',\varepsilon') = \frac{e^2\varepsilon\varepsilon'}{|\mathbf{x}-\mathbf{x}'|}. \tag{2.127}$$

Substitute (2.127) in (2.126), then we obtain

$$\int (dz)(dz')\ \frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}V(z,z')\frac{\delta}{\delta K(z')}\frac{\delta}{\delta S(z')}$$

$$= \sum_{\substack{\alpha,\beta\\ \alpha',\beta'}}\sum_{\varepsilon,\varepsilon'} \varepsilon c_\alpha(\varepsilon)c_\beta(\varepsilon) \int d^3\mathbf{x}\, d^3\mathbf{x}'\ \psi_\alpha(\mathbf{x})\psi_\beta(\mathbf{x})\frac{e^2}{|\mathbf{x}-\mathbf{x}'|}$$

$$\times\ \varepsilon' c_{\alpha'}(\varepsilon')c_{\beta'}(\varepsilon')\psi_{\alpha'}(\mathbf{x}')\psi_{\beta'}(\mathbf{x}')\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}} \tag{2.128}$$

where we use (2.73), i.e.,

$$\sum_{\varepsilon=\pm1}\varepsilon c_\alpha(\varepsilon)c_\beta(\varepsilon) = \begin{cases} 1, & \alpha=0,\ \beta\neq 0 \quad \text{or} \quad \alpha\neq 0,\ \beta=0 \\ 0, & \text{otherwise.}\end{cases} \tag{2.129}$$

Multiply (2.129) by $\sum_{\varepsilon'=\pm1}\varepsilon' c_{\alpha'}(\varepsilon')c_{\beta'}(\varepsilon')$, we obtain

$$\sum_{\varepsilon,\varepsilon'}\varepsilon c_\alpha(\varepsilon)c_\beta(\varepsilon)\varepsilon' c_{\alpha'}(\varepsilon')c_{\beta'}(\varepsilon')$$

$$= \Big[\delta_{\alpha 0}(1-\delta_{\beta 0}) + (1-\delta_{\alpha 0})\delta_{\beta 0}\Big]\ \Big[\delta_{\alpha' 0}(1-\delta_{\beta' 0}) + (1-\delta_{\alpha' 0})\delta_{\beta' 0}\Big]. \tag{2.130}$$

Consider the right-hand side of (2.128), by using the (2.130), we obtain

$$\sum_{\varepsilon,\varepsilon'}\varepsilon c_\alpha(\varepsilon)c_\beta(\varepsilon)\varepsilon' c_{\alpha'}(\varepsilon')c_{\beta'}(\varepsilon')$$

$$\times \int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \psi_\alpha(\mathbf{x})\psi_\beta(\mathbf{x})\frac{e^2}{|\mathbf{x}-\mathbf{x}'|}\psi_{\alpha'}(\mathbf{x}')\psi_{\beta'}(\mathbf{x}')\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}}$$

$$= \Big[\delta_{\alpha 0}(1-\delta_{\beta 0}) + (1-\delta_{\alpha 0})\delta_{\beta 0}\Big]\ \Big[\delta_{\alpha' 0}(1-\delta_{\beta' 0}) + (1-\delta_{\alpha' 0})\delta_{\beta' 0}\Big]$$

$$\times I_{\alpha\beta,\alpha'\beta'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}}$$

$$= \Big[\delta_{\alpha 0}(1-\delta_{\beta 0})\delta_{\alpha' 0}(1-\delta_{\beta' 0}) + \delta_{\alpha 0}(1-\delta_{\beta 0})(1-\delta_{\alpha' 0})\delta_{\beta' 0}$$

$$+(1-\delta_{\alpha 0})\delta_{\beta 0}\delta_{\alpha' 0}(1-\delta_{\beta' 0}) + (1-\delta_{\alpha 0})\delta_{\beta 0}(1-\delta_{\alpha' 0})\delta_{\beta' 0}\Big]$$

$$\times I_{\alpha\beta,\alpha'\beta'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}}$$

$$= \Big[\delta_{\alpha 0}(1-\delta_{\beta 0})\delta_{\alpha' 0}(1-\delta_{\beta' 0}) + \delta_{\alpha 0}(1-\delta_{\beta 0})(1-\delta_{\alpha' 0})\delta_{\beta' 0}$$

$$+(1-\delta_{\alpha 0})\delta_{\beta 0}\delta_{\alpha' 0}(1-\delta_{\beta' 0}) + (1-\delta_{\alpha 0})\delta_{\beta 0}(1-\delta_{\alpha' 0})\delta_{\beta' 0}\Big]$$

$$\times I_{\alpha\beta,\alpha'\beta'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}} \tag{2.131}$$

where

$$I_{\alpha\beta,\alpha'\beta'} = \int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\ \psi_\alpha(\mathbf{x})\psi_\beta(\mathbf{x})\frac{e^2}{|\mathbf{x}-\mathbf{x}'|}\psi_{\alpha'}(\mathbf{x}')\psi_{\beta'}(\mathbf{x}'). \tag{2.132}$$

Multiply (2.131) by $\sum_{\alpha,\beta}\sum_{\alpha',\beta'}$, we obtain

$$\sum_{\substack{\alpha,\beta\\ \alpha',\beta'}}\sum_{\varepsilon,\varepsilon'}\varepsilon c_\alpha(\varepsilon)c_\beta(\varepsilon)\varepsilon' c_{\alpha'}(\varepsilon')c_{\beta'}(\varepsilon')I_{\alpha\beta,\alpha'\beta'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}}$$

$$= \sum_{\substack{\alpha,\beta\\ \alpha',\beta'}}\delta_{\alpha 0}(1-\delta_{\beta 0})\delta_{\alpha' 0}(1-\delta_{\beta' 0})I_{\alpha\beta,\alpha'\beta'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}}$$

$$+\sum_{\substack{\alpha,\beta\\ \alpha',\beta'}}\delta_{\alpha 0}(1-\delta_{\beta 0})(1-\delta_{\alpha' 0})\delta_{\beta' 0}I_{\alpha\beta,\alpha'\beta'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}}$$

$$+\sum_{\substack{\alpha,\beta\\ \alpha',\beta'}}(1-\delta_{\alpha 0})\delta_{\beta 0}\delta_{\alpha' 0}(1-\delta_{\beta' 0})I_{\alpha\beta,\alpha'\beta'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}}$$

$$+\sum_{\substack{\alpha,\beta\\ \alpha',\beta'}}(1-\delta_{\alpha 0})\delta_{\beta 0}(1-\delta_{\alpha' 0})\delta_{\beta' 0}I_{\alpha\beta,\alpha'\beta'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}}$$

$$=\sum_{\beta=1}^{k}\sum_{\beta'=1}^{k}I_{0\beta,0\beta'}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}+\sum_{\beta=1}^{k}\sum_{\alpha'=1}^{k}I_{0\beta,\alpha'0}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_0}$$

$$+\sum_{\alpha=1}^{k}\sum_{\beta'=1}^{k}I_{\alpha 0,0\beta'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}+\sum_{\alpha=1}^{k}\sum_{\alpha'=1}^{k}I_{\alpha 0,\alpha' 0}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_0}. \tag{2.133}$$

From (2.30), we can write

$$I_{\alpha\beta,\alpha'\beta'}=I_{\beta\alpha,\alpha'\beta'}, \tag{2.134}$$

$$I_{\alpha\beta,\alpha'\beta'}=I_{\alpha\beta,\beta'\alpha'}. \tag{2.135}$$

By using (2.134) and (2.135), Eq. (2.133) becomes

$$\sum_{\substack{\alpha,\beta\\ \alpha',\beta'}}\sum_{\varepsilon,\varepsilon'}\varepsilon c_\alpha(\varepsilon)c_\beta(\varepsilon)\varepsilon' c_{\alpha'}(\varepsilon')c_{\beta'}(\varepsilon')I_{\alpha\beta,\alpha'\beta'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}}$$

$$=\sum_{\beta=1}^{k}\sum_{\beta'=1}^{k}I_{0\beta,0\beta'}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}+\sum_{\beta=1}^{k}\sum_{\alpha'=1}^{k}I_{0\beta,0\alpha'}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_0}$$

$$+\sum_{\alpha=1}^{k}\sum_{\beta'=1}^{k}I_{0\alpha,0\beta'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}+\sum_{\alpha=1}^{k}\sum_{\alpha'=1}^{k}I_{0\alpha,0\alpha'}\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_0}$$

$$= \sum_{\beta=1}^{k}\sum_{\beta'=1}^{k} I_{0\beta,0\beta'} \frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}} + \sum_{\beta=1}^{k}\sum_{\beta'=1}^{k} I_{0\beta,0\beta'} \frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\beta'}}\frac{\delta}{\delta S_0}$$

$$+ \sum_{\beta=1}^{k}\sum_{\beta'=1}^{k} I_{0\beta,0\beta'} \frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}} + \sum_{\beta=1}^{k}\sum_{\beta'=1}^{k} I_{0\beta,0\beta'} \frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_{\beta'}}\frac{\delta}{\delta S_0}$$

$$= \sum_{\beta=1}^{k}\sum_{\beta'=1}^{k} I_{0\beta,0\beta'} \left\{ \frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}} + \frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\beta'}}\frac{\delta}{\delta S_0} \right.$$

$$\left. + \frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}} + \frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_{\beta'}}\frac{\delta}{\delta S_0} \right\}. \tag{2.136}$$

We use the symmetric property of $K_\alpha$ and $S_\alpha$ to obtain

$$\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}} = \frac{\delta}{\delta S_0}\frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_{\beta'}} = \frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_{\beta'}}\frac{\delta}{\delta S_0} \tag{2.137}$$

$$\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\beta'}}\frac{\delta}{\delta S_0} = \frac{\delta}{\delta S_0}\frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_{\beta'}}\frac{\delta}{\delta K_0} = \frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}. \tag{2.138}$$

Substitute (2.137) and (2.138) in (2.136), then we obtain

$$\sum_{\substack{\alpha,\beta \\ \alpha',\beta'}}\sum_{\varepsilon,\varepsilon'} \varepsilon c_\alpha(\varepsilon) c_\beta(\varepsilon) \varepsilon' c_{\alpha'}(\varepsilon') c_{\beta'}(\varepsilon') I_{\alpha\beta,\alpha'\beta'} \frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_{\alpha'}}\frac{\delta}{\delta S_{\beta'}}$$

$$= 2\sum_{\beta=1}^{k}\sum_{\beta'=1}^{k} I_{0\beta,0\beta'} \left[ \frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}} + \frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}} \right]$$

$$= 2\sum_{\beta=1}^{k}\sum_{\beta'=1}^{k} I_{0\beta,0\beta'} \left[ \frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta} + \frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0} \right] \frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}. \tag{2.139}$$

Substitute (2.139) in (2.126), then we rewrite (2.125) as below

$$\mathcal{V}(\lambda^2) = \lambda^2 \sum_{\beta=1}^{k}\sum_{\beta'=1}^{k} I_{0\beta,0\beta'} \left( \prod_{\alpha=0}^{k} \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \right)$$

$$\times \frac{1}{2}\left[\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}+\frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\right]\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}\exp\sum_{\alpha=0}^{k}\left(\frac{K_\alpha^2\lambda_\alpha+S_\alpha^2\lambda_\alpha}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right)$$

$$\times\left[\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)+\exp\left(\sum_{\alpha=0}^{k}\frac{-\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)\right] \tag{2.140}$$

where $K_\alpha, S_\alpha \to 0$.

Let

$$A=\exp\sum_{\alpha=0}^{k}\left(\frac{K_\alpha^2\lambda_\alpha+S_\alpha^2\lambda_\alpha}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right)$$

$$\times\left\{\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)+\exp\left(\sum_{\alpha=0}^{k}\frac{-\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)\right\} \tag{2.141}$$

and

$$B=\exp\sum_{\alpha=0}^{k}\left(\frac{K_\alpha^2\lambda_\alpha+S_\alpha^2\lambda_\alpha}{2\left(1-\lambda^2\lambda_\alpha^2\right)}\right)$$

$$\times\left\{\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)-\exp\left(\sum_{\alpha=0}^{k}\frac{-\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)\right\}. \tag{2.142}$$

Substitute (2.141) in (2.140), then we obtain

$$\mathcal{V}(\lambda^2)=\frac{\lambda^2}{2}\sum_{\beta=1}^{k}\sum_{\beta'=1}^{k}I_{0\beta,0\beta'}\left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)$$

$$\times\left[\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}+\frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\right]\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}A. \tag{2.143}$$

We use the functional derivative, for $X \neq Y$,

$$\frac{\delta X_\alpha}{\delta X_{\alpha'}}=\delta_{\alpha\alpha'},\quad \frac{\delta Y_\alpha}{\delta X_\alpha}=0 \tag{2.144}$$

to obtain $\dfrac{\delta A}{\delta S_{\beta'}}$, which is given by

$$\frac{\delta A}{\delta S_{\beta'}} = \frac{\delta}{\delta S_{\beta'}}\left[\exp\sum_{\alpha=0}^{k}\left(\frac{K_\alpha^2\lambda_\alpha + S_\alpha^2\lambda_\alpha}{2\,(1-\lambda^2\lambda_\alpha^2)}\right)\right]$$

$$\times\left\{\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)+\exp\left(\sum_{\alpha=0}^{k}\frac{-\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)\right\}$$

$$+\exp\sum_{\alpha=0}^{k}\left(\frac{K_\alpha^2\lambda_\alpha + S_\alpha^2\lambda_\alpha}{2\,(1-\lambda^2\lambda_\alpha^2)}\right)$$

$$\times\frac{\delta}{\delta S_{\beta'}}\left\{\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)+\exp\left(\sum_{\alpha=0}^{k}\frac{-\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)\right\}. \tag{2.145}$$

Consider the first term in above equation,

$$\frac{\delta}{\delta S_{\beta'}}\exp\sum_{\alpha=0}^{k}\left(\frac{K_\alpha^2\lambda_\alpha + S_\alpha^2\lambda_\alpha}{2\,(1-\lambda^2\lambda_\alpha^2)}\right) = \frac{\lambda_{\beta'}S_{\beta'}}{(1-\lambda^2\lambda_{\beta'}^2)}\exp\sum_{\alpha=0}^{k}\left(\frac{K_\alpha^2\lambda_\alpha + S_\alpha^2\lambda_\alpha}{2\,(1-\lambda^2\lambda_\alpha^2)}\right) \tag{2.146}$$

and the second term,

$$\frac{\delta}{\delta S_{\beta'}}\left\{\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)+\exp\left(\sum_{\alpha=0}^{k}\frac{-\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)\right\}$$

$$=\frac{\lambda\lambda_{\beta'}^2K_{\beta'}}{(1-\lambda^2\lambda_{\beta'}^2)}\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)-\frac{\lambda\lambda_{\beta'}^2K_{\beta'}}{(1-\lambda^2\lambda_{\beta'}^2)}\exp\left(\sum_{\alpha=0}^{k}\frac{-\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)$$

$$=\frac{\lambda\lambda_{\beta'}^2K_{\beta'}}{(1-\lambda^2\lambda_{\beta'}^2)}\left\{\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)-\exp\left(\sum_{\alpha=0}^{k}\frac{-\lambda_\alpha^2\lambda S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)\right\}. \tag{2.147}$$

Then, from (2.141), (2.146) and (2.147), we obtain

$$\frac{\delta}{\delta S_{\beta'}}A = \frac{\lambda_{\beta'}S_{\beta'}}{(1-\lambda^2\lambda_{\beta'}^2)}A + \frac{\lambda\lambda_{\beta'}^2K_{\beta'}}{(1-\lambda^2\lambda_{\beta'}^2)}B \tag{2.148}$$

where $A$ and $B$ are defined in (2.141) and (2.142), respectively.

Operate (2.148) by $\dfrac{\delta}{\delta K_0}$, where $\dfrac{\delta K_\alpha}{\delta K_0} = 0$, $\alpha = 1, 2, \ldots, k$, then we obtain

$$\begin{aligned}
\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}A &= \frac{\delta}{\delta K_0}\left\{\frac{\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)}A + \frac{\lambda\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)}B\right\} \\
&= \frac{\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)}\frac{\delta}{\delta K_0}A + \left(\frac{\delta}{\delta K_0}\frac{\lambda\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)}\right)B \\
&\quad + \frac{\lambda\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)}\frac{\delta}{\delta K_0}B
\end{aligned} \tag{2.149}$$

where

$$\frac{\delta}{\delta K_0}A = \frac{\lambda_0K_0}{(1-\lambda^2\lambda_0^2)}A + \frac{\lambda\lambda_0^2S_0}{(1-\lambda^2\lambda_0^2)}B, \tag{2.150}$$

$$\frac{\delta}{\delta K_0}\frac{\lambda\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)} = 0, \tag{2.151}$$

$$\frac{\delta}{\delta K_0}B = \frac{\lambda_0K_0}{(1-\lambda^2\lambda_0^2)}B + \frac{\lambda\lambda_0^2S_0}{(1-\lambda^2\lambda_0^2)}A. \tag{2.152}$$

Substitute (2.150), (2.151) and (2.152) in (2.149), we obtain

$$\begin{aligned}
\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}A &= \frac{\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)}\left\{\frac{\lambda_0K_0}{(1-\lambda^2\lambda_0^2)}A + \frac{\lambda\lambda_0^2S_0}{(1-\lambda^2\lambda_0^2)}B\right\} \\
&\quad + \frac{\lambda\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)}\left\{\frac{\lambda_0K_0}{(1-\lambda^2\lambda_0^2)}B + \frac{\lambda\lambda_0^2S_0}{(1-\lambda^2\lambda_0^2)}A\right\} \\
&= \frac{\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)}\frac{\lambda_0K_0}{(1-\lambda^2\lambda_0^2)}A + \frac{\lambda\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)}\frac{\lambda\lambda_0^2S_0}{(1-\lambda^2\lambda_0^2)}A \\
&\quad + \frac{\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)}\frac{\lambda\lambda_0^2S_0}{(1-\lambda^2\lambda_0^2)}B + \frac{\lambda\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)}\frac{\lambda_0K_0}{(1-\lambda^2\lambda_0^2)}B \\
&= \frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)(1-\lambda^2\lambda_0^2)}A
\end{aligned}$$

$$+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2 K_0 K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'} S_0 S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}B$$

$$\equiv C \tag{2.153}$$

where

$$C=\frac{\left(\lambda_0\lambda_{\beta'} K_0 S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2 K_{\beta'} S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}A+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2 K_0 K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'} S_0 S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}B. \tag{2.154}$$

From (2.153) and (2.154), Eq. (2.143) becomes

$$\mathcal{V}(\lambda^2)=\frac{\lambda^2}{2}\sum_{\beta=1}^{k}\sum_{\beta'=1}^{k} I_{0\beta,0\beta'}\left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\left[\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}+\frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\right]C. \tag{2.155}$$

Operate $C$ by $\dfrac{\delta}{\delta S_\beta}$, where $\beta=1,2,\ldots,k$ then $\dfrac{\delta S_0}{\delta S_\beta}=0$, we obtain

$$\begin{aligned}
\frac{\delta}{\delta S_\beta}C &= \frac{\delta}{\delta S_\beta}\left\{\frac{\left(\lambda_0\lambda_{\beta'} K_0 S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2 K_{\beta'} S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}A\right.\\
&\qquad\left.+\quad\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2 K_0 K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'} S_0 S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}B\right\}\\
&= \frac{\delta}{\delta S_\beta}\left[\frac{\left(\lambda_0\lambda_{\beta'} K_0 S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2 K_{\beta'} S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]A\\
&\qquad+\left[\frac{\left(\lambda_0\lambda_{\beta'} K_0 S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2 K_{\beta'} S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]\frac{\delta}{\delta S_\beta}A\\
&\qquad+\frac{\delta}{\delta S_\beta}\left[\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2 K_0 K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'} S_0 S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]B\\
&\qquad+\left[\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2 K_0 K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'} S_0 S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]\frac{\delta}{\delta S_\beta}B
\end{aligned} \tag{2.156}$$

where

$$\frac{\delta}{\delta S_\beta}\left[\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]=\frac{\left(\lambda_0\lambda_{\beta'}K_0\frac{\delta}{\delta S_\beta}S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}\frac{\delta}{\delta S_\beta}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}$$

$$=\frac{\lambda_0\lambda_{\beta'}K_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}, \tag{2.157}$$

$$\frac{\delta A}{\delta S_\beta}=\frac{\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}A+\frac{\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}B, \tag{2.158}$$

$$\frac{\delta}{\delta S_\beta}\left[\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]=\frac{\lambda\lambda_0^2\lambda_{\beta'}\frac{\delta S_0}{\delta S_\beta}S_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0\frac{\delta S_{\beta'}}{\delta S_\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}$$

$$=\frac{\lambda\lambda_0^2\lambda_{\beta'}S_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}, \tag{2.159}$$

$$\frac{\delta B}{\delta S_\beta}=\frac{\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}B+\frac{\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}A. \tag{2.160}$$

Substitute the results from (2.157)–(2.160) in (2.156), we obtain

$$\begin{aligned}\frac{\delta}{\delta S_\beta}C=&\frac{\lambda_0\lambda_{\beta'}K_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}A\\&+\left[\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]\left[\frac{\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}A+\frac{\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}B\right]\\&+\frac{\lambda\lambda_0^2\lambda_{\beta'}S_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}B\\&+\left[\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]\left[\frac{\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}B+\frac{\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}A\right]\\=&\frac{\lambda_0\lambda_{\beta'}K_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}A\end{aligned}$$

$$+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}A$$

$$+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}B$$

$$+\frac{\lambda\lambda_0^2\lambda_{\beta'}S_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}B$$

$$+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}B$$

$$+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}A. \tag{2.161}$$

Rewrite (2.161), we obtain

$$\begin{aligned}\frac{\delta}{\delta S_\beta}C=&\left\{\frac{\lambda_0\lambda_{\beta'}K_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\right.\\&\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\right\}A\\&+\left\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\right.\\&\left.+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\right\}B.\end{aligned} \tag{2.162}$$

Operate (2.162) by $\frac{\delta}{\delta K_0}$ where $\frac{\delta K_\beta}{\delta K_0}=0$, then we obtain

$$\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}C$$

$$=\frac{\delta}{\delta K_0}\left\{\frac{\lambda_0\lambda_{\beta'}K_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\right.$$

$$+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\Bigg\}A$$

$$+\Bigg\{\frac{\lambda_0\lambda_{\beta'}K_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\Bigg\}\frac{\delta A}{\delta K_0}$$

$$+\frac{\delta}{\delta K_0}\Bigg\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\Bigg\}B$$

$$+\Bigg\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\Bigg\}\frac{\delta B}{\delta K_0}$$

$$=\Bigg\{\frac{\lambda_0\lambda_{\beta'}\frac{\delta K_0}{\delta K_0}\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}\frac{\delta K_0}{\delta K_0}S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2\frac{\delta K_{\beta'}}{\delta K_0}S_0\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2\frac{\delta K_0}{\delta K_0}K_{\beta'}\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_\beta^2\frac{\delta K_\beta}{\delta K_0}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\Bigg\}A$$

$$+\Bigg\{\frac{\lambda_0\lambda_{\beta'}K_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\Bigg\}\frac{\delta A}{\delta K_0}$$

$$+\Bigg\{\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2\frac{\delta K_0}{\delta K_0}K_{\beta'}\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+\frac{\left(\lambda_0\lambda_{\beta'}\frac{\delta K_0}{\delta K_0}S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2\frac{\delta K_{\beta'}}{\delta K_0}S_0\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_\beta^2\frac{\delta K_\beta}{\delta K_0}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\Bigg\}B$$

$$+\Bigg\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\Bigg\}\frac{\delta B}{\delta K_0}$$

$$=\Bigg\{\frac{\lambda_0\lambda_{\beta'}\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}S_{\beta'}+0\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_{\beta'}\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}+0\Bigg\}A$$

$$+\Bigg\{\frac{\lambda_0\lambda_{\beta'}K_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\Bigg\}\frac{\delta A}{\delta K_0}$$

$$+\Bigg\{\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_{\beta'}\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}$$

$$+ \frac{\left(\lambda_0 \lambda_{\beta'} S_{\beta'} + 0\right) \lambda \lambda_\beta^2 K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)} + 0 \Bigg\} B$$

$$+ \left\{ \frac{\lambda \lambda_0^2 \lambda_{\beta'} S_0 \delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)} + \frac{\left(\lambda\lambda_0\lambda_{\beta'}^2 K_0 K_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'} S_0 S_{\beta'}\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)} \right.$$

$$\left. + \frac{\left(\lambda_0\lambda_{\beta'} K_0 S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2 K_{\beta'} S_0\right)\lambda\lambda_\beta^2 K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)} \right\} \frac{\delta B}{\delta K_0}$$

$$= \left\{ \frac{\lambda_0\lambda_{\beta'}\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)} + \frac{\left(\lambda_0\lambda_\beta\lambda_{\beta'} S_\beta S_{\beta'} + \lambda^2\lambda_0\lambda_\beta^2\lambda_{\beta'}^2 K_{\beta'} K_\beta\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)} \right\} A$$

$$+ \left\{ \frac{\lambda_0\lambda_{\beta'} K_0 \delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)} + \frac{\left(\lambda_0\lambda_{\beta'} K_0 S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2 K_{\beta'} S_0\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)} \right.$$

$$\left. + \frac{\left(\lambda\lambda_0\lambda_{\beta'}^2 K_0 K_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'} S_0 S_{\beta'}\right)\lambda\lambda_\beta^2 K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)} \right\} \frac{\delta A}{\delta K_0}$$

$$+ \left\{ \frac{\left(\lambda\lambda_0\lambda_\beta\lambda_{\beta'}^2 K_{\beta'} S_\beta + \lambda\lambda_0\lambda_\beta^2\lambda_{\beta'} K_\beta S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)} \right\} B$$

$$+ \left\{ \frac{\lambda \lambda_0^2 \lambda_{\beta'} S_0 \delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)} + \frac{\left(\lambda\lambda_0\lambda_{\beta'}^2 K_0 K_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'} S_0 S_{\beta'}\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)} \right.$$

$$\left. + \frac{\left(\lambda_0\lambda_{\beta'} K_0 S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2 K_{\beta'} S_0\right)\lambda\lambda_\beta^2 K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)} \right\} \frac{\delta B}{\delta K_0} \tag{2.163}$$

where

$$\frac{\delta A}{\delta K_0} = \left\{ \frac{\lambda_0 K_0}{\left(1-\lambda^2\lambda_0^2\right)} A + \frac{\lambda\lambda_0^2 S_0}{\left(1-\lambda^2\lambda_0^2\right)} B \right\}, \tag{2.164}$$

$$\frac{\delta B}{\delta K_0} = \left\{ \frac{\lambda_0 K_0}{\left(1-\lambda^2\lambda_0^2\right)} B + \frac{\lambda\lambda_0^2 S_0}{\left(1-\lambda^2\lambda_0^2\right)} A \right\}. \tag{2.165}$$

Substitute (2.164) and (2.165) in (2.163), we obtain

$$
\begin{aligned}
&\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}C \\
&= \left\{\frac{\lambda_0\lambda_{\beta'}\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)} + \frac{\left(\lambda_0\lambda_\beta\lambda_{\beta'}S_\beta S_{\beta'} + \lambda^2\lambda_0\lambda_\beta^2\lambda_{\beta'}^2K_{\beta'}K_\beta\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\right\}A \\
&\quad + \left\{\frac{\lambda_0\lambda_{\beta'}K_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)} + \frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\right. \\
&\quad \left. + \frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\right\}\left\{\frac{\lambda_0K_0}{\left(1-\lambda^2\lambda_0^2\right)}A + \frac{\lambda\lambda_0^2S_0}{\left(1-\lambda^2\lambda_0^2\right)}B\right\} \\
&\quad + \left\{\frac{\left(\lambda\lambda_0\lambda_\beta\lambda_{\beta'}^2K_{\beta'}S_\beta + \lambda\lambda_0\lambda_\beta^2\lambda_{\beta'}K_\beta S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\right\}B \\
&\quad + \left\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_0\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)} + \frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_\beta S_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\right. \\
&\quad \left. + \frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_\beta^2K_\beta}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)\left(1-\lambda^2\lambda_\beta^2\right)}\right\}\left\{\frac{\lambda_0K_0}{\left(1-\lambda^2\lambda_0^2\right)}B + \frac{\lambda\lambda_0^2S_0}{\left(1-\lambda^2\lambda_0^2\right)}A\right\}.
\end{aligned}
\tag{2.166}
$$

Now, we will operate $C$, from (2.153), by $\frac{\delta}{\delta S_0}$ where $\frac{\delta S_\beta}{\delta S_0} = \frac{\delta S_{\beta'}}{\delta S_0} = 0$ for $\beta, \beta' = 1, 2, \ldots, k$, we obtain

$$
\begin{aligned}
\frac{\delta C}{\delta S_0} &= \frac{\delta}{\delta S_0}\left\{\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}A\right. \\
&\qquad\qquad \left. + \frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}B\right\} \\
&= \frac{\left(\lambda_0\lambda_{\beta'}K_0\frac{\delta S_{\beta'}}{\delta S_0} + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}\frac{\delta S_0}{\delta S_0}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}A
\end{aligned}
$$

$$+ \frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\delta A}{\delta S_0}$$

$$+ \frac{\left(\lambda\lambda_0^2\lambda_{\beta'}\frac{\delta S_0}{\delta S_0}S_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'}S_0\frac{\delta S_{\beta'}}{\delta S_0}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}B$$

$$+ \frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\delta B}{\delta S_0}$$

$$= \frac{\left(0 + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}A + \frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\delta A}{\delta S_0}$$

$$+ \frac{\left(\lambda\lambda_0^2\lambda_{\beta'}S_{\beta'} + 0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}B + \frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\delta B}{\delta S_0}$$

$$= \frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}A + \left[\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]\frac{\delta A}{\delta S_0}$$

$$+ \frac{\lambda\lambda_0^2\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}B + \left[\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]\frac{\delta B}{\delta S_0} \tag{2.167}$$

where

$$\frac{\delta A}{\delta S_0} = \left\{\frac{\lambda_0S_0}{(1-\lambda^2\lambda_0^2)}A + \frac{\lambda\lambda_0^2K_0}{(1-\lambda^2\lambda_0^2)}B\right\}, \tag{2.168}$$

$$\frac{\delta B}{\delta S_0} = \left\{\frac{\lambda_0S_0}{(1-\lambda^2\lambda_0^2)}B + \frac{\lambda\lambda_0^2K_0}{(1-\lambda^2\lambda_0^2)}A\right\}. \tag{2.169}$$

Substitute (2.168) and (2.169) in (2.167), we obtain

$$\frac{\delta C}{\delta S_0} = \frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}A$$

$$+ \left[\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]\left\{\frac{\lambda_0S_0}{(1-\lambda^2\lambda_0^2)}A + \frac{\lambda\lambda_0^2K_0}{(1-\lambda^2\lambda_0^2)}B\right\}$$

$$+ \frac{\lambda\lambda_0^2\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}B$$

$$+\left[\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right]\left\{\frac{\lambda_0S_0}{(1-\lambda^2\lambda_0^2)}B+\frac{\lambda\lambda_0^2K_0}{(1-\lambda^2\lambda_0^2)}A\right\}$$

$$=\left\{\frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\lambda_0S_0}{(1-\lambda^2\lambda_0^2)}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\lambda\lambda_0^2K_0}{(1-\lambda^2\lambda_0^2)}\right\}A$$

$$+\left\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\lambda\lambda_0^2K_0}{(1-\lambda^2\lambda_0^2)}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\frac{\lambda_0S_0}{(1-\lambda^2\lambda_0^2)}\right\}B. \tag{2.170}$$

Rewrite above equation

$$\frac{\delta C}{\delta S_0}=\left\{\frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}A$$

$$+\left\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}B. \tag{2.171}$$

Then, operate (2.171) by $\frac{\delta}{\delta K_\beta}$, we obtain

$$\frac{\delta}{\delta K_\beta}\frac{\delta C}{\delta S_0}=\frac{\delta}{\delta K_\beta}\left\{\frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}A$$

$$+\left\{\frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2 K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}\frac{\delta A}{\delta K_\beta}$$

$$+\frac{\delta}{\delta K_\beta}\left\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}B$$

$$+\left\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}\frac{\delta B}{\delta K_\beta}$$

$$=\left\{\frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2\dfrac{\delta K_{\beta'}}{\delta K_\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\delta}{\delta K_\beta}\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\delta}{\delta K_\beta}\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}A$$

$$+\left\{\frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2 K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}\frac{\delta A}{\delta K_\beta}$$

$$+\left\{\frac{\delta}{\delta K_\beta}\frac{\lambda\lambda_0^2\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\right.$$

$$+\frac{\delta}{\delta K_\beta}\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}$$

$$+\frac{\delta}{\delta K_\beta}\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\Bigg\}B$$

$$+\left\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}\frac{\delta B}{\delta K_\beta}$$

$$=\left\{\frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\lambda^2\lambda_0^3\lambda_{\beta'}^2S_0\lambda_0S_0^2\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\lambda^2\lambda_0^3\lambda_{\beta'}^2K_0^2\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}A$$

$$+\left\{\frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}\frac{\delta A}{\delta K_\beta}$$

$$+\left\{\frac{\lambda^3\lambda_0^4\lambda_{\beta'}^2K_0S_0\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}+\frac{\lambda\lambda_0^2\lambda_{\beta'}^2K_0S_0\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}B$$

$$+\left\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}+\frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.$$

$$\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'}+\lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}\frac{\delta B}{\delta K_\beta} \tag{2.172}$$

where

$$\frac{\delta A}{\delta K_\beta}=\left\{\frac{\lambda_\beta K_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}A+\frac{\lambda\lambda_\beta^2S_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}B\right\}, \tag{2.173}$$

$$\frac{\delta B}{\delta K_\beta}=\left\{\frac{\lambda_\beta K_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}B+\frac{\lambda\lambda_\beta^2S_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}A\right\}. \tag{2.174}$$

Substitute (2.173) and (2.174) in (2.172), we obtain

$$\begin{aligned}
\frac{\delta}{\delta K_\beta}\frac{\delta C}{\delta S_0} = &\left\{\frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)} + \frac{\lambda^2\lambda_0^3\lambda_{\beta'}^2 S_0\lambda_0 S_0^2\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.\\
&\left.+\frac{\lambda^2\lambda_0^3\lambda_{\beta'}^2 K_0^2\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}A\\
&+\left\{\frac{\lambda^2\lambda_0^2\lambda_{\beta'}^2 K_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)} + \frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.\\
&\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}\left\{\frac{\lambda_\beta K_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}A + \frac{\lambda\lambda_\beta^2S_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}B\right\}\\
&+\left\{\frac{\lambda^3\lambda_0^4\lambda_{\beta'}^2K_0S_0\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2} + \frac{\lambda\lambda_0^2\lambda_{\beta'}^2K_0S_0\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}B\\
&+\left\{\frac{\lambda\lambda_0^2\lambda_{\beta'}S_{\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)} + \frac{\left(\lambda_0\lambda_{\beta'}K_0S_{\beta'} + \lambda^2\lambda_0^2\lambda_{\beta'}^2K_{\beta'}S_0\right)\lambda\lambda_0^2K_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right.\\
&\left.+\frac{\left(\lambda\lambda_0\lambda_{\beta'}^2K_0K_{\beta'} + \lambda\lambda_0^2\lambda_{\beta'}S_0S_{\beta'}\right)\lambda_0S_0}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)^2}\right\}\left\{\frac{\lambda_\beta K_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}B + \frac{\lambda\lambda_\beta^2S_\beta}{\left(1-\lambda^2\lambda_\beta^2\right)}A\right\}.
\end{aligned} \tag{2.175}$$

Because

$$K_\alpha = \sum_{\varepsilon=\pm1} c_\alpha(\varepsilon)\int \mathrm{d}^3\mathbf{x}\;\psi_\alpha(\mathbf{x})K(z)$$

then

$$\lim_{K(z)\to 0} K_\alpha = 0, \tag{2.176}$$

$$\lim_{S(z)\to 0} S_\alpha = 0. \tag{2.177}$$

By using (2.176) and (2.177), from (2.141) and (2.142), we obtain

$$\lim_{K(z),S(z)\to 0} A = 2, \tag{2.178}$$

$$\lim_{K(z),S(z)\to 0} B = 0. \tag{2.179}$$

Then, substitute (2.178) and (2.179) in (2.166), we obtain

$$\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}A = \frac{2\lambda_0\lambda_{\beta'}\delta_{\beta\beta'}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)} \tag{2.180}$$

and (2.175) becomes

$$\frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}A = \frac{2\lambda^2\lambda_0^2\lambda_{\beta'}^2\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}. \tag{2.181}$$

Therefore

$$\begin{aligned}\frac{1}{2}\left\{\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_\beta}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}+\frac{\delta}{\delta K_\beta}\frac{\delta}{\delta S_0}\frac{\delta}{\delta K_0}\frac{\delta}{\delta S_{\beta'}}\right\}A &= \frac{1}{2}\frac{\left(2\lambda_0\lambda_{\beta'}\delta_{\beta\beta'}+2\lambda^2\lambda_0^2\lambda_{\beta'}^2\delta_{\beta'\beta}\right)}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\\ &= \frac{\left(\lambda_0\lambda_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2\right)\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}.\end{aligned} \tag{2.182}$$

Substitute (2.182) in (2.155), where $C$ is from (2.153), we obtain

$$\begin{aligned}\mathcal{V}(\lambda^2) &= \lambda^2\sum_{\beta=1}^{k}\sum_{\beta'=1}^{k} I_{0\beta,0\beta'}\left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\frac{\left(\lambda_0\lambda_{\beta'}+\lambda^2\lambda_0^2\lambda_{\beta'}^2\right)\delta_{\beta'\beta}}{\left(1-\lambda^2\lambda_{\beta'}^2\right)\left(1-\lambda^2\lambda_0^2\right)}\\ &= \left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\lambda^2\sum_{\beta=1}^{k} I_{0\beta,0\beta}\frac{\left(\lambda_0\lambda_\beta+\lambda^2\lambda_0^2\lambda_\beta^2\right)}{\left(1-\lambda^2\lambda_\beta^2\right)\left(1-\lambda^2\lambda_0^2\right)}.\end{aligned} \tag{2.183}$$

## C: Kinetic Energy

Consider the kinetic energy part $\left\langle \Psi_{2N} \left| \sum_{\alpha=1}^{2N} \left( -\frac{\hbar^2}{2m} \boldsymbol{\nabla}_\alpha^2 \right) \right| \Psi_{2N} \right\rangle \equiv T$,

$$
\begin{aligned}
T = & \int (\mathrm{d}z_1) \ldots (\mathrm{d}z_{2N}) \; \Psi_{2N}(z_1, \ldots, z_{2N}) \sum_{\alpha=1}^{2N} \left( -\frac{\hbar^2}{2m} \boldsymbol{\nabla}_\alpha^2 \right) \Psi_{2N}(z_1, \ldots, z_{2N}) \\
= & \int (\mathrm{d}z_1) \ldots (\mathrm{d}z_{2N}) \; \frac{\delta}{\delta K(z_1)} \cdots \frac{\delta}{\delta K(z_{2N})} \\
& \times \sum_{\alpha=1}^{2N} \left( -\frac{\hbar^2}{2m} \boldsymbol{\nabla}_\alpha^2 \right) \frac{\delta}{\delta S(z_1)} \cdots \frac{\delta}{\delta S(z_{2N})} F[K]_0 F[S]_0 \\
= & \left[ \int (\mathrm{d}z_1) \; \frac{\delta}{\delta K(z_1)} \left( -\frac{\hbar^2}{2m} \boldsymbol{\nabla}_1^2 \right) \frac{\delta}{\delta S(z_1)} \right] \\
& \times \int (\mathrm{d}z_2) \ldots (\mathrm{d}z_{2N}) \frac{\delta}{\delta K(z_2)} \frac{\delta}{\delta S(z_2)} \cdots \frac{\delta}{\delta K(z_{2N})} \frac{\delta}{\delta S(z_{2N})} F[K]_0 F[S]_0 \\
& + \\
& \vdots \\
& + \\
& \left[ \int (\mathrm{d}z_{2N}) \; \frac{\delta}{\delta K(z_{2N})} \left( -\frac{\hbar^2}{2m} \boldsymbol{\nabla}_{2N}^2 \right) \frac{\delta}{\delta S(z_{2N})} \right] \\
& \times \int (\mathrm{d}z_1) \ldots (\mathrm{d}z_{2N-1}) \frac{\delta}{\delta K(z_1)} \frac{\delta}{\delta S(z_1)} \cdots \frac{\delta}{\delta K(z_{2N-1})} \frac{\delta}{\delta S(z_{2N-1})} F[K]_0 F[S]_0 \\
= & (2N) \left( \int (\mathrm{d}z_1) \frac{\delta}{\delta K(z_1)} T^1 \frac{\delta}{\delta S(z_1)} \right) \left( \int (\mathrm{d}z) \frac{\delta}{\delta K(z)} \frac{\delta}{\delta S(z)} \right)^{2N-1} F[K]_0 F[S]_0
\end{aligned}
\tag{2.184}
$$

where

$$
T^1 = \left( -\frac{\hbar^2}{2m} \boldsymbol{\nabla}_1^2 \right). \tag{2.185}
$$

Multiply (2.184) by $\sum_{N=0}^{\infty}\frac{(\lambda)^{2N}}{(2N)!}$ and $\Theta(N-1)$, we obtain

$$\sum_{N=0}^{\infty}\frac{(\lambda)^{2N}}{(2N)!}\Theta(N-1)\left\langle\Psi_{2N}\left|\sum_{\alpha=1}^{2N}\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_\alpha^2\right)\right|\Psi_{2N}\right\rangle$$

$$=\left(\int(\mathrm{d}z_1)\frac{\delta}{\delta K(z_1)}T^1\frac{\delta}{\delta S(z_1)}\right)\sum_{N=0}^{\infty}\frac{(2N)(\lambda)^{2N}}{(2N)!}$$

$$\times\left(\int(\mathrm{d}z)\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)^{2N-1}\Theta(N-1)F[K]_0F[S]_0$$

$$\equiv\mathcal{T}(\lambda^2). \tag{2.186}$$

Let $M=2N-1$, for $X=\int(\mathrm{d}z)\;\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}$,

$$\sum_{N=0}^{\infty}\frac{(\lambda)^{2N}}{(2N)!}(2N)X^{2N-1}\Theta(N-1)$$

$$=\sum_{M=1,3,5,\ldots}^{\infty}\frac{(\lambda)^{M+1}}{(M+1)!}(M+1)X^M$$

$$=\lambda\sum_{M=1,3,5,\ldots}^{\infty}\frac{(\lambda)^{M}}{M!}X^M$$

$$=\frac{\lambda}{2}\left\{\left[\frac{\lambda^0}{0!}X^0+\frac{\lambda^1}{1!}X^1+\frac{\lambda^2}{2!}X^2+\frac{\lambda^3}{3!}X^3+\cdots\right]\right.$$

$$\left.-\left[\frac{\lambda^0}{0!}X^0-\frac{\lambda^1}{1!}X^1+\frac{\lambda^2}{2!}X^2-\frac{\lambda^3}{3!}X^3+\cdots\right]\right\}$$

$$=\frac{\lambda}{2}\left\{\sum_{M=0}^{\infty}\frac{\lambda^M}{M!}X^M-\sum_{M=0}^{\infty}\frac{(-\lambda)^M}{M!}X^M\right\}$$

$$=\frac{\lambda}{2}\left\{\exp\left(\lambda X\right)-\exp\left(-\lambda X\right)\right\}. \tag{2.187}$$

Substitute (2.187) in (2.186), then we obtain

$$\mathcal{T}(\lambda^2) = \frac{\lambda}{2}\left(\int(\mathrm{d}z_1)\frac{\delta}{\delta K(z_1)}T^1\frac{\delta}{\delta S(z_1)}\right)\left[\exp\left(\lambda\int(\mathrm{d}z)\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)\right.$$
$$\left. - \exp\left(-\lambda\int(\mathrm{d}z)\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)\right] F[K]_0 F[S]_0. \qquad (2.188)$$

From the last section, we have

$$\exp\left(\pm\lambda\int(\mathrm{d}z)\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)F[K]F[S]$$
$$= \left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\exp\left(\sum_{\alpha=0}^{k}\frac{K_\alpha^2\lambda_\alpha}{2\,(1-\lambda^2\lambda_\alpha^2)}\right)$$
$$\times\exp\left(\sum_{\alpha=0}^{k}\frac{S_\alpha^2\lambda_\alpha}{2\,(1-\lambda^2\lambda_\alpha^2)}\right)\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda_\alpha^2(\pm\lambda)S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)$$
$$= \left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\exp\left(\sum_{\alpha=0}^{k}\frac{(\lambda_\alpha K_\alpha^2+\lambda_\alpha S_\alpha^2)}{2\,(1-\lambda^2\lambda_\alpha^2)}\right)$$
$$\times\exp\left(\sum_{\alpha=0}^{k}\frac{\pm\lambda\lambda_\alpha^2 S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right). \qquad (2.189)$$

By using (2.189), we obtain

$$\left[\exp\left(\lambda\int(\mathrm{d}z)\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right) - \exp\left(-\lambda\int(\mathrm{d}z)\frac{\delta}{\delta K(z)}\frac{\delta}{\delta S(z)}\right)\right]F[K]F[S]$$
$$= \left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\exp\left(\sum_{\alpha=0}^{k}\frac{(\lambda_\alpha K_\alpha^2+\lambda_\alpha S_\alpha^2)}{2\,(1-\lambda^2\lambda_\alpha^2)}\right)\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda\lambda_\alpha^2 S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)$$
$$- \left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\exp\left(\sum_{\alpha=0}^{k}\frac{(\lambda_\alpha K_\alpha^2+\lambda_\alpha S_\alpha^2)}{2\,(1-\lambda^2\lambda_\alpha^2)}\right)\exp\left(\sum_{\alpha=0}^{k}\frac{-\lambda\lambda_\alpha^2 S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)$$
$$= \left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)\exp\left(\sum_{\alpha=0}^{k}\frac{(\lambda_\alpha K_\alpha^2+\lambda_\alpha S_\alpha^2)}{2\,(1-\lambda^2\lambda_\alpha^2)}\right)$$

$$\times\left[\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda\lambda_\alpha^2 S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)-\exp\left(\sum_{\alpha=0}^{k}\frac{-\lambda\lambda_\alpha^2 S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)\right]$$

$$=\left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)B \tag{2.190}$$

where $B$ is defined in (2.142) and expressed by

$$B=\exp\left(\sum_{\alpha=0}^{k}\frac{(\lambda_\alpha K_\alpha^2+\lambda_\alpha S_\alpha^2)}{2\,(1-\lambda^2\lambda_\alpha^2)}\right)$$
$$\times\left[\exp\left(\sum_{\alpha=0}^{k}\frac{\lambda\lambda_\alpha^2 S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)-\exp\left(\sum_{\alpha=0}^{k}\frac{-\lambda\lambda_\alpha^2 S_\alpha K_\alpha}{(1-\lambda^2\lambda_\alpha^2)}\right)\right].$$

Substitute (2.190) in (2.188), then we obtain

$$\mathcal{T}(\lambda^2)=\frac{\lambda}{2}\left(\int(\mathrm{d}z)\frac{\delta}{\delta K(z)}\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\right)\frac{\delta}{\delta S(z)}\right)\left(\prod_{\alpha=0}^{k}\frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}}\right)B. \tag{2.191}$$

From (2.98) we have

$$\frac{\delta}{\delta K(z)}=\sum_\alpha c_\alpha(\varepsilon)\psi_\alpha(\mathbf{x})\frac{\delta}{\delta K_\alpha}$$

then

$$\int(\mathrm{d}z)\frac{\delta}{\delta K(z)}\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\right)\frac{\delta}{\delta S(z)}$$
$$=\sum_{\varepsilon=\pm1}\int\mathrm{d}^3\mathbf{x}\,\sum_\alpha c_\alpha(\varepsilon)\psi_\alpha(\mathbf{x})\frac{\delta}{\delta K_\alpha}\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\right)\sum_\beta c_\beta(\varepsilon)\psi_\beta(\mathbf{x})\frac{\delta}{\delta S_\beta}$$
$$=\sum_\alpha\sum_\beta\sum_{\varepsilon=\pm1}c_\alpha(\varepsilon)c_\beta(\varepsilon)\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\int\mathrm{d}^3\mathbf{x}\,\psi_\alpha(\mathbf{x})\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\right)\psi_\beta(\mathbf{x})$$
$$=\sum_{\alpha,\beta}\sum_{\varepsilon=\pm1}c_\alpha(\varepsilon)c_\beta(\varepsilon)\frac{\delta}{\delta K_\alpha}\frac{\delta}{\delta S_\beta}\left\langle\psi_\alpha\left|\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\right)\right|\psi_\beta\right\rangle$$

$$= \sum_{\alpha,\beta} \sum_{\varepsilon=\pm 1} c_\alpha(\varepsilon) c_\beta(\varepsilon) T_{\alpha\beta} \frac{\delta}{\delta K_\alpha} \frac{\delta}{\delta S_\beta} \tag{2.192}$$

where

$$\left\langle \psi_\alpha \middle| \left( -\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 \right) \middle| \psi_\beta \right\rangle \equiv T_{\alpha\beta}. \tag{2.193}$$

Substitute (2.192) in (2.191), then we obtain

$$\mathcal{T}(\lambda^2) = \frac{\lambda}{2} \left( \prod_{\alpha=0}^{k} \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \right) \sum_{\alpha,\beta} \sum_{\varepsilon=\pm 1} c_\alpha(\varepsilon) c_\beta(\varepsilon) T_{\alpha\beta} \frac{\delta}{\delta K_\alpha} \frac{\delta}{\delta S_\beta} B \tag{2.194}$$

and from (2.160) we have

$$\frac{\delta B}{\delta S_\beta} = \frac{\lambda_\beta S_\beta}{(1-\lambda^2\lambda_\beta^2)} B + \frac{\lambda\lambda_\beta^2 K_\beta}{(1-\lambda^2\lambda_\beta^2)} A.$$

Then

$$\frac{\delta}{\delta K_\alpha} \frac{\delta B}{\delta S_\beta} = \frac{\lambda_\beta S_\beta}{(1-\lambda^2\lambda_\beta^2)} \frac{\delta B}{\delta K_\alpha} + \frac{\lambda\lambda_\beta^2 \frac{\delta K_\beta}{\delta K_\alpha}}{(1-\lambda^2\lambda_\beta^2)} A + \frac{\lambda\lambda_\beta^2 K_\beta}{(1-\lambda^2\lambda_\beta^2)} \frac{\delta A}{\delta K_\alpha}$$

$$= \frac{\lambda_\beta S_\beta}{(1-\lambda^2\lambda_\beta^2)} \left\{ \frac{\lambda_\beta K_\alpha}{(1-\lambda^2\lambda_\alpha^2)} B + \frac{\lambda\lambda_\alpha^2 S_\alpha}{(1-\lambda^2\lambda_\alpha^2)} A \right\}$$

$$+ \frac{\lambda\lambda_\beta^2 \delta_{\alpha\beta}}{(1-\lambda^2\lambda_\beta^2)} A + \frac{\lambda\lambda_\beta^2 K_\beta}{(1-\lambda^2\lambda_\beta^2)} \left\{ \frac{\lambda_\beta K_\alpha}{(1-\lambda^2\lambda_\alpha^2)} A + \frac{\lambda\lambda_\alpha^2 S_\alpha}{(1-\lambda^2\lambda_\alpha^2)} B \right\}$$

$$= \frac{2\lambda\lambda_\beta^2 \delta_{\alpha\beta}}{(1-\lambda^2\lambda_\beta^2)} \tag{2.195}$$

since $K_\alpha, S_\alpha \to 0$. Substitute (2.195) in (2.194), then we obtain

$$\mathcal{T}(\lambda^2) = \frac{\lambda}{2} \left( \prod_{\alpha=0}^{k} \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \right) \sum_{\alpha,\beta} \sum_{\varepsilon=\pm 1} c_\alpha(\varepsilon) c_\beta(\varepsilon) T_{\alpha\beta} \frac{2\lambda\lambda_\beta^2 \delta_{\alpha\beta}}{(1-\lambda^2\lambda_\beta^2)}$$

$$= \lambda \left( \prod_{\alpha=0}^{k} \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \right) \sum_{\alpha=0}^{k} \sum_{\varepsilon=\pm 1} c_\alpha(\varepsilon) c_\alpha(\varepsilon) T_{\alpha\alpha} \frac{\lambda\lambda_\alpha^2}{(1-\lambda^2\lambda_\alpha^2)}$$

$$= \lambda \left( \prod_{\alpha=0}^{k} \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \right) \sum_{\alpha=0}^{k} T_\alpha \frac{\lambda\lambda_\alpha^2}{(1-\lambda^2\lambda_\alpha^2)} \tag{2.196}$$

where $\sum_{\varepsilon=\pm 1} c_\alpha(\varepsilon)c_\alpha(\varepsilon) = \sum_{\varepsilon=\pm 1} |c_\alpha(\varepsilon)|^2 = 1$, $T_{\alpha\alpha} \equiv T_\alpha$.

## D: The Expectation Value of $H$

From (2.183) and (2.196) we have

$$\begin{aligned}
\mathcal{H}(\lambda^2) &= \mathcal{T}(\lambda^2) + \mathcal{V}(\lambda^2) \\
&= \lambda \left( \prod_{\alpha=0}^{k} \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \right) \sum_{\alpha=0}^{k} T_\alpha \frac{\lambda\lambda_\alpha^2}{(1-\lambda^2\lambda_\alpha^2)} \\
&\quad + \left( \prod_{\alpha=0}^{k} \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \right) \lambda^2 \sum_{\beta=1}^{k} I_{0\beta,0\beta} \frac{\left(\lambda_0\lambda_\beta + \lambda^2\lambda_0^2\lambda_\beta^2\right)}{\left(1-\lambda^2\lambda_\beta^2\right)\left(1-\lambda^2\lambda_0^2\right)} \\
&= \left( \prod_{\alpha=0}^{k} \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \right) \\
&\quad \times \left\{ \sum_{\beta=1}^{k} \left[ \frac{T_\beta\lambda_\beta^2\lambda^2}{1-\lambda_\beta^2\lambda^2} + I_{0\beta,0\beta}\lambda^2 \frac{(\lambda_0\lambda_\beta + \lambda_0^2\lambda_\beta^2\lambda^2)}{(1-\lambda^2\lambda_\beta^2)(1-\lambda^2\lambda_0^2)} \right] + \frac{T_0\lambda_0^2\lambda^2}{1-\lambda_0^2\lambda^2} \right\}.
\end{aligned} \tag{2.197}$$

From (2.111), we have

$$\mathcal{N}(\lambda^2) = \left( \prod_{\alpha=0}^{k} \frac{1}{\sqrt{1-\lambda^2\lambda_\alpha^2}} \right)$$

and $\lambda_0 = 1, \lambda_\alpha = -\xi$, where $\xi > 0, \alpha = 1, \ldots, k$. Then, rewrite (2.197) as below

$$\mathcal{H}(\lambda^2) = \mathcal{N}(\lambda^2) \left\{ \sum_{\beta=1}^{k} \left[ \frac{T_\beta\xi^2\lambda^2}{1-\xi^2\lambda^2} + I_{0\beta,0\beta}\lambda^2 \frac{(-\xi + \xi^2\lambda^2)}{(1-\lambda^2\xi^2)(1-\lambda^2)} \right] + \frac{T_0\lambda^2}{1-\lambda^2} \right\}. \tag{2.198}$$

From (2.100) and (2.101), we have

$$\mathcal{N}(\lambda^2) = \sum_{N=0}^{\infty} \frac{(\lambda)^{2N}}{(2N)!} \|\Psi_{2N}\|^2 \tag{2.199}$$

and from (2.15) we define

$$\frac{\langle \Psi_{2N} | H | \Psi_{2N} \rangle}{\|\Psi\|^2} \equiv H_{2N}.$$

From (2.184), (2.186), (2.117) and (2.118), we have

$$\begin{aligned}
\mathcal{H}(\lambda^2) &= \sum_{N \geqslant 0} \frac{(\lambda)^{2N}}{(2N)!} \langle \Psi_{2N} | T + V | \Psi_{2N} \rangle \\
&= \sum_{N \geqslant 0} \frac{(\lambda)^{2N}}{(2N)!} \langle \Psi_{2N} | H | \Psi_{2N} \rangle .
\end{aligned} \tag{2.200}$$

Therefore, the expectation value $H_{2N}$ from (2.15) and be obtained from (2.199) and (2.200)

$$H_{2N} = \frac{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{H}(\lambda^2)}{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)}. \tag{2.201}$$

Consider the coefficient of $I_{0\beta,0\beta}$ in (2.198)

$$\begin{aligned}
\frac{\lambda^2(-\xi + \xi^2\lambda^2)}{(1-\lambda^2\xi^2)(1-\lambda^2)} &= \frac{-\lambda^2\xi}{(1-\lambda^2\xi^2)(1-\lambda^2)}(1-\xi\lambda^2) \\
&= \frac{-\lambda^2\xi}{(1-\lambda^2\xi^2)(1-\lambda^2)(1+\xi)} \left[(1+\xi) - (1+\xi)\xi\lambda^2\right] \\
&= \frac{-\lambda^2\xi}{(1-\lambda^2\xi^2)(1-\lambda^2)(1+\xi)} \left[\xi(1-\lambda^2) + (1-\lambda^2\xi^2)\right] \\
&= \frac{-\lambda^2\xi}{(1+\xi)} \left[\frac{\xi}{1-\lambda^2\xi^2} + \frac{1}{1-\lambda^2}\right]
\end{aligned}$$

$$= \frac{\xi}{(1+\xi)} \left[ \frac{\lambda^2\xi^2 k}{1-\lambda^2\xi^2} - \frac{\lambda^2\xi^2 k}{1-\lambda^2\xi^2} - \frac{\lambda^2\xi}{1-\lambda^2\xi^2} - \frac{\lambda^2}{1-\lambda^2} \right]. \tag{2.202}$$

By using the result from (2.202), Eq. (2.198) will be rewritten as

$$\begin{aligned}
\mathcal{H}(\lambda^2) &= \mathcal{N}(\lambda^2) \left\{ \sum_{\beta=1}^{k} \left[ \frac{T_\beta \xi^2 \lambda^2}{1-\xi^2\lambda^2} + I_{0\beta} \frac{\xi}{(1+\xi)} \right.\right. \\
&\quad \left.\left. \times \left( \frac{\lambda^2\xi^2 k}{1-\lambda^2\xi^2} - \frac{\lambda^2\xi^2 k}{1-\lambda^2\xi^2} - \frac{\lambda^2\xi}{1-\lambda^2\xi^2} - \frac{\lambda^2}{1-\lambda^2} \right) \right] + \frac{T_0\lambda^2}{1-\lambda^2} \right\} \\
&= \mathcal{N}(\lambda^2) \left\{ \frac{\xi^2\lambda^2}{1-\xi^2\lambda^2} \left[ \sum_{\beta=1}^{k} T_\beta + \frac{\xi}{(1+\xi)} \sum_{\beta=1}^{k} I_{0\beta} \left( k - \frac{1}{\xi} \right) \right] + \frac{T_0\lambda^2}{1-\lambda^2} \right. \\
&\quad \left. - \left( \frac{\lambda^2}{1-\lambda^2} + \frac{\lambda^2\xi^2 k}{1-\lambda^2\xi^2} \right) \frac{\xi}{1+\xi} \sum_{\beta=1}^{k} I_{0\beta} \right\} \\
&= \mathcal{N}(\lambda^2) \left\{ \frac{\xi^2\lambda^2}{1-\xi^2\lambda^2} \left[ \sum_{\beta=1}^{k} T_\beta - kT_0 + \frac{\xi}{(1+\xi)} \left( k - \frac{1}{\xi} \right) \sum_{\beta=1}^{k} I_{0\beta} \right] \right. \\
&\quad \left. + T_0 \left( \frac{\lambda^2}{1-\lambda^2} + \frac{\lambda^2\xi^2 k}{1-\lambda^2\xi^2} \right) - \frac{\xi}{(1+\xi)} \left( \frac{\lambda^2}{1-\lambda^2} + \frac{\lambda^2\xi^2 k}{1-\lambda^2\xi^2} \right) \sum_{\beta=1}^{k} I_{0\beta} \right\} \\
&= \mathcal{N}(\lambda^2) \left\{ \frac{\xi^2\lambda^2}{1-\xi^2\lambda^2} \left[ \sum_{\beta=1}^{k} T_\beta - kT_0 + \frac{\xi}{(1+\xi)} \left( k - \frac{1}{\xi} \right) \sum_{\beta=1}^{k} I_{0\beta} \right] \right. \\
&\quad \left. + \left[ \frac{\lambda^2}{1-\lambda^2} + \frac{\lambda^2\xi^2 k}{1-\lambda^2\xi^2} \right] \left( T_0 - \frac{\xi}{(1+\xi)} \sum_{\beta=1}^{k} I_{0\beta} \right) \right\}.
\end{aligned} \tag{2.203}$$

Let

$$\mathcal{A}(\lambda^2) = \frac{\lambda^2}{1-\lambda^2} + \frac{\lambda^2\xi^2 k}{1-\lambda^2\xi^2} \tag{2.204}$$

and the expansion of $\mathcal{N}(\lambda^2)$ in (2.111) gives

$$\mathcal{N}(\lambda^2) = \frac{1}{\sqrt{1-\lambda^2}} \cdot \frac{1}{[1-\lambda^2\xi^2]^{k/2}} \tag{2.205}$$

where $\lambda_0 = 1$ and $\lambda_\alpha = -\xi, \alpha = 1, 2, \ldots$ result (2.205). By using (2.204) and (2.205), then we obtain

$$\mathcal{H}(\lambda^2) = \mathcal{N}(\lambda^2)\frac{\xi^2\lambda^2}{1-\xi^2\lambda^2}\left[\sum_{\beta=1}^{k} T_\beta - kT_0 + \frac{\xi}{(1+\xi)}\left(k-\frac{1}{\xi}\right)\sum_{\beta=1}^{k} I_{0\beta}\right]$$
$$+\mathcal{N}(\lambda^2)\mathcal{A}(\lambda^2)\left(T_0 - \frac{\xi}{(1+\xi)}\sum_{\beta=1}^{k} I_{0\beta}\right). \tag{2.206}$$

We can see from (2.206) that

$$\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{H}(\lambda^2) = \left(\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)\frac{\lambda^2\xi^2}{1-\lambda^2\xi^2}\right)$$
$$\times\left[\sum_{\beta=1}^{k} T_\beta - kT_0 + \frac{\xi}{(1+\xi)}\left(k-\frac{1}{\xi}\right)\sum_{\beta=1}^{k} I_{0\beta}\right]$$
$$+\left(\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)\mathcal{A}(\lambda^2)\right)\left(T_0 - \frac{\xi}{(1+\xi)}\sum_{\beta=1}^{k} I_{0\beta}\right). \tag{2.207}$$

Substitute (2.207) in (2.201), we obtain

$$H_{2N} = \left(\frac{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)\dfrac{\lambda^2\xi^2}{1-\lambda^2\xi^2}}{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)}\right)$$
$$\times\left[\sum_{\beta=1}^{k} T_\beta - kT_0 + \frac{\xi}{(1+\xi)}\left(k-\frac{1}{\xi}\right)\sum_{\beta=1}^{k} I_{0\beta}\right]$$

$$+\left(\frac{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)\mathcal{A}(\lambda^2)}{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)}\right)\left(T_0 - \frac{\xi}{(1+\xi)}\sum_{\beta=1}^{k} I_{0\beta}\right). \tag{2.208}$$

Now, we will consider (2.205)

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\lambda^2}\mathcal{N}(\lambda^2) &= \frac{1}{2}\frac{1}{(1-\lambda^2)^{\frac{3}{2}}}\frac{1}{[1-\lambda^2\xi^2]^{\frac{k}{2}}} + \frac{k}{2}\frac{\xi^2}{\sqrt{1-\lambda^2}}\frac{1}{[1-\lambda^2\xi^2]^{\frac{k}{2}+1}} \\
&= \frac{1}{2\lambda^2}\left\{\frac{\lambda^2}{(1-\lambda^2)^{\frac{3}{2}}[1-\lambda^2\xi^2]^{\frac{k}{2}}} + \frac{k\xi^2\lambda^2}{\sqrt{1-\lambda^2}\,[1-\lambda^2\xi^2]^{\frac{k}{2}+1}}\right\} \\
&= \frac{1}{2\lambda^2}\frac{1}{\sqrt{1-\lambda^2}\,[1-\lambda^2\xi^2]}\left\{\frac{\lambda^2}{(1-\lambda^2)} + \frac{k\xi^2\lambda^2}{[1-\lambda^2\xi^2]^{\frac{k}{2}}}\right\} \\
&= \frac{1}{2\lambda^2}\mathcal{N}(\lambda^2)\mathcal{A}(\lambda^2). 
\end{aligned} \tag{2.209}$$

Let

$$\mathcal{N}(\lambda^2) = \sum_{N\geqslant 0} a_N(\lambda^2)^N \tag{2.210}$$

where $a_N$ is the coefficient of $(\lambda^2)^N$ of $\mathcal{N}(\lambda^2)$, then

$$\frac{\mathrm{d}}{\mathrm{d}\lambda^2}\mathcal{N}(\lambda^2) = \sum_{N\geqslant 0} a_N N(\lambda^2)^{N-1}. \tag{2.211}$$

Multiply (2.211) by $2\lambda^2$ and compare the result with (2.209)

$$2\lambda^2\frac{\mathrm{d}}{\mathrm{d}\lambda^2}\mathcal{N}(\lambda^2) = \sum_{N\geqslant 0} a_N 2N(\lambda^2)^N \equiv \mathcal{N}(\lambda^2)\mathcal{A}(\lambda^2). \tag{2.212}$$

Then, from (2.210) and (2.212), we obtain

$$\begin{aligned}
\frac{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)\mathcal{A}(\lambda^2)}{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)} &= \frac{(2N)a_N}{a_N} \\
&= 2N.
\end{aligned} \tag{2.213}$$

Substitute (2.213) in (2.208), we obtain

$$H_{2N} = \left( \frac{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2) \dfrac{\lambda^2\xi^2}{1-\lambda^2\xi^2}}{\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)} \right) \left[ \sum_{\beta=1}^{k} T_\beta - kT_0 \right.$$

$$\left. + \frac{\xi}{(1+\xi)} \left(k - \frac{1}{\xi}\right) \sum_{\beta=1}^{k} I_{0\beta} \right] + 2N \left( T_0 - \frac{\xi}{(1+\xi)} \sum_{\beta=1}^{k} I_{0\beta} \right). \quad (2.214)$$

## Binomial Expansion

We can use the binomial expansion[*)] to find such coefficients. Some useful expressions are given below

$$\text{Binomial series:} \quad (1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \frac{n(n-1)(n-2)}{3!}x^3 + \ldots, \quad (2.215)$$

$$\text{Binomial coefficient:} \quad {}^nC_r \equiv \binom{n}{r} \equiv \frac{n!}{r!(n-r)!}, \quad (2.216)$$

$$\text{Binomial theorem:} \quad (a+b)^n = \sum_{k=0}^{n} \binom{n}{k} a^{n-k} b^k, \quad (2.217)$$

$$\text{Taylor series:} \quad f(a+x) = f(a) + xf'(a) + \frac{x^2}{2!} f^2(a) + \ldots + \frac{x^{n-1}}{(n-1)!} f^{n-1}(a) + \ldots, \quad (2.218)$$

$$\text{Taylor series:} \quad f(\mathbf{a}+\mathbf{x}) = f(\mathbf{a}) + (\mathbf{x}\cdot\boldsymbol{\nabla})f|_{\mathbf{a}} + \frac{(\mathbf{x}\cdot\boldsymbol{\nabla})^2}{2!} f\Big|_{\mathbf{a}} + \ldots. \quad (2.219)$$

Now, we will define

$$\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2) \frac{\lambda^2\xi^2}{1-\lambda^2\xi^2} \equiv b_N \quad (2.220)$$

*) See Woan (2000) p. 28.

$$\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2) \equiv D_N \tag{2.221}$$

and

$$\beta_N = \frac{b_N}{D_N}. \tag{2.222}$$

Substitute (2.222) in (2.214), we obtain

$$H_{2N} = \beta_N \left[ \sum_{\beta=1}^{k} T_\beta - kT_0 + \frac{\xi}{(1+\xi)} \left( k - \frac{1}{\xi} \right) \sum_{\beta=1}^{k} I_{0\beta} \right]$$

$$+ 2N \left( T_0 - \frac{\xi}{(1+\xi)} \sum_{\beta=1}^{k} I_{0\beta} \right). \tag{2.223}$$

Then, we will consider $b_N$ : let $\lambda^2 \equiv x$, by using Taylor series (about 0), for any functions $f(x)$ and $g(x)$

$$f(x)g(x) = \sum_{N=0}^{\infty} \left[ \frac{x^N}{N!} \left( \frac{\mathrm{d}^N f(x)g(x)}{\mathrm{d}x^N} \right) \bigg|_{x\to 0} \right] \tag{2.224}$$

where

$$\left( \frac{\mathrm{d}^N f(x)g(x)}{\mathrm{d}x^N} \right) \bigg|_{x\to 0} = f^{(N)}(0)g(0) + \frac{N!}{1!(N-1)!} f^{(N-1)}(0)g^{(1)}(0)$$

$$+ \frac{N!}{2!(N-2)!} f^{(N-2)}(0)g^{(2)}(0) + \cdots$$

$$+ \frac{N!}{(N-1)!1!} f^{(1)}(0)g^{(N-1)}(0) + \frac{N!}{N!0!} f(0)g^{(N)}(0)$$

$$= \sum_{r=0}^{N} \frac{N!}{r!(N-r)!} f^{(N-r)}(0)g^{(r)}(0) \tag{2.225}$$

and

$$f^{(t)}(0) = \frac{\mathrm{d}^t f(x)}{\mathrm{d}x^t} \bigg|_{x\to 0}. \tag{2.226}$$

By using (2.225), Eq. (2.224) becomes

$$f(x)g(x) = \sum_{N=0}^{\infty} \left[ \frac{x^N}{N!} \sum_{r=0}^{N} \frac{N!}{r!(N-r)!} f^{(N-r)}(0) g^{(r)}(0) \right] \tag{2.227}$$

and from (2.215) we have

$$\begin{aligned} (1+x)^n &= 1 + nx + \frac{n(n-1)}{2!}x^2 + \frac{n(n-1)(n-2)}{3!}x^3 + \dots \\ &= \sum_{t=0}^{\infty} \left[ \frac{x^t}{t!} \frac{1}{(n+1)} \prod_{i=0}^{t} \Big( n - (i-1) \Big) \right]. \end{aligned} \tag{2.228}$$

Then, for $f(x)g(x) = (1+x)^n$, we compare (2.224) with (2.228), we obtain

$$\left. \frac{\mathrm{d}^t (1+x)^n}{\mathrm{d}t^n} \right|_{x \to 0} = \frac{1}{(n+1)} \prod_{i=0}^{t} \Big( n - (i-1) \Big). \tag{2.229}$$

Let

$$f(x) = (1-x)^{-\frac{1}{2}}, \tag{2.230}$$

$$g(x) = (1 - x\xi^2)^{-\frac{k+2}{2}}. \tag{2.231}$$

By using (2.229), we obtain Eq. (2.230), for $n = -\dfrac{1}{2}$, $x \to -x$,

$$\begin{aligned} f(x) = \Big( 1 + (-x) \Big)^{-\frac{1}{2}} &= \sum_{t=0}^{\infty} \left[ \frac{(-x)^t}{t!} \frac{1}{\left( -\frac{1}{2} + 1 \right)} \prod_{i=0}^{t} \left( -\frac{1}{2} - (i-1) \right) \right] \\ &= \sum_{t=0}^{\infty} \frac{x^t}{t!} \frac{(-1)^t}{\frac{1}{2}} \prod_{i=0}^{t} \left( \frac{1}{2} - i \right) \\ &= \sum_{t=0}^{\infty} \frac{x^t}{t!} (-1)^t \left( \frac{1}{2} \right)^t \prod_{i=0}^{t} \Big( 1 - 2i \Big). \end{aligned} \tag{2.232}$$

Compare (2.232) with (2.224), we obtain

$$f^{(t)}(0) = (-1)^t \left(\frac{1}{2}\right)^t \prod_{i=0}^{t} \Big(1 - 2i\Big). \tag{2.233}$$

Consider $g(x)$ in (2.231) and use (2.229), we obtain

$$\begin{aligned}
g(x) &= \left[1 + (-x\xi^2)\right]^{-\frac{k+2}{2}} \\
&= \sum_{s=0}^{\infty} \left\{ \frac{(-x\xi^2)^s}{s!} \frac{1}{\left(-\dfrac{k+2}{2} + 1\right)} \prod_{j=0}^{s} \left[-\frac{k+2}{2} - (j-1)\right] \right\} \\
&= \sum_{s=0}^{\infty} \left[ \frac{x^s}{s!} (-\xi^2)^s \left(-\frac{2}{k}\right) \prod_{j=0}^{s} \left(\frac{-k-2j}{2}\right) \right] \\
&= \sum_{s=0}^{\infty} \left[ \frac{x^s}{s!} (-\xi^2)^s \left(-\frac{2}{k}\right) \left(\frac{1}{2}\right)^{s+1} \prod_{j=0}^{s} (-k-2j) \right] \\
&= \sum_{s=0}^{\infty} \left[ \frac{x^s}{s!} (-\xi^2)^s \left(-\frac{1}{k}\right) \left(\frac{1}{2}\right)^{s} \prod_{j=0}^{s} (-k-2j) \right] \\
&= \sum_{s=0}^{\infty} \left[ \frac{x^s}{s!} (-1)^s \left(-\frac{1}{k}\right) \left(\frac{\xi^2}{2}\right)^{s} \prod_{j=0}^{s} (-k-2j) \right].
\end{aligned} \tag{2.234}$$

Compare (2.234) with (2.224), we obtain

$$g^{(s)}(0) = (-1)^s \left(-\frac{1}{k}\right) \left(\frac{\xi^2}{2}\right)^s \prod_{j=0}^{s} \Big(-k - 2j\Big). \tag{2.235}$$

By using (2.225), (2.233), (2.235) and (2.227) we have

$$f(x)g(x) = (1-x)^{-\frac{1}{2}} \left(1 - x\xi^2\right)^{-\frac{k+2}{2}}$$

$$= \sum_{N=0}^{\infty} x^N \sum_{r=0}^{N} \frac{1}{r!(N-r)!}(-1)^{N-r}\left(\frac{1}{2}\right)^{N-r}\left[\prod_{i=0}^{N-r}(1-2i)\right]$$

$$\times (-1)^r \left(-\frac{1}{k}\right)\left(\frac{\xi^2}{2}\right)^r \prod_{j=0}^{r}(-k-2j)\,. \tag{2.236}$$

Multiply (2.236) by $x\xi^2$, we obtain

$$x\xi^2 f(x)g(x) = \frac{x\xi^2}{\sqrt{1-x}\,[1-x\xi^2]^{\frac{k}{2}+1}}$$

$$= \sum_{N=0}^{\infty} x^{N+1}\xi^2 \sum_{r=0}^{N} \frac{(-1)^{N-r}}{r!(N-r)!\,2^{N-r}}\left[\prod_{i=0}^{N-r}(1-2i)\right]$$

$$\times (-1)^r \left(-\frac{1}{k}\right)\left(\frac{\xi^2}{2}\right)^r \prod_{j=0}^{r}(-k-2j)$$

$$= \sum_{N=1}^{\infty} x^{N}\xi^2 \sum_{r=0}^{N-1} \frac{(-1)^{N-1-r}}{r!(N-1-r)!\,2^{N-1-r}}\left[\prod_{i=0}^{N-1-r}(1-2i)\right]$$

$$\times (-1)^r \left(-\frac{1}{k}\right)\left(\frac{\xi^2}{2}\right)^r \prod_{j=0}^{r}(-k-2j)$$

$$= \sum_{N=1}^{\infty} x^{N}\xi^2 \sum_{r=0}^{N-1} \frac{(-1)^{N-1}}{r!(N-1-r)!\,2^{N-1-r}}\left(\frac{\xi^2}{2}\right)^r\left(-\frac{1}{k}\right)$$

$$\times \left[\prod_{i=0}^{N-1-r}(1-2i)\right]\prod_{j=0}^{r}(-k-2j)\,. \tag{2.237}$$

From (2.205) and (2.220), where $x=\lambda^2$, we can write

$$x\xi^2 f(x)g(x) = \mathcal{N}(\lambda^2)\frac{\lambda^2\xi^2}{1-\lambda^2\xi^2}. \tag{2.238}$$

By comparing (2.237) with (2.238), we obtain $b_N$ as follow

$$b_N = (-1)^{N-1}\left(-\frac{1}{k}\right)\xi^2 \sum_{r=0}^{N-1}\left\{\frac{1}{r!(N-1-r)!\,2^{N-1-r}}\ \left(\frac{\xi^2}{2}\right)^r\right.$$

$$\left.\times\left[\prod_{i=0}^{N-1-r}(1-2i)\right]\prod_{j=0}^{r}(-k-2j)\right\} \tag{2.239}$$

where $N \geqslant 1, b_0 = 0$.

For $\xi^2 = \dfrac{1}{4}$, $\xi = \dfrac{1}{2}$, we have

$$b_N = (-1)^{N-1}\left(-\frac{1}{k}\right)\frac{1}{4}\ \sum_{r=0}^{N-1}\frac{1}{r!(N-1-r)!\,2^{N-1-r}}\ \left(\frac{1}{4}\cdot\frac{1}{2}\right)^r$$

$$\times\left[\prod_{i=0}^{N-1-r}(1-2i)\right]\prod_{j=0}^{r}(-k-2j)$$

$$= \frac{1}{4}(-1)^{N-1}\left(-\frac{1}{k}\right)\ \sum_{r=0}^{N-1}\frac{1}{r!(N-1-r)!\,2^{N-1-r}}\ \left(\frac{1}{8}\right)^r$$

$$\times\left[\prod_{i=0}^{N-1-r}(1-2i)\right]\prod_{j=0}^{r}(-k-2j)\,. \tag{2.240}$$

Simplify (2.240), we obtain

$$b_N = \left(\frac{1}{2}\right)^2(-1)^{N-1}\ \frac{(-1)}{k}\ \sum_{r=0}^{N-1}\left\{\frac{1}{2^{N-1}\,r!(N-1-r)!\,2^{-r}}\ \left(\frac{1}{2}\right)^{3r}\right.$$

$$\left.\times\ (-1)^{N-r}\ (-1)^{r+1}\ \left[\prod_{i=0}^{N-1-r}(2i-1)\right]\prod_{j=0}^{r}(2j+k)\right\}$$

$$= \left(\frac{1}{2}\right)^{N-1+2}\ \frac{(-1)^N}{k}\ \sum_{r=0}^{N-1}\left\{\frac{(-1)^{N+1}}{2^{2r}\,r!(N-1-r)!}\right.$$

$$\times \left[\prod_{i=0}^{N-1-r}(2i-1)\right]\prod_{j=0}^{r}(2j+k)\Bigg\}$$

$$= \frac{(-1)^{N+N+1}}{2^{N+1}}\,\frac{1}{k}\sum_{r=0}^{N-1}\Bigg\{\frac{1}{2^{2r}\,r!(N-1-r)!}$$

$$\times \left[\prod_{i=0}^{N-1-r}(2i-1)\right]\prod_{j=0}^{r}(2j+k)\Bigg\}$$

$$= -\frac{1}{k}\,\frac{1}{2^{N+1}}\sum_{r=0}^{N-1}\frac{\left[\prod_{i=0}^{N-1-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}r!(N-1-r)!}. \tag{2.241}$$

Rewrite (2.223) with $\xi = \dfrac{1}{2}$, we obtain

$$H_{2N} = \beta_N\left[\sum_{\alpha=1}^{k}T_\alpha - kT_0 + \frac{\frac{1}{2}}{\left(1+\frac{1}{2}\right)}(k-2)\sum_{\alpha=1}^{k}I_{0\alpha}\right]$$
$$+\,2N\left[T_0 - \frac{\frac{1}{2}}{\left(1+\frac{1}{2}\right)}\sum_{\alpha=1}^{k}I_{0\alpha}\right]$$

$$= \beta_N\left[\sum_{\alpha=1}^{k}T_\alpha - kT_0 + \frac{1}{3}(k-2)\sum_{\alpha=1}^{k}I_{0\alpha}\right] + 2N\left[T_0 - \frac{1}{3}\sum_{\alpha=1}^{k}I_{0\alpha}\right] \tag{2.242}$$

and

$$T_\alpha = \int \mathrm{d}^3\mathbf{x}\;\psi_\alpha^*(\mathbf{x})\left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}\right)\psi_\alpha(\mathbf{x}),\quad \alpha = 0,1,\ldots,k, \tag{2.243}$$

$$I_{0\alpha} = \int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\;\psi_0^*(\mathbf{x})\psi_\alpha^*(\mathbf{x})\frac{e^2}{|\mathbf{x}-\mathbf{x}'|}\psi_0(\mathbf{x}')\psi_\alpha(\mathbf{x}'),\quad \alpha = 1,\ldots,k. \tag{2.244}$$

The purpose of this work is to carry out a rigorous analysis of the expression in (2.242) in conjunction with the inequality in (2.34) to finally obtain an upper bound for $E_{N,N}$. To this end basic estimates are derived in Sect. 2.2 followed in

Sect. 2.3 by the derivation of the upper bound. Such an upper bound will be useful if it is, for example, less than the ground-state energy of $N$ isolated boson-equivalent of positronium atoms. This, as we will see, puts a self-consistency restriction on $N$. We were able to obtain a sharp estimate on the Dyson coefficient (cf. (2.222)) $\beta_n$ (Proposition 3), and have developed a way of counting (Proposition 6) the quantum states which is of central importance in establishing the upper bound of the ground-state energy.

## 2.2 Basic Estimates

For $\xi^2 = \dfrac{1}{4}$, we have

$$\frac{\lambda^2\xi^2}{1-\lambda^2\xi^2} = \frac{\frac{1}{4}\lambda^2}{1-\frac{1}{4}\lambda^2} = \frac{\lambda^2}{4-\lambda^2} \tag{2.245}$$

then

$$\text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)\frac{\lambda^2\xi^2}{1-\lambda^2\xi^2} = \text{coeff. of } (\lambda^2)^N \text{ of } \mathcal{N}(\lambda^2)\frac{\lambda^2}{4-\lambda^2} \equiv b_N. \tag{2.246}$$

Let

$$\mathcal{N}(\lambda^2)\frac{\lambda^2}{4-\lambda^2} = \sum_{N\geqslant 1} b_N(\lambda^2)^N \tag{2.247}$$

where $b_0 = 0$.

**Proposition 1**

$$D_N = 4b_{N+1} - b_N. \tag{2.248}$$

To establish this result, we multiply $\mathcal{N}(\lambda^2)$ by $\dfrac{4-\lambda^2}{\lambda^2}\dfrac{\lambda^2}{4-\lambda^2}$, we obtain

$$\begin{aligned}
\mathcal{N}(\lambda^2) &= \frac{4-\lambda^2}{\lambda^2}\mathcal{N}(\lambda^2)\frac{\lambda^2}{4-\lambda^2} \\
&= \frac{4}{\lambda^2}\mathcal{N}(\lambda^2)\frac{\lambda^2}{4-\lambda^2} - \mathcal{N}(\lambda^2)\frac{\lambda^2}{4-\lambda^2} \\
&= \frac{4}{\lambda^2}\sum_{N\geqslant 1} b_N(\lambda^2)^N - \sum_{N\geqslant 1} b_N(\lambda^2)^N \\
&= \sum_{N\geqslant 1} 4b_N(\lambda^2)^{N-1} - \sum_{N\geqslant 1} b_N(\lambda^2)^N \\
&= \sum_{N\geqslant 0} 4b_{N+1}(\lambda^2)^N - \sum_{N\geqslant 0} b_N(\lambda^2)^N \\
&= \sum_{N\geqslant 0}(4b_{N+1} - b_N)(\lambda^2)^N. \qquad (2.249)
\end{aligned}$$

From (2.221) and (2.249), Eq. (2.248) follows. □

Also, together with (2.222), we have the important equality

$$\beta_N = \frac{b_N}{4b_{N+1} - b_N}. \tag{2.250}$$

**Proposition 2**

*For $N \geqslant 2$, $k < 2N$*

$$\frac{3}{4}b_N \leqslant b_{N+1} \leqslant b_N \tag{2.251}$$

*where $b_N$ is defined in (2.241).*

By using (2.241), we obtain

$$b_{N+1} = -\frac{1}{k}\,\frac{1}{2^{(N+1)+1}}\sum_{r=0}^{(N+1)-1}\frac{\left[\prod_{i=0}^{(N+1)-1-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!\,\big[(N+1)-1-r\big]!}$$

$$= -\frac{1}{k}\,\frac{1}{2^{N+2}}\sum_{r=0}^{N}\frac{\left[\prod_{i=0}^{N-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!(N-r)!}$$

$$= -\frac{1}{k}\,\frac{1}{2^{N+2}}\sum_{r=0}^{N-1}\frac{\left[\prod_{i=0}^{N-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!(N-r)!}$$

$$-\frac{1}{k}\,\frac{1}{2^{N+2}}\,\frac{(-1)}{2^{2N}\,N!}\prod_{j=0}^{N}(2j+k)$$

$$= -\frac{1}{k}\,\frac{1}{2^{N+1}}\,\frac{1}{2}\sum_{r=0}^{N-1}\frac{\left[\prod_{i=0}^{N-1-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!(N-1-r)!}\cdot\frac{\big[2(N-r)-1\big]}{N-r}$$

$$-\frac{1}{k}\,\frac{1}{2^{N+1}}\,\frac{1}{2}\,\frac{(-1)}{2^{2(N-1)}\,(N-1)!}\left[\prod_{j=0}^{N-1}(2j+k)\right]\cdot\frac{(2N+k)}{2^2\,N}$$

$$= -\frac{1}{k}\,\frac{1}{2^{N+1}}\sum_{r=0}^{N-1}\frac{\left[\prod_{i=0}^{N-1-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!(N-1-r)!}\cdot\frac{[2(N-r)-1]}{2(N-r)}$$

$$-\frac{1}{k}\,\frac{1}{2^{N+1}}\,\frac{(-1)}{2^{2(N-1)}\,(N-1)!}\left[\prod_{j=0}^{N-1}(2j+k)\right]\cdot\frac{(2N+k)}{8N}$$

$$= -\frac{1}{k\,2^{N+1}}\sum_{r=0}^{N-2}\frac{\left[\prod_{i=0}^{N-1-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!(N-1-r)!}\cdot\frac{[2(N-r)-1]}{2(N-r)}$$

$$-\frac{1}{k\ 2^{N+1}}\ \frac{(-1)}{2^{2(N-1)}\,(N-1)!}\left[\prod_{j=0}^{r-1}(2j+k)\right]\cdot\frac{[2(N-(N-1))-1]}{2[N-(N-1)]}$$

$$-\frac{1}{k\ 2^{N+1}}\ \frac{(-1)}{2^{2(N-1)}\,(N-1)!}\left[\prod_{j=0}^{N-1}(2j+k)\right]\cdot\frac{(2N+k)}{8N}. \qquad (2.252)$$

Accordingly, by a rearrangement and a grouping of terms, we have

$$b_{N+1}=-\frac{1}{k\ 2^{N+1}}\left\{\sum_{r=0}^{N-2}\frac{\left[\prod_{i=0}^{N-1-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!(N-1-r)!}\cdot\frac{[2(N-r)-1]}{2(N-r)}\right\}$$

$$-\frac{1}{k\ 2^{N+1}}\ \frac{(-1)}{2^{2(N-1)}\,(N-1)!}\left[\prod_{j=0}^{N-1}(2j+k)\right]\left(\frac{1}{2}+\frac{2N+k}{8N}\right). \qquad (2.253)$$

Consider $\dfrac{2(N-r)-1}{2(N-r)}$ on the right-hand side of first term in (2.253) for $N \geqslant 2$, for

$$0 \leqslant r \leqslant N-2,$$

we multiply above inequality by $(-1)$, and then add the result by $N$, we obtain

$$N \geqslant N-r \geqslant N-(N-2).$$

The above inequality leads to

$$-\frac{1}{2N} \geqslant -\frac{1}{2(N-r)} \geqslant -\frac{1}{4}.$$

By adding above inequality by 1 leads to

$$\frac{3}{4} \leqslant 1-\frac{1}{2(N-r)} \equiv \frac{2(N-r)-1}{2(N-r)} < 1. \qquad (2.254)$$

Consider $\left(\frac{1}{2}+\frac{2N+k}{8N}\right)$ on the right-hand side of second term in (2.253), for $N \geqslant 2$, $k < 2N$, we have

$$0 \leqslant k < 2N.$$

Add above inequality by $2N$ and multiply the result by $\frac{1}{8N}$, then add the result by $\frac{1}{2}$, we obtain

$$\frac{1}{2}+\frac{1}{4} \leqslant \frac{1}{2}+\frac{2N+k}{8N} < \frac{1}{2}+\frac{1}{2}$$

then

$$\frac{3}{4} \leqslant \frac{1}{2}+\frac{2N+k}{8N} < 1. \tag{2.255}$$

From (2.253)–(2.255)

$$\begin{aligned}
&\frac{3}{4}\left(-\frac{1}{k\,2^{N+1}}\right)\sum_{r=0}^{N-2}\frac{\left[\prod_{i=0}^{N-1-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!(N-1-r)!}\\
&\leqslant\left(-\frac{1}{k\,2^{N+1}}\right)\sum_{r=0}^{N-2}\frac{\left[\prod_{i=0}^{N-1-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!(N-1-r)!}\cdot\frac{[2(N-r)-1]}{2(N-r)}\\
&<\left(-\frac{1}{k\,2^{N+1}}\right)\sum_{r=0}^{N-2}\frac{\left[\prod_{i=0}^{N-1-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!(N-1-r)!}
\end{aligned} \tag{2.256}$$

and

$$\frac{3}{4}\left(-\frac{1}{k\,2^{N+1}}\right)\frac{(-1)}{2^{2(N-1)}\,(N-1)!}\prod_{j=0}^{N-1}(2j+k)$$

$$\leqslant \left(-\frac{1}{k\,2^{N+1}}\right) \frac{(-1)}{2^{2(N-1)}\,(N-1)!} \left[\prod_{j=0}^{N-1} (2j+k)\right] \left(\frac{1}{2} + \frac{2N+k}{8N}\right)$$

$$< \left(-\frac{1}{k\,2^{N+1}}\right) \frac{(-1)}{2^{2(N-1)}\,(N-1)!} \prod_{j=0}^{N-1} (2j+k)\,. \tag{2.257}$$

The addition of inequalities in (2.256) and (2.257) gives

$$\frac{3}{4}\left\{\left(-\frac{1}{k\,2^{N+1}}\right) \sum_{r=0}^{N-2} \frac{\left[\prod_{i=0}^{N-1-r} (2i-1)\right]\left[\prod_{j=0}^{r} (2j+k)\right]}{2^{2r}\,r!(N-1-r)!}\right.$$

$$\left. + \left(-\frac{1}{k\,2^{N+1}}\right)(-1)\,\frac{\left[\prod_{j=0}^{N-1} (2j+k)\right]}{2^{2(N-1)}\,(N-1)!}\right\}$$

$$\leqslant -\frac{1}{k\,2^{N+1}} \sum_{r=0}^{N-2} \left\{\frac{\left[\prod_{i=0}^{N-1-r} (2i-1)\right]\left[\prod_{j=0}^{r} (2j+k)\right]}{2^{2r}\,r!(N-1-r)!} \cdot \frac{[2(N-r)-1]}{2(N-r)}\right\}$$

$$-\frac{1}{k\,2^{N+1}}\,\frac{(-1)}{2^{2(N-1)}\,(N-1)!} \left[\prod_{j=0}^{N-1} (2j+k)\right] \left(\frac{1}{2} + \frac{2N+k}{8N}\right). \tag{2.258}$$

Grouping the left-hand side of above inequality leads to

$$\frac{3}{4}\left(-\frac{1}{k\,2^{N+1}}\right) \sum_{r=0}^{N-1} \frac{\left[\prod_{i=0}^{N-1-r} (2i-1)\right]\left[\prod_{j=0}^{r} (2j+k)\right]}{2^{2r}\,r!(N-1-r)!}$$

$$\leqslant -\frac{1}{k\ 2^{N+1}} \sum_{r=0}^{N-2} \left\{ \frac{\left[\prod_{i=0}^{N-1-r} (2i-1)\right] \left[\prod_{j=0}^{r} (2j+k)\right]}{2^{2r}\, r!(N-1-r)!} \cdot \frac{[2(N-r)-1]}{2(N-r)} \right\}$$

$$- \frac{1}{k\ 2^{N+1}} \frac{(-1)}{2^{2(N-1)}(N-1)!} \left[\prod_{j=0}^{N-1} (2j+k)\right] \left(\frac{1}{2} + \frac{2N+k}{8N}\right). \tag{2.259}$$

Compare (2.259) with (2.241) and (2.253), then

$$\frac{3}{4} b_N \leqslant b_{N+1}. \tag{2.260}$$

Again, the addition of inequalities in (2.256) and (2.257) gives

$$-\frac{1}{k\ 2^{N+1}} \sum_{r=0}^{N-2} \left\{ \frac{\left[\prod_{i=0}^{N-1-r} (2i-1)\right] \left[\prod_{j=0}^{r} (2j+k)\right]}{2^{2r}\, r!(N-1-r)!} \cdot \frac{[2(N-r)-1]}{2(N-r)} \right\}$$

$$- \frac{1}{k\ 2^{N+1}} (-1) \frac{\left[\prod_{j=0}^{N-1} (2j+k)\right]}{2^{2(N-1)}\,(N-1)!} \left(\frac{1}{2} + \frac{2N+k}{8N}\right)$$

$$< \quad \left(-\frac{1}{k\ 2^{N+1}}\right) \sum_{r=0}^{N-2} \left\{ \frac{\left[\prod_{i=0}^{N-1-r} (2i-1)\right] \left[\prod_{j=0}^{r} (2j+k)\right]}{2^{2r}\, r!(N-1-r)!} \cdot \right\}$$

$$+ \left(-\frac{1}{k\ 2^{N+1}}\right) (-1) \frac{\left[\prod_{j=0}^{N-1} (2j+k)\right]}{2^{2(N-1)}\,(N-1)!} \tag{2.261}$$

Grouping the right-hand side of above inequality leads to

$$-\frac{1}{k\ 2^{N+1}}\sum_{r=0}^{N-2}\left\{\frac{\left[\prod_{i=0}^{N-1-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!(N-1-r)!}\cdot\frac{[2(N-r)-1]}{2(N-r)}\right\}$$

$$-\frac{1}{k\ 2^{N+1}}(-1)\,\frac{\left[\prod_{j=0}^{N-1}(2j+k)\right]}{2^{2(N-1)}\,(N-1)!}\left(\frac{1}{2}+\frac{2N+k}{8N}\right)$$

$$<\left(-\frac{1}{k\ 2^{N+1}}\right)\sum_{r=0}^{N-1}\frac{\left[\prod_{i=0}^{N-1-r}(2i-1)\right]\left[\prod_{j=0}^{r}(2j+k)\right]}{2^{2r}\,r!(N-1-r)!}. \tag{2.262}$$

Again, compare (2.262) with (2.241) and (2.253), then

$$b_{N+1}<b_N. \tag{2.263}$$

From (2.260) and (2.263), we obtain Proposition 2

$$\frac{3}{4}b_N\leqslant b_{N+1}<b_N. \tag{2.264}$$

□

**Proposition 3**

$$\frac{1}{3}<\beta_N\leqslant\frac{1}{2} \tag{2.265}$$

*where $\beta_N$ is defined in (2.222) and is the critical coefficient appearing in (2.242), for $N\geqslant 2,\ k<2N$.*

To obtain above inequality, we multiply (2.264) by 4 and then add by $(-b_N)$

$$3b_N - b_N \leqslant 4b_{N+1} - b_N < b4_N - b_N.$$

Rewrite above inequality

$$2b_N \leqslant 4b_{N+1} - b_N < 3b_N$$

then, multiply above inequality by $\frac{1}{b_N}$, we obtain

$$\frac{2b_N}{b_N} \leqslant \frac{4b_{N+1} - b_N}{b_N} < \frac{3b_N}{b_N}$$

then

$$2 \leqslant \frac{4b_{N+1} - b_N}{b_N} < 3. \tag{2.266}$$

We obtain the useful bound

$$\frac{1}{2} \geqslant \frac{b_N}{4b_{N+1} - b_N} > \frac{1}{3} \tag{2.267}$$

and from (2.250) we rewrite (2.267)

$$\frac{1}{3} < \beta_N \leqslant \frac{1}{2}. \tag{2.268}$$

Then, Proposition 3 is obtained and is of central importance in the entire investigation and (2.267) embodies basic inequalities used below. □

We rewrite the expression in Eq. (2.242) as

$$H_{2N} = \left[\beta_N \sum_{\alpha=1}^{k} T_\alpha - \beta_N k T_0 - \frac{1}{3}\beta_N (k-2)\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right)\right]$$

$$+ \left[2NT_0 + \frac{1}{3}2N\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right)\right]$$

$$= \beta_N \sum_{\alpha=1}^{k} T_\alpha + (2N - k\beta_N)T_0 + \frac{1}{3}[2N - (k-2)\beta_N]\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right). \quad (2.269)$$

Later in (2.398), we will bound $\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right)$ above by a strictly negative expression. Also, $\sum_{\alpha=1}^{k} T_\alpha$ and $T_0$ are positive. With $k$ chosen such that $k < 2N$, as before, we find, from the inequalities in (2.268), bound (2.269) will be derived below:

$$\beta_N \sum_{\alpha=1}^{k} T_\alpha \leqslant \frac{1}{2} \sum_{\alpha=1}^{k} T_\alpha. \quad (2.270)$$

Since $kT_0 > 0$ and $-\beta_N < -\frac{1}{3}$, then

$$-\beta_N k T_0 < -\frac{1}{3} k T_0$$

add $2NT_0$ to above inequality, we obtain

$$(2N - k\beta_N)T_0 < \left(2N - \frac{k}{3}\right) T_0. \quad (2.271)$$

Since $(k-2) > 0$ and $\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right)$ is strictly negative, then

$$(k-2)\beta_N \leqslant \frac{1}{2}(k-2).$$

Multiply above inequality by $-1$, we obtain

$$-(k-2)\beta_N \geqslant -\frac{(k-2)}{2}$$

then, add above inequality by $2N$, we obtain

$$2N-(k-2)\beta_N \geqslant 2N-\frac{(k-2)}{2}.$$

Multiply above inequality by $\frac{1}{3}\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right)$, we obtain

$$\frac{1}{3}[2N-(k-2)\beta_N]\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right) \leqslant \frac{1}{3}\left[2N-\frac{(k-2)}{2}\right]\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right). \qquad (2.272)$$

The addition of (2.270), (2.271) and (2.272), by comparing with (2.269), gives

$$H_{2N} < \frac{1}{2}\sum_{\alpha=1}^{k} T_\alpha + \left(2N-\frac{k}{3}\right)T_0 + \frac{1}{3}\left[2N-\frac{(k-2)}{2}\right]\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right) \qquad (2.273)$$

where $N \geqslant 2$. We replace $2N$ by $N$ in (2.273), then we obtain our basic bound

$$E_{N,N} < \frac{1}{2}\sum_{\alpha=1}^{k} T_\alpha + \left(N-\frac{k}{3}\right)T_0 + \frac{1}{3}\left[N-\frac{(k-2)}{2}\right]\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right) \qquad (2.274)$$

where we note that with $k < N$, in particular, that the coefficients of $T_0$ and $\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right)$ are strictly positive.

To the above end, for each triplet $(n_1, n_2, n_3)$ of *natural* numbers, we define a state specified by the tip of the vector $\mathbf{n} = (n_1, n_2, n_3)$. A non-trivial permutation of $(n_1, n_2, n_3)$ defines a different state. For example, $(1,1,2), (1,2,1)$ and $(2,1,1)$ define three distinct states all satisfying, however, the constraint $n^2 = n_1^2 + n_2^2 + n_3^2 = 6$.

For any given such an allowed $n^2$ (a natural number), let $k$ denote the number of distinct states, *excluding* the state $(1,1,1)$, with the constraint that the length squared of each vector specifying such a state is less or equal to $n^2$. These are the total number of states, excluding the state $(1,1,1)$, lying within, or falling on, the surface of $\dfrac{1}{8}$ of a sphere of radius $n$ in the so-called first quadrant, i.e., for which $n_1 \geqslant 1$, $n_2 \geqslant 1$, $n_3 \geqslant 1$.

Since, by definition, the state $(1,1,1)$ is excluded, the lowest possible value of $n^2$ is 6. For $n^2 = 6$, we have $k = 3$, corresponding to the non-trivial permutations of $(1,1,2)$. The next allowed value for $n^2$ is 9, with $k = 6$ corresponding to the non-trivial permutations of the states $(1,1,2)$ and $(1,2,2)$, and so on for the other allowed values of $n^2 = 11, 12, 14, \ldots$. We now establish the following.

**Proposition 4**

*For any allowed $n^2$, as defined above, we have the following inequality for the number of states $k$, also defined above, in terms of $n$:*

$$\frac{k}{n^3} \geqslant \sqrt{1 - \frac{2}{n^2}} \left( \frac{1}{3} - \frac{\sqrt{2}}{n} \right) - \frac{(3 + 2\sqrt{2})}{4n} - \frac{(3 - 2\sqrt{2})}{2} \frac{1}{n^3}. \qquad (2.275)$$

*Further, the right-hand side of this inequality is strictly positive for allowed values of $n^2 \geqslant 76$.*

To establish this inequality, we consider $s$ boxes each of height of one unit with square bases of areas $N_1 \times N_1, \ldots, N_s \times N_s$ with $1 \leqslant N_s \leqslant \cdots \leqslant N_1$ are stacked on top of each other as shown in the Fig. 2.1 inside a $\dfrac{1}{8}$ section of a sphere of radius $n$.

Since the height of each box is one unit, we choose $N_1, \ldots, N_s$ to be the *largest* positive integers such that

$$2N_1^2 + 1 \leqslant n^2, \ldots, 2N_s^2 + s^2 \leqslant n^2 \tag{2.276}$$

to make sure that the boxes fall within or touch the surface of a $\frac{1}{8}$ section of a sphere of radius $n$. That is, we take

$$N_1 + 1 \geqslant \sqrt{\frac{n^2 - 1}{2}} \geqslant N_1, \ldots, N_s + 1 \geqslant \sqrt{\frac{n^2 - s^2}{2}} \geqslant N_s. \tag{2.277}$$

We obtain from (2.277) that,

$$N_j + 1 \geqslant \sqrt{\frac{n^2 - j^2}{2}} \geqslant N_j \tag{2.278}$$

where $1 \leqslant j \leqslant s$. Also, $N_s \geqslant 1$, requires that $1 \leqslant \sqrt{\frac{n^2 - s^2}{2}}$. Hence $s$ is taken to be the largest positive integer such that

$$s \leqslant \sqrt{n^2 - 2} < s + 1. \tag{2.279}$$

For any $N_j$, $1 \leqslant j \leqslant s$, we have $N_j^2$ states such that

$$\begin{gathered}(j, 1, 1), (j, 1, 2), (j, 1, 3), \ldots, (j, 1, N_j), \\ (j, 2, 1), (j, 2, 2), (j, 2, 3), \ldots, (j, 2, N_j), \\ \vdots \\ (j, N_j, 1), (j, N_j, 2), (j, N_j, 3), \ldots, (j, N_j, N_j).\end{gathered} \tag{2.280}$$

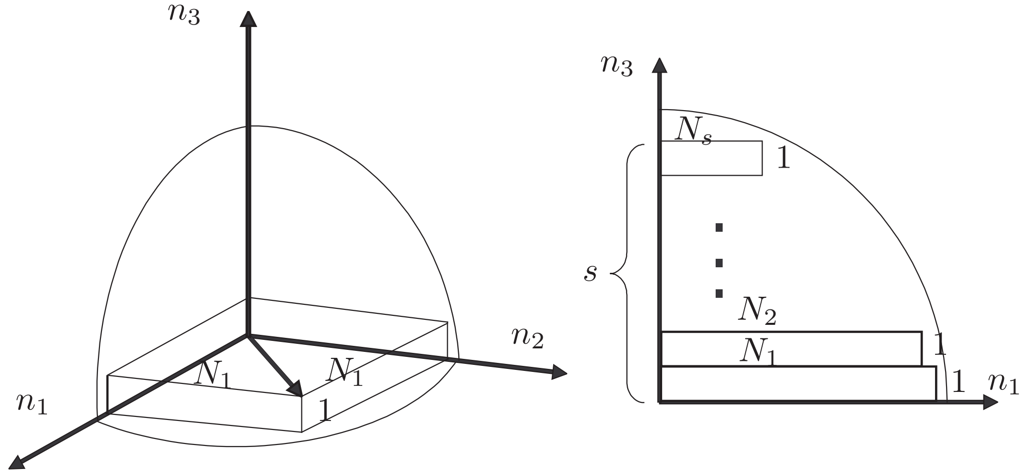


Figure 2.1: $s$ boxes of unit height and square bases of area $N_1 \times N_1, \ldots, N_s \times N_s$, with $1 \leqslant N_s \leqslant \cdots \leqslant N_1$, are stacked on top of each other inside a 1/8 section of a sphere of radius $n$. Bounds are obtained on $N_1, \ldots, N_s$ and $s$ in the text such that the boxes are within or just touch the surface of the 1/8 section of the sphere.

Excluding the state $(1, 1, 1)$, the total number $k$ of state $(n_1, n_2, n_3)$ which lie within or on the surface of a $\frac{1}{8}$ section of a sphere of radius $n$ clearly satisfies

$$k = \sum_{j=1}^{s} N_j^2 - 1. \tag{2.281}$$

Upon using the left-hand side of the inequalities in (2.278),

$$N_j \geqslant \sqrt{\frac{n^2 - j^2}{2}} - 1 \tag{2.282}$$

then

$$N_j^2 \geqslant \left( \sqrt{\frac{n^2 - j^2}{2}} - 1 \right)^2,$$

$$\sum_{j=1}^{s} N_j^2 \geqslant \sum_{j=1}^{s} \left( \sqrt{\frac{n^2 - j^2}{2}} - 1 \right)^2,$$

$$\sum_{j=1}^{s} N_j^2 - 1 \geqslant \sum_{j=1}^{s} \left( \sqrt{\frac{n^2 - j^2}{2}} - 1 \right)^2 - 1. \tag{2.283}$$

Eq. (2.281) yields

$$k \geqslant \sum_{j=1}^{s} \left( \sqrt{\frac{n^2 - j^2}{2}} - 1 \right)^2 - 1. \tag{2.284}$$

We have

$$\begin{aligned} \left( \sqrt{\frac{n^2 - j^2}{2}} - 1 \right)^2 &= \frac{n^2 - j^2}{2} - 2\sqrt{\frac{n^2 - j^2}{2}} + 1 \\ &= \frac{n^2 - j^2}{2} - \sqrt{2}\sqrt{(n-j)(n+j)} + 1. \end{aligned} \tag{2.285}$$

Since $(n - j) \leqslant (n + j)$, then

$$\sqrt{(n-j)(n+j)} \leqslant (n+j).$$

Multiply above inequality by $-\sqrt{2}$ and add the result by $\dfrac{(n^2 - j^2)}{2} + 1$, we obtain

$$\frac{n^2 - j^2}{2} - \sqrt{2}\sqrt{(n-j)(n+j)} + 1 \geqslant \frac{n^2 - j^2}{2} - \sqrt{2}(n+j) + 1.$$

Using the right-hand side of (2.285), we can rewrite above inequality

$$\left( \sqrt{\frac{n^2 - j^2}{2}} - 1 \right)^2 \geqslant \frac{n^2 - j^2}{2} - \sqrt{2}(n+j) + 1$$

then multiply above inequality by $\sum_{j=1}^{s}$, we obtain

$$\sum_{j=1}^{s} \left( \sqrt{\frac{n^2 - j^2}{2}} - 1 \right)^2 \geqslant \sum_{j=1}^{s} \left[ \frac{n^2 - j^2}{2} - \sqrt{2}(n+j) + 1 \right].$$

Add above inequality by $-1$, we obtain

$$\sum_{j=1}^{s}\left(\sqrt{\frac{n^2-j^2}{2}}-1\right)^2-1 \geqslant \sum_{j=1}^{s}\left[\frac{n^2-j^2}{2}-\sqrt{2}(n+j)+1\right]-1. \tag{2.286}$$

Substitute (2.286) in (2.284), we obtain

$$k \geqslant \sum_{j=1}^{s}\left[\frac{n^2-j^2}{2}-\sqrt{2}(n+j)+1\right]-1. \tag{2.287}$$

To obtain the bound of $k$, we use some elementary sums

$$\sum_{j=1}^{s} j = \frac{s(s+1)}{2}, \tag{2.288}$$

$$\sum_{j=1}^{s} j^2 = \frac{s(s+1)(2s+1)}{6}. \tag{2.289}$$

Consider the right-hand side of (2.287), by using the help of (2.288) and (2.289), we obtain

$$\begin{aligned}
&\sum_{j=1}^{s}\left[\frac{n^2-j^2}{2}-\sqrt{2}(n+j)+1\right]-1 \\
&\quad= \sum_{j=1}^{s}\frac{n^2}{2}-\sum_{j=1}^{s}\frac{j^2}{2}-\sqrt{2}\sum_{j=1}^{s}n-\sqrt{2}\sum_{j=1}^{s}j+\sum_{j=1}^{s}1-1 \\
&\quad= \frac{n^2 s}{2}-\frac{s(s+1)(2s+1)}{12}-\sqrt{2}ns-\frac{\sqrt{2}s(s+1)}{2}+s-1 \\
&\quad= \frac{n^2 s}{2}-\frac{2s^3+3s^2+s}{12}-\sqrt{2}ns-\frac{s^2}{\sqrt{2}}-\frac{s}{\sqrt{2}}+s-1 \\
&\quad= \left(\frac{n^2}{2}+1\right)s-\left[\frac{s^3}{6}+\left(\frac{1}{4}+\frac{1}{\sqrt{2}}\right)s^2+\left(\frac{1}{12}+\sqrt{2}n+\frac{1}{\sqrt{2}}\right)s+1\right] \\
&\quad= \left(\frac{n^2}{2}+1\right)s-\frac{1}{12}\left[2s^3+\left(3+6\sqrt{2}\right)s^2+\left(1+12\sqrt{2}n+6\sqrt{2}\right)s+12\right]
\end{aligned}$$

$$= \left(\frac{n^2}{2}+1\right) s - \frac{1}{12}\left[2s^3 + 3\left(1+2\sqrt{2}\right)s^2 + \left(1+6\sqrt{2}(2n+1)\right)s + 12\right]. \tag{2.290}$$

By using (2.279), we can find the bounds of $s$

$$s \leqslant \sqrt{n^2-2} = n\sqrt{1-\frac{2}{n^2}} \equiv s_{\max}, \tag{2.291}$$

$$s \geqslant \sqrt{n^2-2} - 1 \equiv s_{\max} - 1. \tag{2.292}$$

Using (2.291) and (2.292), Eq. (2.290) will be rewritten and the substitution of (2.290) in (2.287) gives

$$k \geqslant \left(\frac{n^2}{2}+1\right)(s_{\max}-1)$$

$$- \frac{1}{12}\left[2s_{\max}^3 + 3\left(1+2\sqrt{2}\right)s_{\max}^2 + \left(1+6\sqrt{2}(2n+1)\right)s_{\max} + 12\right]$$

$$= \left(\frac{n^2}{2}+1\right)s_{\max} - \left(\frac{n^2}{2}+1\right)$$

$$- \frac{1}{12}\left[2s_{\max}^3 + 3\left(1+2\sqrt{2}\right)s_{\max}^2 + \left(1+6\sqrt{2}(2n+1)\right)s_{\max} + 12\right]$$

$$= -\frac{1}{12}\left[2s_{\max}^3 + 3\left(1+2\sqrt{2}\right)s_{\max}^2\right.$$

$$\left. + \left(1+6\sqrt{2}(2n+1) - 6(n^2+2)\right)s_{\max} + 12\right] - \frac{n^2+2}{2}$$

$$= -\frac{1}{12}\left[2s_{\max}^3 + 3\left(1+2\sqrt{2}\right)s_{\max}^2\right.$$

$$\left. + \left(1+6\sqrt{2}(2n+1) - 6(n^2+2)\right)s_{\max} + 12 + 6(n^2+2)\right]$$

$$= -\frac{1}{12}\left[2s_{\max}^3 + 3\left(1+2\sqrt{2}\right)s_{\max}^2\right.$$

$$+\left(-6n^2+12\sqrt{2}n+(6\sqrt{2}-11)\right)s_{\max}+6(n^2+4)\Big]. \tag{2.293}$$

Substitute $s_{\max}$ from (2.291) in (2.293), we obtain

$$k \geqslant -\frac{1}{12}\left[2\left(n\sqrt{1-\frac{2}{n^2}}\right)^3+3\left(1+2\sqrt{2}\right)\left(n\sqrt{1-\frac{2}{n^2}}\right)^2\right.$$

$$\left.+\left(-6n^2+12\sqrt{2}n+(6\sqrt{2}-11)\right)\left(n\sqrt{1-\frac{2}{n^2}}\right)+6(n^2+4)\right]$$

$$=-\frac{1}{12}\left[2n^3\left(1-\frac{2}{n^2}\right)^{\frac{3}{2}}+3n^2\left(1+2\sqrt{2}\right)\left(1-\frac{2}{n^2}\right)\right.$$

$$\left.+n\left(-6n^2+12\sqrt{2}n+(6\sqrt{2}-11)\right)\left(1-\frac{2}{n^2}\right)^{\frac{1}{2}}+6(n^2+4)\right]$$

$$=-\frac{n^3}{12}\left[2\left(1-\frac{2}{n^2}\right)^{\frac{3}{2}}+\frac{3}{n}\left(1+2\sqrt{2}\right)\left(1-\frac{2}{n^2}\right)\right.$$

$$\left.+\frac{1}{n^2}\left(-6n^2+12\sqrt{2}n+(6\sqrt{2}-11)\right)\left(1-\frac{2}{n^2}\right)^{\frac{1}{2}}+\frac{6}{n^3}(n^2+4)\right]. \tag{2.294}$$

Multiply (2.294) by $\dfrac{1}{n^3}$ then

$$\frac{k}{n^3} \geqslant -\frac{1}{12}\left(1-\frac{2}{n^2}\right)^{\frac{1}{2}}\left[2\left(1-\frac{2}{n^2}\right)+\frac{1}{n^2}\left(-6n^2+12\sqrt{2}n+(6\sqrt{2}-11)\right)\right]$$

$$-\frac{1}{4n}\left(1+2\sqrt{2}\right)\left(1-\frac{2}{n^2}\right)-\frac{1}{2n^3}(n^2+4)$$

$$=\left(1-\frac{2}{n^2}\right)^{\frac{1}{2}}\left[\frac{1}{6}\left(\frac{2}{n^2}-1\right)+\frac{1}{12n^2}\left(6n^2-12\sqrt{2}n-6\sqrt{2}+11\right)\right]$$

$$-\frac{1}{4n}\left(1-\frac{2}{n^2}+2\sqrt{2}-\frac{4\sqrt{2}}{n^2}\right)-\left(\frac{1}{2n}+\frac{2}{n^3}\right)$$

$$= \left(1 - \frac{2}{n^2}\right)^{\frac{1}{2}} \left[\frac{1}{3n^2} - \frac{1}{6} + \frac{1}{2} - \frac{\sqrt{2}}{n} + \frac{(11 - 6\sqrt{2})}{12n^2}\right]$$

$$- \frac{1}{4n}\left[\left(1 + 2\sqrt{2}\right) - \frac{2}{n^2}\left(1 + 2\sqrt{2}\right)\right] - \left(\frac{1}{2n} + \frac{2}{n^3}\right)$$

$$= \left(1 - \frac{2}{n^2}\right)^{\frac{1}{2}} \left[\frac{1}{3} - \frac{\sqrt{2}}{n} + \frac{(15 - 6\sqrt{2})}{12n^2}\right]$$

$$- \frac{\left(1 + 2\sqrt{2}\right)}{4n}\left[1 - \frac{2}{n^2}\right] - \left(\frac{1}{2n} + \frac{2}{n^3}\right)$$

$$= \left(1 - \frac{2}{n^2}\right)^{\frac{1}{2}} \left[\frac{1}{3} - \frac{\sqrt{2}}{n} + \frac{(5 - 2\sqrt{2})}{4n^2}\right]$$

$$- \frac{\left(1 + 2\sqrt{2}\right)}{4n} - \frac{1}{2n} + \frac{2\left(1 + 2\sqrt{2}\right)}{4n^3} - \frac{2}{n^3}$$

$$= \left(1 - \frac{2}{n^2}\right)^{\frac{1}{2}} \left[\frac{1}{3} - \frac{\sqrt{2}}{n} + \frac{(5 - 2\sqrt{2})}{4n^2}\right] - \frac{\left(3 + 2\sqrt{2}\right)}{4n} - \frac{\left(3 - 2\sqrt{2}\right)}{2n^3}. \quad (2.295)$$

The coefficient of $\frac{1}{n^2}$ in the first brackets in (2.295) is positive value, i.e.,

$$\frac{(5 - 2\sqrt{2})}{4n^2} \geqslant 0. \quad (2.296)$$

Eq. (2.295) becomes

$$\frac{k}{n^3} \geqslant \left(1 - \frac{2}{n^2}\right)^{\frac{1}{2}} \left[\frac{1}{3} - \frac{\sqrt{2}}{n}\right] - \frac{\left(3 + 2\sqrt{2}\right)}{4n} - \frac{\left(3 - 2\sqrt{2}\right)}{2n^3}. \quad (2.297)$$

Then, Proposition 4 follows. □

Estimates of the sort in (2.295), involving corrections, are available in the literature. A classic example of this is filling a sphere with smaller ones (the so-called Swiss-Cheese theorem) see, e.g., Thirring (1983), Fisher (1964). For further reading, see Pfender and Ziegler (2004) and Casselman (2004). The estimate in (2.295), as it stands, is not, however, what is ultimately needed. What we need is a more involved one which allows to count $(k - k')$ states corresponding to two consecutive $n^2 > n'^2$ values which is of central importance in deriving the upper bound for the ground-state energy in Sect. 2.3. This is established in Proposition 6 and will be used extensively in Sect. 2.3, particularly, in (2.388) and (2.398).

**Proposition 5**

*Let $n'^2 < n^2$ be consecutive allowed values of $n^2$. Then*

$$n - n' \leqslant 1 + \frac{3}{2n'} \tag{2.298}$$

*and*

$$n\left[1 - \frac{1}{n'}\left(1 + \frac{3}{2n'}\right)\right] \leqslant n' \tag{2.299}$$

*where the coefficient of $n$ on the left-hand side of the latter inequality is positive for all allowed $n'^2$.*

To establish the validity of (2.298), note that although $n'^2$ is a natural number, $n'$ is not necessarily so. Accordingly, let $n'_0$ be the largest positive integer such that $n'_0 \leqslant n'$. That is, we have

$$n' = n'_0 + x, \quad 0 \leqslant x < 1 \tag{2.300}$$

then

$$n' < n'_0 + 1. \tag{2.301}$$

Next, consider the state specified by the vector $\mathbf{n}''$, where

$$\mathbf{n}'' = (n'_0 + 1, 1, 1). \tag{2.302}$$

The length of $\mathbf{n}''$ is $n''$ where

$$n''^2 = (n_0' + 1)^2 + 1^2 + 1^2 = (n_0' + 1)^2 + 2 > n'^2 + 2. \tag{2.303}$$

Clearly,

$$n''^2 > n'^2. \tag{2.304}$$

Since, $n^2$ and $n'^2$ are consecutive, with $n > n'$, it follows that $n \leqslant n''$.

From (2.300) and (2.303) we have

$$\begin{aligned} n''^2 - n'^2 &= (n_0' + 1)^2 + 2 - (n_0' + x)^2 \\ &= n_0'^2 + 2n_0' + 1 + 2 - n_0'^2 - 2n_0'x - x^2 \\ &= 2n_0'(1 - x) + (3 - x^2). \end{aligned} \tag{2.305}$$

Since

$$(n'' - n')^2 = n''^2 + n'^2 - 2n''n' \geqslant 0 \tag{2.306}$$

then

$$2n''n' \leqslant n''^2 + n'^2. \tag{2.307}$$

We have

$$2n'(n'' - n') = 2n'n'' - 2n'^2. \tag{2.308}$$

By adding (2.307) with $-2n'^2$, we obtain the right-hand side of (2.308) and by comparing with (2.305)

$$\begin{aligned} 2n'n'' - 2n'^2 &\leqslant n''^2 + n'^2 - 2n'^2 \\ &= n''^2 - n'^2 \end{aligned}$$

$$= 2n_0'(1-x) + (3-x^2). \tag{2.309}$$

Then, from (2.308), Eq. (2.309) can be rewritten as

$$2n'(n''-n') \leqslant 2n_0'(1-x) + (3-x^2). \tag{2.310}$$

Multiply (2.310) by $\dfrac{1}{2n'}$, therefore, with (2.300), we obtain

$$\begin{aligned}
n''-n' &\leqslant \frac{2n_0'(1-x)}{2n'} + \frac{(3-x^2)}{2n'} \\
&= \frac{2n_0'(1-x)}{2\left(n_0'+x\right)} + \frac{(3-x^2)}{2n'} \\
&= \frac{2n_0'(1-x)}{2n_0'\left(1+\dfrac{x}{n_0'}\right)} + \frac{(3-x^2)}{2n'} \\
&= \frac{1-x}{1+\dfrac{x}{n_0'}} + \frac{(3-x^2)}{2n'}.
\end{aligned} \tag{2.311}$$

For $x \geqslant 0$, we have

$$1-x \leqslant 1. \tag{2.312}$$

Since $\dfrac{x}{n_0'} \geqslant 0$ then

$$\frac{1}{1+\dfrac{x}{n_0'}} \leqslant 1. \tag{2.313}$$

Since $x^2 \geqslant 0$ then

$$\frac{3-x^2}{2n'} \leqslant \frac{3}{2n'}. \tag{2.314}$$

We multiply (2.312) by (2.313) and then add by (2.314), we obtain

$$\frac{1-x}{1+\dfrac{x}{n_0'}} \leqslant 1,$$

$$\frac{1-x}{1+\dfrac{x}{n_0'}}+\frac{(3-x^2)}{2n'}\leqslant 1+\frac{3}{2n'}. \tag{2.315}$$

Substitute (2.315) in (2.311) we get

$$n''-n'\leqslant 1+\frac{3}{2n'}. \tag{2.316}$$

For $n\leqslant n''$, we have

$$n-n'\leqslant n''-n'\leqslant 1+\frac{3}{2n'}$$

then

$$n-n'\leqslant 1+\frac{3}{2n'}. \tag{2.317}$$

The above expression is the first inequality expressed in Proposition 5. Eq. (2.317) can be rewritten as

$$n-\left(1+\frac{3}{2n'}\right)\leqslant n',$$

$$n\left[1-\frac{1}{n}\left(1+\frac{3}{2n'}\right)\right]\leqslant n'. \tag{2.318}$$

For $n>n'$, we have

$$-\frac{1}{n}>-\frac{1}{n'},$$

$$-\frac{1}{n}\left(1+\frac{3}{2n'}\right)\geqslant -\frac{1}{n'}\left(1+\frac{3}{2n'}\right),$$

$$1-\frac{1}{n}\left(1+\frac{3}{2n'}\right)\geqslant 1-\frac{1}{n'}\left(1+\frac{3}{2n'}\right),$$

$$n\left[1-\frac{1}{n}\left(1+\frac{3}{2n'}\right)\right]\geqslant n\left[1-\frac{1}{n'}\left(1+\frac{3}{2n'}\right)\right]. \tag{2.319}$$

Then, by comparing (2.318) with (2.319), the latter inequality in Proposition 5 follows,

$$n' \geqslant n\left[1 - \frac{1}{n'}\left(1 + \frac{3}{2n'}\right)\right]. \tag{2.320}$$

□

For any consecutive $n^2 > n'^2$, we label the $(k - k')$ state specified by those vectors *all* of length squared equal to $n^2$, in arbitrary orders, as $\alpha = k' + 1, k' + 2, \ldots, k$

$$k \geqslant \alpha > k' \tag{2.321}$$

where $k' \equiv$ number of states in $\dfrac{1}{8}$ sphere of radius $n'$.

**Proposition 6**

*We have the inequality*

$$\alpha > n^3 \left[1 - \frac{1}{n'}\left(1 + \frac{3}{2n'}\right)\right]^3 C(n') \tag{2.322}$$

*where*

$$C(n') = \left(1 - \frac{2}{n'^2}\right)^{\frac{1}{2}} \left[\frac{1}{3} - \frac{\sqrt{2}}{n'}\right] - \frac{3 + 2\sqrt{2}}{4n'} - \frac{3 - 2\sqrt{2}}{2n'^3} \tag{2.323}$$

*for* $n'^2 \geqslant 76$.

From (2.297), let

$$\left(1 - \frac{2}{n^2}\right)^{\frac{1}{2}} \left[\frac{1}{3} - \frac{\sqrt{2}}{n}\right] - \frac{3 + 2\sqrt{2}}{4n} - \frac{3 - 2\sqrt{2}}{2n^3} \equiv C(n) \tag{2.324}$$

then Eq. (2.297) can be rewritten as

$$k' \geqslant n'^3 C(n'). \tag{2.325}$$

From (2.320), we can rewrite (2.325) as

$$k' \geqslant n^3 \left[1 - \frac{1}{n'}\left(1 + \frac{3}{2n'}\right)\right]^3 C(n'). \tag{2.326}$$

Using (2.321), $\alpha > k'$, then, with (2.326), Proposition 6 follows, i.e.,

$$\alpha > n^3 \left[1 - \frac{1}{n'}\left(1 + \frac{3}{2n'}\right)\right]^3 C(n'). \tag{2.327}$$

The constraint $n'^2 \geqslant 76$ just ensures the positivity of $C(n')$. (As an example, note that $n'^2 = 76$ for the state specified by the vector $\mathbf{n}' = (2, 6, 6)$.) $\square$

Proposition 3 and 6 contain two of the key new estimates obtained in this work. For example for $n^2 \geqslant 100^2$, $\mathbf{n} = (36, 48, 80)$, the consecutive allowed values is $\mathbf{n}' = (1, 14, 99)$, $n' = 99.9899$ then, for $n \geqslant 100$,

$$\begin{aligned} \alpha &> n^3 \left[1 - \frac{1}{n'}\left(1 + \frac{3}{2n'}\right)\right]^3 C(n') \\ &> \frac{n^3}{3.3852}. \end{aligned} \tag{2.328}$$

## 2.3 Derivation of the Upper Bounds

For orthonormal trial functions, we choose the Dyson ones (Dyson, 1967):

$$\phi_{\mathbf{n}}(\mathbf{x}) = \left(\frac{2}{L}\right)^{\frac{3}{2}} \prod_{i=1}^{3} \sin\left(\frac{n_i \pi x_i}{L}\right) \tag{2.329}$$

for $0 < x_i < L$, and vanishing outside this interval, we label the states as $\alpha = 0$ for $\mathbf{n}_0 = (1,1,1)$, $\alpha = 1,2,3$ for $\mathbf{n} = (1,1,2),(1,2,1),(2,1,1)$, respectively, and so on.

With our effort in deriving the bound given in this work, we have found the Dyson trial functions most suitable for the problem at hand for the following reasons:

(1) We need an *orthonormal* set of functions defined on a bounded interval, vanishing at its endpoints, with the length of the interval (chosen optimally) becoming smaller and smaller as $N$ increases, representing the localization of the particles and eventual collapse for large $N$.

(2) The trial orthonormal functions in (2.329) are simple enough to allow for explicit sharp analytical estimates, as seen below.

(3) We have tried other orthonormal trial functions, such as the Hermite functions with an arbitrary scale parameter, and in all cases, we have found that the negative interaction becomes very small in comparison to the kinetic energy part for large $n$ and hence that these functions are not appropriate as trial functions. In particular, while the normalization constant in (2.329) is independent of $n$, this is not true, for example, with Hermite functions.

(4) The trial functions in (2.329) overlap. This is necessary for the interaction term in (2.331) to be non-vanishing, and thus non-overlapping orthonormal states defined on sub-intervals of $(0, L)$ are not useful.

(5) Based on the estimates established in Sect. 2.2, the trial functions in (2.329) already lead to an improvement to the classic Dyson bound.

Let

$$
\begin{aligned}
T^{(\mathbf{n})} &= \left\langle \phi_{\mathbf{n}} \middle| \left( -\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} \right) \middle| \phi_{\mathbf{n}} \right\rangle \\
&= \frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{x}\ \left| \boldsymbol{\nabla} \phi_{\mathbf{n}}(\mathbf{x}) \right|^2 , \qquad (2.330)
\end{aligned}
$$

$$I^{(\mathbf{n})} = \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\ \phi_{\mathbf{n_0}}(\mathbf{x})\phi_{\mathbf{n}}(\mathbf{x}) \frac{e^2}{|\mathbf{x}-\mathbf{x}'|} \phi_{\mathbf{n_0}}(\mathbf{x}')\phi_{\mathbf{n}}(\mathbf{x}'). \tag{2.331}$$

For $\mathbf{x} = (x_1, x_2, x_3)$, we have

$$\boldsymbol{\nabla} = \frac{\partial}{\partial x_1}\hat{\mathbf{i}} + \frac{\partial}{\partial x_2}\hat{\mathbf{j}} + \frac{\partial}{\partial x_3}\hat{\mathbf{k}} \tag{2.332}$$

then

$$\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x}) = \frac{\partial \phi_{\mathbf{n}}(\mathbf{x})}{\partial x_1}\hat{\mathbf{i}} + \frac{\partial \phi_{\mathbf{n}}(\mathbf{x})}{\partial x_2}\hat{\mathbf{j}} + \frac{\partial \phi_{\mathbf{n}}(\mathbf{x})}{\partial x_3}\hat{\mathbf{k}}, \tag{2.333}$$

$$|\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x})|^2 = \left|\frac{\partial \phi_{\mathbf{n}}(\mathbf{x})}{\partial x_1}\right|^2 + \left|\frac{\partial \phi_{\mathbf{n}}(\mathbf{x})}{\partial x_2}\right|^2 + \left|\frac{\partial \phi_{\mathbf{n}}(\mathbf{x})}{\partial x_3}\right|^2, \tag{2.334}$$

$$\int \mathrm{d}^3\mathbf{x}\ |\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x})|^2 = \sum_{i=1}^{3} \int \mathrm{d}^3\mathbf{x}\ \left|\frac{\partial \phi_{\mathbf{n}}(\mathbf{x})}{\partial x_i}\right|^2. \tag{2.335}$$

We consider only for the case of $i = 1$ :

$$\begin{aligned} \frac{\partial \phi_{\mathbf{n}}(\mathbf{x})}{\partial x_1} &= \left(\frac{2}{L}\right)^{\frac{3}{2}} \frac{\partial}{\partial x_1} \sin\left(\frac{n_1\pi x_1}{L}\right) \sin\left(\frac{n_2\pi x_2}{L}\right) \sin\left(\frac{n_3\pi x_3}{L}\right) \\ &= \left(\frac{2}{L}\right)^{\frac{3}{2}} \left(\frac{n_1\pi}{L}\right) \cos\left(\frac{n_1\pi x_1}{L}\right) \sin\left(\frac{n_2\pi x_2}{L}\right) \sin\left(\frac{n_3\pi x_3}{L}\right) \end{aligned} \tag{2.336}$$

then

$$\left|\frac{\partial \phi_{\mathbf{n}}(\mathbf{x})}{\partial x_1}\right|^2 = \left(\frac{2}{L}\right)^{3} \left(\frac{n_1\pi}{L}\right)^2 \cos^2\left(\frac{n_1\pi x_1}{L}\right) \sin^2\left(\frac{n_2\pi x_2}{L}\right) \sin^2\left(\frac{n_3\pi x_3}{L}\right). \tag{2.337}$$

Multiply above equation by $\int \mathrm{d}^3\mathbf{x}$, then

$$\begin{aligned} &\int \mathrm{d}^3\mathbf{x}\ \left|\frac{\partial \phi_{\mathbf{n}}(\mathbf{x})}{\partial x_1}\right|^2 \\ &\qquad = \left(\frac{2}{L}\right)^{3} \left(\frac{n_1\pi}{L}\right)^2 \int_0^L \mathrm{d}x_1\ \cos^2\left(\frac{n_1\pi x_1}{L}\right) \end{aligned}$$

$$\times \int_0^L \mathrm{d}x_2 \ \sin^2\left(\frac{n_2\pi x_2}{L}\right) \int_0^L \mathrm{d}x_3 \ \sin^2\left(\frac{n_3\pi x_3}{L}\right)$$

$$= \left(\frac{2}{L}\right)^3 \left(\frac{n_1\pi}{L}\right)^2 \left(\frac{L}{2}\right)^3$$

$$= \left(\frac{n_1\pi}{L}\right)^2. \tag{2.338}$$

Then, from (2.338), we have

$$\int \mathrm{d}^3\mathbf{x} \ \left|\frac{\partial \phi_{\mathbf{n}}(\mathbf{x})}{\partial x_i}\right|^2 = \left(\frac{n_i\pi}{L}\right)^2. \tag{2.339}$$

Substitute (2.339) in (2.335), then we obtain

$$\int \mathrm{d}^3\mathbf{x} \ |\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x})|^2 = \left(\frac{n_1\pi}{L}\right)^2 + \left(\frac{n_2\pi}{L}\right)^2 + \left(\frac{n_3\pi}{L}\right)^2$$

$$= \left(\frac{n\pi}{L}\right)^2 \tag{2.340}$$

where $n^2 = n_1^2 + n_2^2 + n_3^2$. Then, by using (2.340), we obtain

$$T^{(\mathbf{n})} = \frac{\pi^2\hbar^2 n^2}{2mL^2}. \tag{2.341}$$

From (2.329), we obtain

$$\phi_{\mathbf{n}}(\mathbf{x}) = \left(\frac{2}{L}\right)^{\frac{3}{2}} \sin\left(\frac{n_1\pi x_1}{L}\right) \sin\left(\frac{n_2\pi x_2}{L}\right) \sin\left(\frac{n_3\pi x_3}{L}\right), \tag{2.342}$$

$$\phi_{\mathbf{m}}(\mathbf{x}) = \left(\frac{2}{L}\right)^{\frac{3}{2}} \sin\left(\frac{m_1\pi x_1}{L}\right) \sin\left(\frac{m_2\pi x_2}{L}\right) \sin\left(\frac{m_3\pi x_3}{L}\right) \tag{2.343}$$

then

$$\int \mathrm{d}^3\mathbf{x} \ |\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2$$

$$= \left(\frac{2}{L}\right)^6 \left[\int_0^L \mathrm{d}x_1 \ \sin^2\left(\frac{n_1\pi x_1}{L}\right) \sin^2\left(\frac{m_1\pi x_1}{L}\right)\right]$$

$$\times \left[\int_0^L \mathrm{d}x_2 \ \sin^2\left(\frac{n_2\pi x_2}{L}\right) \sin^2\left(\frac{m_2\pi x_2}{L}\right)\right]$$

$$\times \left[\int_0^L \mathrm{d}x_3 \ \sin^2\left(\frac{n_3\pi x_3}{L}\right) \sin^2\left(\frac{m_3\pi x_3}{L}\right)\right]$$

$$= \left(\frac{2}{L}\right)^6 \prod_{i=1}^{3} \left[\int_0^L \mathrm{d}x_i \ \sin^2\left(\frac{n_i\pi x_i}{L}\right) \sin^2\left(\frac{m_i\pi x_i}{L}\right)\right] \tag{2.344}$$

where the integral on the right-hand side of (2.344) is given by

$$\int_0^L \mathrm{d}x_i \ \sin^2\left(\frac{n_i\pi x_i}{L}\right) \sin^2\left(\frac{m_i\pi x_i}{L}\right) = \frac{L}{4}. \tag{2.345}$$

Substitute (2.345) in (2.344), then we obtain

$$\begin{aligned}\int \mathrm{d}^3\mathbf{x} \ |\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2 &= \left(\frac{2}{L}\right)^6 \left(\frac{L}{4}\right)^3 \\ &= \frac{1}{L^3}.\end{aligned} \tag{2.346}$$

Let

$$\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \ F(\mathbf{k}) \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{2.347}$$

then

$$\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x}) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \ F(\mathbf{k})(\mathrm{i}\mathbf{k}) \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{2.348}$$

We square above equation, then

$$\begin{aligned}|\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2 &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3} \ (\mathrm{i}\mathbf{k}) \cdot (-\mathrm{i}\mathbf{k}') F(\mathbf{k}) F^*(\mathbf{k}') \, \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3} \ \mathbf{k}\cdot\mathbf{k}' \ F(\mathbf{k}) F^*(\mathbf{k}') \, \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}.\end{aligned} \tag{2.349}$$

Multiply above equation by $\int \mathrm{d}^3\mathbf{x}$, we obtain

$$\begin{aligned}\int \mathrm{d}^3\mathbf{x}\ |\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2 &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\ \mathbf{k}\cdot\mathbf{k}' F(\mathbf{k})F^*(\mathbf{k}') \int \mathrm{d}^3\mathbf{x}\ \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k}'\ \mathbf{k}\cdot\mathbf{k}' F(\mathbf{k})F^*(\mathbf{k}') \left(\int \frac{\mathrm{d}^3\mathbf{x}}{(2\pi)^3}\ \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}\right) \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k}'\ \mathbf{k}\cdot\mathbf{k}' F(\mathbf{k})F^*(\mathbf{k}')\delta(\mathbf{k}-\mathbf{k}') \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ |\mathbf{k}|^2\, |F(\mathbf{k})|^2 . \end{aligned} \tag{2.350}$$

From (2.347), we obtain

$$|\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2 = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\ F(\mathbf{k})F^*(\mathbf{k}')\ \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}. \tag{2.351}$$

Multiply (2.351) by $\int \mathrm{d}^3\mathbf{x}$, we obtain

$$\begin{aligned}\int \mathrm{d}^3\mathbf{x}\ |\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2 &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k}'\ F(\mathbf{k})F^*(\mathbf{k}') \left(\int \frac{\mathrm{d}^3\mathbf{x}}{(2\pi)^3}\ \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}\right) \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k}'\ F(\mathbf{k})F^*(\mathbf{k}')\delta(\mathbf{k}-\mathbf{k}') \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ |F(\mathbf{k})|^2 . \end{aligned} \tag{2.352}$$

From Schwarz inequality (Woan, 2000),

$$\left(\int_a^b \mathrm{d}x\ f(x)g(x)\right)^2 \leqslant \int_a^b \mathrm{d}x\ \ [f(x)]^2 \int_a^b \mathrm{d}x\ \ [g(x)]^2 . \tag{2.353}$$

Eq. (2.352) can be rewritten as

$$\int \mathrm{d}^3\mathbf{x}\ |\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2 = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ |F(\mathbf{k})|^2$$

$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ |F(\mathbf{k})|\,|\mathbf{k}|\,\frac{1}{|\mathbf{k}|}\,|F(\mathbf{k})|\,. \tag{2.354}$$

By using (2.353), we obtain

$$\begin{aligned}\left(\int \mathrm{d}^3\mathbf{x}\ |\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2\right)^2 &\leqslant \left(\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ |F(\mathbf{k})|^2\,|\mathbf{k}|^2\right)\left(\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ \frac{|F(\mathbf{k})|^2}{|\mathbf{k}|^2}\right)\\ &= \left(\int \mathrm{d}^3\mathbf{x}\ |\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2\right)\left(\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\ \frac{|F(\mathbf{k})|^2}{|\mathbf{k}|^2}\right).\end{aligned} \tag{2.355}$$

Consider

$$\begin{aligned}\int \mathrm{d}^3\mathbf{x}\ \frac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}{|\mathbf{k}|^2} &= \int_0^{2\pi}\mathrm{d}\phi\ \int_{\pi/2}^{-\pi/2}\mathrm{d}\theta\ \int_0^{\infty}\mathrm{d}k\ k^2\sin\theta\frac{\mathrm{e}^{-\mathrm{i}|\mathbf{k}||\mathbf{R}|\cos\theta}}{|\mathbf{k}|^2-\varepsilon^2}\\ &= 2\pi\int_0^{\infty}\mathrm{d}k\ k^2\int_{-1}^{1}\mathrm{d}(\cos\theta)\ \frac{\mathrm{e}^{-\mathrm{i}kR\cos\theta}}{k^2-\varepsilon^2}\end{aligned} \tag{2.356}$$

where $\varepsilon \to 0$, $\mathbf{R} = \mathbf{x} - \mathbf{x}'$, let $\cos\theta \equiv p$, then (2.356) becomes

$$\begin{aligned}\int \mathrm{d}^3\mathbf{x}\ \frac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}{|\mathbf{k}|^2} &= 2\pi\int_0^{\infty}\mathrm{d}k\ k^2\int_{-1}^{1}\mathrm{d}p\ \frac{\mathrm{e}^{-\mathrm{i}kRp}}{k^2-\varepsilon^2}\\ &= 2\pi\int_0^{\infty}\frac{\mathrm{d}k\ k^2}{-\mathrm{i}kR}\left(\frac{\mathrm{e}^{-\mathrm{i}kRp}}{k^2-\varepsilon^2}\right)\Bigg|_{p=-1}^{p=1}\\ &= \frac{2\pi}{-\mathrm{i}R}\int_0^{\infty}\mathrm{d}k\ k\left(\frac{\mathrm{e}^{-\mathrm{i}kR}-\mathrm{e}^{\mathrm{i}kR}}{k^2-\varepsilon^2}\right)\\ &= -\frac{2\pi}{\mathrm{i}R}\int_0^{\infty}\mathrm{d}k\ k\frac{\mathrm{e}^{-\mathrm{i}kR}}{k^2-\varepsilon^2}+\frac{2\pi}{\mathrm{i}R}\int_0^{\infty}\mathrm{d}k\ k\frac{\mathrm{e}^{\mathrm{i}kR}}{k^2-\varepsilon^2}\\ &= -\frac{2\pi}{\mathrm{i}R}(-1)\int_{\infty}^{0}\mathrm{d}k\ k\frac{\mathrm{e}^{-\mathrm{i}kR}}{k^2-\varepsilon^2}+\frac{2\pi}{\mathrm{i}R}\int_0^{\infty}\mathrm{d}k\ k\frac{\mathrm{e}^{\mathrm{i}kR}}{k^2-\varepsilon^2}\\ &= \frac{2\pi}{\mathrm{i}R}\int_{-\infty}^{0}\mathrm{d}(-k)\ (-k)\frac{\mathrm{e}^{-\mathrm{i}(-k)R}}{(-k)^2-\varepsilon^2}+\frac{2\pi}{\mathrm{i}R}\int_0^{\infty}\mathrm{d}k\ k\frac{\mathrm{e}^{\mathrm{i}kR}}{k^2-\varepsilon^2}\end{aligned}$$

$$= \frac{2\pi}{\mathrm{i}R}\int_{-\infty}^{0}\mathrm{d}k\; k\frac{\mathrm{e}^{\mathrm{i}kR}}{k^2-\varepsilon^2} + \frac{2\pi}{\mathrm{i}R}\int_{0}^{\infty}\mathrm{d}k\; k\frac{\mathrm{e}^{\mathrm{i}kR}}{k^2-\varepsilon^2}$$

$$= \frac{2\pi}{\mathrm{i}R}\int_{-\infty}^{\infty}\mathrm{d}k\; k\frac{\mathrm{e}^{\mathrm{i}kR}}{k^2-\varepsilon^2}$$

$$= \frac{2\pi}{\mathrm{i}R}\oint\mathrm{d}k\; k\frac{\mathrm{e}^{\mathrm{i}kR}}{k^2-\varepsilon^2}$$

$$= \frac{2\pi}{\mathrm{i}^2R}\oint\mathrm{d}k\; \frac{\partial}{\partial R}\frac{\mathrm{e}^{\mathrm{i}kR}}{k^2-\varepsilon^2}$$

$$= -\frac{2\pi}{R}\frac{\partial}{\partial R}\oint\mathrm{d}k\; \frac{\mathrm{e}^{\mathrm{i}kR}}{(k-\varepsilon)(k+\varepsilon)}$$

$$= -\frac{2\pi}{R}\frac{\partial}{\partial R}(2\pi\mathrm{i})\frac{\mathrm{e}^{\mathrm{i}\varepsilon R}}{2\varepsilon}$$

$$= \frac{2\pi^2}{R}\mathrm{e}^{\mathrm{i}\varepsilon R} \tag{2.357}$$

for $\varepsilon \to 0$. Then (2.357) becomes

$$\int \mathrm{d}^3\mathbf{x}\; \frac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}{|\mathbf{k}|^2} = \frac{2\pi^2}{|\mathbf{x}-\mathbf{x}'|}. \tag{2.358}$$

From (2.347) we have

$$F(\mathbf{k}) = \int \mathrm{d}^3\mathbf{x}\; \phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{2.359}$$

We square above expression, then we obtain

$$|F(\mathbf{k})|^2 = \int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\; \phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\; \phi_{\mathbf{n}}(\mathbf{x}')\phi_{\mathbf{m}}(\mathbf{x}'). \tag{2.360}$$

Multiply (2.360) by $\int d^3\mathbf{k}\ |\mathbf{k}|^{-2}$, we obtain

$$\int d^3\mathbf{k}\ \frac{|F(\mathbf{k})|^2}{|\mathbf{k}|^2} = \int d^3\mathbf{x}\, d^3\mathbf{x}'\ \phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x}) \left( \int d^3\mathbf{k}\ \frac{e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}{|\mathbf{k}|^2} \right) \phi_{\mathbf{n}}(\mathbf{x}')\phi_{\mathbf{m}}(\mathbf{x}'). \tag{2.361}$$

Substitute (2.358) in (2.361), then we obtain

$$\begin{aligned} \int d^3\mathbf{k}\ \frac{|F(\mathbf{k})|^2}{|\mathbf{k}|^2} &= \int d^3\mathbf{x}\, d^3\mathbf{x}'\ \phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x}) \left( \frac{2\pi^2}{|\mathbf{x}-\mathbf{x}'|} \right) \phi_{\mathbf{n}}(\mathbf{x}')\phi_{\mathbf{m}}(\mathbf{x}') \\ &= 2\pi^2 \int d^3\mathbf{x}\, d^3\mathbf{x}'\ \phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_{\mathbf{n}}(\mathbf{x}')\phi_{\mathbf{m}}(\mathbf{x}'). \end{aligned} \tag{2.362}$$

Multiply (2.362) by $\frac{e^2}{2\pi^2}$ then

$$\begin{aligned} \int d^3\mathbf{x}\, d^3\mathbf{x}'\ \phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x}) \frac{e^2}{|\mathbf{x}-\mathbf{x}'|} \phi_{\mathbf{n}}(\mathbf{x}')\phi_{\mathbf{m}}(\mathbf{x}') &= e^2 \int \frac{d^3\mathbf{k}}{2\pi^2}\ \frac{|F(\mathbf{k})|^2}{|\mathbf{k}|^2} \\ &= 4\pi e^2 \int \frac{d^3\mathbf{k}}{(2\pi)^3}\ \frac{|F(\mathbf{k})|^2}{|\mathbf{k}|^2}. \end{aligned} \tag{2.363}$$

Let $\mathbf{m} = (1,1,1) = \mathbf{n}_0$, Eq. (2.363) becomes

$$\begin{aligned} \int d^3\mathbf{x}\, d^3\mathbf{x}'\ \phi_{\mathbf{n}_0}(\mathbf{x})\phi_{\mathbf{n}}(\mathbf{x}) \frac{e^2}{|\mathbf{x}-\mathbf{x}'|} \phi_{\mathbf{n}_0}(\mathbf{x}')\phi_{\mathbf{n}}(\mathbf{x}') &= e^2 \int \frac{d^3\mathbf{k}}{2\pi^2}\ \frac{|F(\mathbf{k})|^2}{|\mathbf{k}|^2} \\ &= 4\pi e^2 \int \frac{d^3\mathbf{k}}{(2\pi)^3}\ \frac{|F(\mathbf{k})|^2}{|\mathbf{k}|^2} \\ &= I^{(\mathbf{n})} \end{aligned} \tag{2.364}$$

where

$$\int d^3\mathbf{x}\, d^3\mathbf{x}'\ \phi_{\mathbf{n}_0}(\mathbf{x})\phi_{\mathbf{n}}(\mathbf{x}) \frac{e^2}{|\mathbf{x}-\mathbf{x}'|} \phi_{\mathbf{n}_0}(\mathbf{x}')\phi_{\mathbf{n}}(\mathbf{x}') \equiv I^{(\mathbf{n})}. \tag{2.365}$$

Substitute (2.364) in (2.355), we obtain

$$I^{(\mathbf{n})} \geqslant 4\pi e^2 \frac{\left(\displaystyle\int \mathrm{d}^3\mathbf{x}\ |\phi_{\mathbf{n}_0}(\mathbf{x})\phi_{\mathbf{n}}(\mathbf{x})|^2\right)^2}{\displaystyle\int \mathrm{d}^3\mathbf{x}\ |\boldsymbol{\nabla}\phi_{\mathbf{n}_0}(\mathbf{x})\phi_{\mathbf{n}}(\mathbf{x})|^2}. \tag{2.366}$$

From (2.346), Eq. (2.366) becomes

$$I^{(\mathbf{n})} \geqslant \frac{4\pi e^2 \left(\dfrac{1}{L^3}\right)^2}{\displaystyle\int \mathrm{d}^3\mathbf{x}\ |\boldsymbol{\nabla}\phi_{\mathbf{n}_0}(\mathbf{x})\phi_{\mathbf{n}}(\mathbf{x})|^2}. \tag{2.367}$$

We can find the denominator of above equation by consider, for $\mathbf{x} = (x_1, x_2, x_3)$,

$$\begin{aligned}
\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x}) = \left(\frac{2}{L}\right)^3 \Bigg\{ & \hat{\mathbf{i}}\frac{\partial}{\partial x_1}\left[\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{m_1\pi x_1}{L}\right)\right] \\
& \times \sin\left(\frac{n_2\pi x_2}{L}\right)\sin\left(\frac{m_2\pi x_2}{L}\right)\sin\left(\frac{n_3\pi x_3}{L}\right)\sin\left(\frac{m_3\pi x_3}{L}\right) \\
& + \hat{\mathbf{j}}\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{m_1\pi x_1}{L}\right)\frac{\partial}{\partial x_2}\left[\sin\left(\frac{n_2\pi x_2}{L}\right)\sin\left(\frac{m_2\pi x_2}{L}\right)\right] \\
& \times \sin\left(\frac{n_3\pi x_3}{L}\right)\sin\left(\frac{m_3\pi x_3}{L}\right) \\
& + \hat{\mathbf{k}}\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{m_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right)\sin\left(\frac{m_2\pi x_2}{L}\right) \\
& \times \frac{\partial}{\partial x_3}\left[\sin\left(\frac{n_3\pi x_3}{L}\right)\sin\left(\frac{m_3\pi x_3}{L}\right)\right]\Bigg\}.
\end{aligned} \tag{2.368}$$

The square of above equation is given by

$$\begin{aligned}
& |\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2 \\
& = \left(\frac{2}{L}\right)^6 \Bigg\{\left[\frac{\mathrm{d}}{\mathrm{d}x_1}\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{m_1\pi x_1}{L}\right)\right]^2
\end{aligned}$$

$$\times \sin^2\left(\frac{n_2\pi x_2}{L}\right)\sin^2\left(\frac{m_2\pi x_2}{L}\right)\sin^2\left(\frac{n_3\pi x_3}{L}\right)\sin^2\left(\frac{m_3\pi x_3}{L}\right)$$

$$+ \sin^2\left(\frac{n_1\pi x_1}{L}\right)\sin^2\left(\frac{m_1\pi x_1}{L}\right)\left[\frac{\mathrm{d}}{\mathrm{d}x_2}\sin\left(\frac{n_2\pi x_2}{L}\right)\sin\left(\frac{m_2\pi x_2}{L}\right)\right]^2$$

$$\times \sin^2\left(\frac{n_3\pi x_3}{L}\right)\sin^2\left(\frac{m_3\pi x_3}{L}\right)$$

$$+ \sin^2\left(\frac{n_1\pi x_1}{L}\right)\sin^2\left(\frac{m_1\pi x_1}{L}\right)\sin^2\left(\frac{n_2\pi x_2}{L}\right)\sin^2\left(\frac{m_2\pi x_2}{L}\right)$$

$$\times \left[\frac{\mathrm{d}}{\mathrm{d}x_3}\sin\left(\frac{n_3\pi x_3}{L}\right)\sin\left(\frac{m_3\pi x_3}{L}\right)\right]^2\Bigg\}. \tag{2.369}$$

Multiply (2.369) by $\int \mathrm{d}^3\mathbf{x}$, we obtain

$$\int \mathrm{d}^3\mathbf{x}\ |\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2$$

$$= \left(\frac{2}{L}\right)^6 \Bigg\{\int_0^L \mathrm{d}x_1\ \left[\frac{\mathrm{d}}{\mathrm{d}x_1}\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{m_1\pi x_1}{L}\right)\right]^2$$

$$\times \int_0^L \mathrm{d}x_2\ \sin^2\left(\frac{n_2\pi x_2}{L}\right)\sin^2\left(\frac{m_2\pi x_2}{L}\right)$$

$$\times \int_0^L \mathrm{d}x_3\ \sin^2\left(\frac{n_3\pi x_3}{L}\right)\sin^2\left(\frac{m_3\pi x_3}{L}\right)$$

$$+ \int_0^L \mathrm{d}x_1\ \sin^2\left(\frac{n_1\pi x_1}{L}\right)\sin^2\left(\frac{m_1\pi x_1}{L}\right)$$

$$\times \int_0^L \mathrm{d}x_2\ \left[\frac{\mathrm{d}}{\mathrm{d}x_2}\sin\left(\frac{n_2\pi x_2}{L}\right)\sin\left(\frac{m_2\pi x_2}{L}\right)\right]^2$$

$$\times \int_0^L \mathrm{d}x_3\ \sin^2\left(\frac{n_3\pi x_3}{L}\right)\sin^2\left(\frac{m_3\pi x_3}{L}\right)$$

$$+ \int_0^L \mathrm{d}x_1\ \sin^2\left(\frac{n_1\pi x_1}{L}\right)\sin^2\left(\frac{m_1\pi x_1}{L}\right)$$

$$\times \int_0^L \mathrm{d}x_2 \ \sin^2\left(\frac{n_2\pi x_2}{L}\right)\sin^2\left(\frac{m_2\pi x_2}{L}\right)$$

$$\left.\times \int_0^L \mathrm{d}x_3 \ \left[\frac{\mathrm{d}}{\mathrm{d}x_3}\sin\left(\frac{n_3\pi x_3}{L}\right)\sin\left(\frac{m_3\pi x_3}{L}\right)\right]^2\right\}$$

$$= \left(\frac{2}{L}\right)^6\left(\frac{L}{4}\right)^2\sum_{i=1}^{3}\int_0^L \mathrm{d}x_i \ \left[\frac{\mathrm{d}}{\mathrm{d}x_i}\sin\left(\frac{n_i\pi x_i}{L}\right)\sin\left(\frac{m_i\pi x_i}{L}\right)\right]^2. \tag{2.370}$$

The integral on the right-hand side of (2.370) can be derived as follow

$$\frac{\mathrm{d}}{\mathrm{d}x_i}\sin\left(\frac{n_i\pi x_i}{L}\right)\sin\left(\frac{m_i\pi x_i}{L}\right)$$

$$= \left[\frac{\mathrm{d}}{\mathrm{d}x_i}\sin\left(\frac{n_i\pi x_i}{L}\right)\right]\sin\left(\frac{m_i\pi x_i}{L}\right) + \sin\left(\frac{n_i\pi x_i}{L}\right)\left[\frac{\mathrm{d}}{\mathrm{d}x_i}\sin\left(\frac{m_i\pi x_i}{L}\right)\right]$$

$$= \left(\frac{n_i\pi}{L}\right)\cos\left(\frac{n_i\pi x_i}{L}\right)\sin\left(\frac{m_i\pi x_i}{L}\right) + \left(\frac{m_i\pi}{L}\right)\sin\left(\frac{n_i\pi x_i}{L}\right)\cos\left(\frac{m_i\pi x_i}{L}\right). \tag{2.371}$$

The square of (2.371) gives

$$\left[\frac{\mathrm{d}}{\mathrm{d}x_i}\sin\left(\frac{n_i\pi x_i}{L}\right)\sin\left(\frac{m_i\pi x_i}{L}\right)\right]^2$$

$$= \left(\frac{n_i\pi}{L}\right)^2\cos^2\left(\frac{n_i\pi x_i}{L}\right)\sin^2\left(\frac{m_i\pi x_i}{L}\right) + \left(\frac{m_i\pi}{L}\right)^2\sin^2\left(\frac{n_i\pi x_i}{L}\right)\cos^2\left(\frac{m_i\pi x_i}{L}\right)$$

$$+ 2\left(\frac{n_i\pi}{L}\right)\left(\frac{m_i\pi}{L}\right)\cos\left(\frac{n_i\pi x_i}{L}\right)\sin\left(\frac{m_i\pi x_i}{L}\right)\sin\left(\frac{n_i\pi x_i}{L}\right)\cos\left(\frac{m_i\pi x_i}{L}\right). \tag{2.372}$$

Multiply (2.372) by $\int_0^L \mathrm{d}x_i$, we obtain

$$\int_0^L \mathrm{d}x_i \ \left[\frac{\mathrm{d}}{\mathrm{d}x_i}\sin\left(\frac{n_i\pi x_i}{L}\right)\sin\left(\frac{m_i\pi x_i}{L}\right)\right]^2$$

$$
\begin{aligned}
&= \left(\frac{n_i\pi}{L}\right)^2 \int_0^L \mathrm{d}x_i \ \cos^2\left(\frac{n_i\pi x_i}{L}\right)\sin^2\left(\frac{m_i\pi x_i}{L}\right) \\
&\quad + \left(\frac{m_i\pi}{L}\right)^2 \int_0^L \mathrm{d}x_i \ \sin^2\left(\frac{n_i\pi x_i}{L}\right)\cos^2\left(\frac{m_i\pi x_i}{L}\right) \\
&\quad + 2\left(\frac{n_i\pi}{L}\right)\left(\frac{m_i\pi}{L}\right)\left\{\int_0^L \mathrm{d}x_i \ \cos\left(\frac{n_i\pi x_i}{L}\right)\sin\left(\frac{m_i\pi x_i}{L}\right)\right. \\
&\quad \left. \times \sin\left(\frac{n_i\pi x_i}{L}\right)\cos\left(\frac{m_i\pi x_i}{L}\right)\right\} \\
&= \left(\frac{L}{4}\right)\left(\frac{\pi}{L}\right)^2\left(n_i^2+m_i^2\right). \qquad (2.373)
\end{aligned}
$$

Substitute (2.373) in (2.370) then

$$
\begin{aligned}
\int \mathrm{d}^3\mathbf{x} \ |\boldsymbol{\nabla}\phi_{\mathbf{n}}(\mathbf{x})\phi_{\mathbf{m}}(\mathbf{x})|^2 &= \left(\frac{2}{L}\right)^6\left(\frac{L}{4}\right)^2\sum_{i=1}^{3}\left(\frac{L}{4}\right)\left(\frac{\pi}{L}\right)^2\left(n_i^2+m_i^2\right) \\
&= \frac{\pi^2}{L^5}\left(n_1^2+n_2^2+n_3^2+m_1^2+m_2^2+m_3^2\right) \\
&= \frac{\pi^2}{L^5}\left(n^2+m^2\right). \qquad (2.374)
\end{aligned}
$$

For $\mathbf{m} = \mathbf{n}_0$, $m^2 = n_0^2 = 3$, then (2.374) becomes

$$
\int \mathrm{d}^3\mathbf{x} \ |\boldsymbol{\nabla}\phi_{\mathbf{n}_0}(\mathbf{x})\phi_{\mathbf{n}}(\mathbf{x})|^2 = \frac{\pi^2}{L^5}\left(n^2+3\right). \qquad (2.375)
$$

Substitute (2.375) in (2.367), then we obtain

$$
\begin{aligned}
I^{(\mathbf{n})} &\geqslant \frac{4\pi e^2\left(\dfrac{1}{L^3}\right)^2}{\dfrac{\pi^2}{L^5}\left(n^2+3\right)} \\
&= \frac{4e^2}{\pi L}\frac{1}{(n^2+3)}. \qquad (2.376)
\end{aligned}
$$

From (2.327), let

$$\left[1 - \frac{1}{n'}\left(1 + \frac{3}{2n'}\right)\right]^{-2} C^{-\frac{2}{3}}(n') \equiv c \tag{2.377}$$

then we can rewrite (2.327) as

$$\alpha > \frac{n^3}{c^{3/2}} \tag{2.378}$$

or

$$n^2 < \alpha^{2/3} c \tag{2.379}$$

from which $c$ is determined. For example, for $n' \geqslant 100$, $c = 2.25456$. Accordingly, we may write from (2.243) and (2.341),

$$\sum_n T^{(\mathbf{n})} = \sum_{\alpha=1}^{k} T_\alpha. \tag{2.380}$$

Let $k_n$ is the number of distinct state in state $n$ (see Appendix A), then

$$\begin{aligned}\sum_{\alpha=1}^{k} T_\alpha &= T_1 + T_2 + \cdots + T_k \\ &= \frac{\hbar^2\pi^2}{2mL^2}\Big\{(n^2 = 6)[k_6 = 3] + (n^2 = 9)[k_9 = 3] + (n^2 = 11)[k_{11} = 3] \\ &+ (n^2 = 12)[k_{12} = 1] + \cdots + (n^2 = n'^2)[k_{n'}] + (n^2)[k_n = (k - k')]\Big\}\end{aligned} \tag{2.381}$$

where $k' \equiv$ number of state in $\frac{1}{8}$ sphere of radius $n'$ exclude state $(1, 1, 1)$, then

$$k' = \sum_{n > \sqrt{3}}^{n'} [k_n]. \tag{2.382}$$

Eq. (2.381) can be rewritten as

$$\sum_{\alpha=1}^{k} T_\alpha = \frac{\hbar^2\pi^2}{2mL^2} \sum_{n>\sqrt{3}}^{n'} \left(n^2 k_n\right) + \frac{\hbar^2\pi^2}{2mL^2} n^2(k-k')$$

$$= \frac{\hbar^2\pi^2}{2mL^2} \left[a + (k-k')n^2\right] \tag{2.383}$$

where

$$a = \sum_{n>\sqrt{3}}^{n'} \left(n^2 k_n\right). \tag{2.384}$$

The quantity $k_n$ multiplying $n^2$ corresponds to all those vectors representing states with length squared precisely equal to $n^2$.

Because

$$\alpha \leqslant k \tag{2.385}$$

and from (2.379), we obtain

$$n^2 < \alpha^{2/3} c \leqslant k^{2/3} c. \tag{2.386}$$

Multiply (2.386) by $(k-k')$, then

$$n^2(k-k') < k^{2/3} c(k-k')$$

add above inequality by $a$, we obtain

$$\left[a + (k-k')n^2\right] < \left[a + k^{2/3} c(k-k')\right].$$

Multiply above inequality by $\frac{\hbar^2\pi^2}{2mL^2}$, we obtain

$$\frac{\hbar^2\pi^2}{2mL^2} \left[a + (k-k')n^2\right] < \frac{\hbar^2\pi^2}{2mL^2} \left[a + k^{2/3} c(k-k')\right]. \tag{2.387}$$

Compare (2.387) with (2.383), then we obtain

$$\sum_{\alpha=1}^{k} T_\alpha < \frac{\hbar^2\pi^2}{2mL^2}\left[a + k^{2/3}c(k-k')\right]. \tag{2.388}$$

Similarly, from (2.365) and (2.376), we have

$$\sum_{n>\sqrt{3}} I^{(\mathbf{n})} = \sum_{\alpha=1}^{k} I_{0\alpha}. \tag{2.389}$$

Multiplying (2.376) by $(-1)$ gives

$$-I^{(\mathbf{n})} \leqslant -\frac{4e^2}{\pi L}\,\frac{1}{(n^2+3)}$$

then

$$-\sum_{n>\sqrt{3}} I^{(\mathbf{n})} = -\sum_{\alpha=1}^{k} I_{0\alpha} \leqslant -\frac{4e^2}{\pi L}\sum_{n>\sqrt{3}} \frac{[k_n]}{n^2+3}. \tag{2.390}$$

Consider the right-hand side of (2.390)

$$\sum_{n>\sqrt{3}} \frac{[k_n]}{n^2+3} = \sum_{n>\sqrt{3}}^{n'} \frac{[k_n]}{n^2+3} + \sum_{\alpha=k'+1}^{k} \frac{1}{n^2+3}. \tag{2.391}$$

Let

$$\sum_{n>\sqrt{3}}^{n'} \frac{[k_n]}{n^2+3} \equiv b \tag{2.392}$$

and we have

$$\sum_{\alpha=k'+1}^{k} \frac{1}{n^2+3} = \frac{(k-k')}{n^2+3}. \tag{2.393}$$

Then, by using (2.391), (2.392) and (2.393), Eq. (2.390) becomes

$$-\sum_{\alpha=1}^{k} I_{0\alpha} \leqslant -\frac{4e^2}{\pi L}\left[b + \frac{(k-k')}{n^2+3}\right]. \tag{2.394}$$

From (2.378) and (2.385), we obtain

$$\frac{n^3}{c^{3/2}} < \alpha \leqslant k$$

then

$$\frac{n^2}{c} < \alpha^{2/3} \leqslant k^{2/3}.$$

Multiply above inequality by $c$, we obtain

$$n^2 < c\alpha^{2/3} \leqslant ck^{2/3}$$

add above inequality by 3, we obtain

$$n^2 + 3 < c\alpha^{2/3} + 3 \leqslant ck^{2/3} + 3 \leqslant ck^{2/3} + 3k^{2/3} = (c+3)k^{2/3} \tag{2.395}$$

then

$$n^2 + 3 < (c+3)k^{2/3}, \tag{2.396}$$

$$\frac{1}{n^2+3} > \frac{1}{(c+3)k^{2/3}}.$$

Multiply above inequality by $(k - k')$, we obtain

$$\frac{k-k'}{n^2+3} > \frac{k-k'}{(c+3)k^{2/3}}$$

add above inequality by $b$, we obtain

$$b + \frac{k-k'}{n^2+3} > b + \frac{k-k'}{(c+3)k^{2/3}}$$

multiply above inequality by $-\frac{4e^2}{\pi L}$, we obtain

$$-\frac{4e^2}{\pi L}\left[b + \frac{k-k'}{n^2+3}\right] < -\frac{4e^2}{\pi L}\left[b + \frac{k-k'}{(c+3)k^{2/3}}\right]. \tag{2.397}$$

Compare (2.397) with (2.394), then we obtain

$$-\sum_{\alpha=1}^{k} I_{0\alpha} \leqslant -\frac{4e^2}{\pi L}\left[b + \frac{k-k'}{(c+3)k^{2/3}}\right]. \tag{2.398}$$

Multiply (2.388) by $\frac{1}{2}$, we obtain

$$\frac{1}{2}\sum_{\alpha=1}^{k} T_\alpha < \frac{1}{2}\frac{\hbar^2\pi^2}{2mL^2}\left[a + k^{2/3}c(k-k')\right] \tag{2.399}$$

and we have

$$\left(N - \frac{k}{3}\right)T_0 = \frac{3\hbar^2\pi^2}{2mL^2}\left(N - \frac{k}{3}\right). \tag{2.400}$$

Multiply (2.398) by $\frac{1}{3}\left[N-(k-2)\frac{1}{2}\right]$, we obtain

$$\frac{1}{3}\left[N-(k-2)\frac{1}{2}\right]\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right) \leqslant \frac{1}{3}\left[N-(k-2)\frac{1}{2}\right]\left(-\frac{4e^2}{\pi L}\right)\left[b + \frac{k-k'}{(c+3)k^{2/3}}\right]. \tag{2.401}$$

The addition of (2.399)–(2.401) leads to the following bound

$$\begin{aligned}
&\frac{1}{2}\sum_{\alpha=1}^{k} T_\alpha + \left(N-\frac{k}{3}\right)T_0 + \frac{1}{3}\left[N-(k-2)\frac{1}{2}\right]\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right) \\
&\qquad < \frac{1}{2}\left(\frac{\hbar^2\pi^2}{2mL^2}\right)\left[a + k^{2/3}c(k-k')\right] + \frac{3\hbar^2\pi^2}{2mL^2}\left(N-\frac{k}{3}\right) \\
&\qquad + \frac{1}{3}\left[N-(k-2)\frac{1}{2}\right]\left(-\frac{4e^2}{\pi L}\right)\left[b + \frac{k-k'}{(c+3)k^{2/3}}\right].
\end{aligned} \tag{2.402}$$

Compare (2.274) and (2.402), we obtain

$$\begin{aligned}
E_{N,N} &< \frac{\hbar^2\pi^2}{4mL^2}\left[a + k^{2/3}c(k-k')\right] + \frac{3\hbar^2\pi^2}{2mL^2}\left(N-\frac{k}{3}\right) \\
&\quad + \frac{1}{3}\left[N-(k-2)\frac{1}{2}\right]\left(-\frac{4e^2}{\pi L}\right)\left[b + \frac{k-k'}{(c+3)k^{2/3}}\right]
\end{aligned}$$

$$\equiv f(A) \tag{2.403}$$

where $f(A)$ is defined by

$$f(A) = \frac{\hbar^2\pi^2}{4mL^2}\left[a + k^{2/3}c(k-k')\right] + \frac{3\hbar^2\pi^2}{2mL^2}\left(N - \frac{k}{3}\right)$$

$$+\frac{1}{3}\left[N-(k-2)\frac{1}{2}\right]\left(-\frac{4e^2}{\pi L}\right)\left[b + \frac{k-k'}{(c+3)k^{2/3}}\right]$$

$$\equiv pA^2 - qA \tag{2.404}$$

where $p$, $q > 0$. We want to find the minimum point of the right-hand side of (2.404). The optimization of $f(A)$ is given below

$$\left.\frac{\mathrm{d}f(A)}{\mathrm{d}A}\right|_{A=A_0} = 2pA_0 - q = 0, \tag{2.405}$$

$$\frac{\mathrm{d}^2 f(A)}{\mathrm{d}A^2} = 2p \geqslant 0. \tag{2.406}$$

From (2.405), we obtain

$$A_0 = \frac{q}{2p} \tag{2.407}$$

gives the minimum point $f(A_0)$ then

$$E_{N,N} < f(A_0). \tag{2.408}$$

Let

$$\frac{1}{L} = \left(\frac{me^2}{\hbar^2\pi^3}\right)N^{1/5}A \tag{2.409}$$

where $A$ will be determined optimally. Substitute $\frac{1}{L}$ in (2.404), we obtain

$$f(A) = \frac{\hbar^2\pi^2}{4m}\left(\frac{m^2e^4N^{2/5}}{\hbar^4\pi^6}\right)A^2\left[a + k^{2/3}c(k-k')\right]$$

$$+\frac{3\hbar^2\pi^2}{2m}\left(\frac{m^2e^4N^{2/5}}{\hbar^4\pi^6}\right)A^2\left(N-\frac{k}{3}\right)$$

$$+\frac{1}{3}\left[N-(k-2)\frac{1}{2}\right]\left(-\frac{4e^2}{\pi}\frac{me^2N^{1/5}}{\hbar^2\pi^3}\right)A\left[b+\frac{k-k'}{(c+3)k^{2/3}}\right]$$

$$=\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\frac{A^2}{2N}\left[a+k^{2/3}c(k-k')\right]+\frac{me^4}{2\hbar^2}\left(\frac{N^{7/5}}{\pi^4}\right)\frac{3A^2}{N}\left(N-\frac{k}{3}\right)$$

$$+\frac{1}{3}\left[N-(k-2)\frac{1}{2}\right]\left(-\frac{me^4}{2\hbar^2}\frac{N^{7/5}}{\pi^4}\right)\frac{8A}{N^{6/5}}\left[b+\frac{k-k'}{(c+3)k^{2/3}}\right]$$

$$=\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\left\{\frac{A^2}{2N}\left[a+k^{2/3}c(k-k')\right]+\frac{3A^2}{N}\left(N-\frac{k}{3}\right)\right.$$

$$\left.-\frac{1}{3}\left[N-(k-2)\frac{1}{2}\right]\frac{8A}{N^{6/5}}\left[b+\frac{k-k'}{(c+3)k^{2/3}}\right]\right\}$$

$$=\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\left\{A^2\left[3\left(1-\frac{k}{3N}\right)+\left[a+k^{2/3}c(k-k')\right]\frac{1}{2N}\right]\right.$$

$$\left.-\frac{8}{3}A\left[1-(k-2)\frac{1}{2N}\right]\frac{1}{N^{1/5}}\left[b+\frac{k-k'}{(c+3)k^{2/3}}\right]\right\}$$

$$=\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\{\,\cdot\,\} \tag{2.410}$$

where

$$\{\,\cdot\,\}=\left\{A^2\left[3\left(1-\frac{k}{3N}\right)+\left[a+k^{2/3}c(k-k')\right]\frac{1}{2N}\right]\right.$$

$$\left.-\frac{8}{3}A\left[1-(k-2)\frac{1}{2N}\right]\frac{1}{N^{1/5}}\left[b+\frac{k-k'}{(c+3)k^{2/3}}\right]\right\}. \tag{2.411}$$

Since $k<N$, then

$$1-\frac{k}{3N}>1-\frac{N}{3N}=\frac{2}{3}>0. \tag{2.412}$$

For $k>k'$, then

$$\left[a+k^{2/3}c(k-k')\right]\frac{1}{2N}>\frac{a}{2N}>0. \tag{2.413}$$

Compare (2.411) with (2.404), we have

$$p = \left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\left[3\left(1-\frac{k}{3N}\right)+\left[a+k^{2/3}c(k-k')\right]\frac{1}{2N}\right] > 0 \tag{2.414}$$

where (2.412)–(2.413) imply that $p > 0$.

For $\left[1-(k-2)\frac{1}{2N}\right]$ is strictly positive, then

$$\left[b+\frac{k-k'}{(c+3)k^{2/3}}\right] > b > 0. \tag{2.415}$$

Then

$$q = \left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\frac{8}{3}\left[1-(k-2)\frac{1}{2N}\right]\frac{1}{N^{1/5}}\left[b+\frac{k-k'}{(c+3)k^{2/3}}\right] > 0 \tag{2.416}$$

where (2.415) imply that $q > 0$.

By using (2.414) and (2.416), and from (2.407), we obtain

$$A_0 = \frac{\frac{8}{3}\left[1-(k-2)\frac{1}{2N}\right]\frac{1}{N^{1/5}}\left[b+\frac{k-k'}{(c+3)k^{2/3}}\right]}{2\left[3\left(1-\frac{k}{3N}\right)+\left[a+k^{2/3}c(k-k')\right]\frac{1}{2N}\right]}. \tag{2.417}$$

From (2.408), we obtain

$$\begin{aligned} f(A_0) &= pA_0^2 - qA_0 \\ &= p\left(\frac{q}{2p}\right)^2 - q\left(\frac{q}{2p}\right) \\ &= -\frac{1}{4}\frac{q^2}{p}. \end{aligned} \tag{2.418}$$

Substitute $p$, $q$ in (2.418) then

$$f(A_0) = -\frac{1}{4}\frac{\left\{\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\frac{8}{3}\left[1-(k-2)\frac{1}{2N}\right]\frac{1}{N^{1/5}}\left[b+\frac{k-k'}{(c+3)k^{2/3}}\right]\right\}^2}{\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\left[3\left(1-\frac{k}{3N}\right)+\left[a+k^{2/3}c(k-k')\right]\frac{1}{2N}\right]}$$

$$= -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\left(\frac{16}{27}\right)$$

$$\times\frac{\left[1-\frac{k}{2N}+\frac{1}{N}\right]^2\frac{1}{N^{2/5}}\left[\frac{b(c+3)}{(c+3)}+\frac{k^{1/3}}{(c+3)}-\frac{k'}{(c+3)k^{2/3}}\right]^2}{1-\frac{k}{3N}+\frac{a+k^{5/3}c}{6N}-\frac{k^{2/3}k'c}{6N}}$$

$$= -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\left(\frac{16}{27}\right)\frac{1}{(c+3)^2}$$

$$\times\frac{\left(1-\frac{k}{2N}+\frac{1}{N}\right)^2\left[\frac{b(c+3)}{N^{1/5}}+\frac{k^{1/3}}{N^{1/5}}-\frac{k'}{N^{1/5}k^{2/3}}\right]^2}{1-\frac{k}{3N}+\frac{a+k^{5/3}c}{6N}-\frac{k^{2/3}k'c}{6N}}$$

$$= -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\left(\frac{16}{27}\right)\frac{1}{(c+3)^2}[\,\cdot\,] \tag{2.419}$$

where

$$[\,\cdot\,] = \frac{\left(1-\frac{k}{2N}+\frac{1}{N}\right)^2\left[\frac{b(c+3)}{N^{1/5}}+\frac{k^{1/3}}{N^{1/5}}-\frac{k'}{N^{1/5}k^{2/3}}\right]^2}{1-\frac{k}{3N}+\frac{a+k^{5/3}c}{6N}-\frac{k^{2/3}k'c}{6N}}. \tag{2.420}$$

For $N > 0$, we have

$$\left(1-\frac{k}{2N}+\frac{1}{N}\right)^2 > \left(1-\frac{k}{2N}\right)^2. \tag{2.421}$$

For $\dfrac{b(c+3)}{N^{1/5}} > 0$, we have

$$\left[\frac{b(c+3)}{N^{1/5}} + \frac{k^{1/3}}{N^{1/5}} - \frac{k'}{N^{1/5}k^{2/3}}\right]^2 > \left[\frac{k^{1/3}}{N^{1/5}} - \frac{k'}{N^{1/5}k^{2/3}}\right]^2. \tag{2.422}$$

For $\dfrac{k}{3N} > 0$, we have

$$-\frac{k}{3N} < 0. \tag{2.423}$$

For $\dfrac{k^{2/3}k'c}{6N} > 0$, we obtain

$$\frac{1}{1 - \dfrac{k}{3N} + \dfrac{a + k^{5/3}c}{6N} - \dfrac{k^{2/3}k'c}{6N}} > \frac{1}{1 + \dfrac{a + k^{5/3}c}{6N}}. \tag{2.424}$$

From (2.421)–(2.424), we obtain

$$\frac{\left(1 - \dfrac{k}{2N} + \dfrac{1}{N}\right)^2 \left[\dfrac{b(c+3)}{N^{1/5}} + \dfrac{k^{1/3}}{N^{1/5}} - \dfrac{k'}{N^{1/5}k^{2/3}}\right]^2}{1 - \dfrac{k}{3N} + \dfrac{a + k^{5/3}c}{6N} - \dfrac{k^{2/3}k'c}{6N}}$$

$$\geqslant \frac{\left(1 - \dfrac{k}{2N}\right)^2 \left[\dfrac{k^{1/3}}{N^{1/5}} - \dfrac{k'}{N^{1/5}k^{2/3}}\right]^2}{1 + \dfrac{a + k^{5/3}c}{6N}}. \tag{2.425}$$

Compare (2.425) with (2.420), then we obtain

$$[\,\cdot\,] \geqslant \frac{\left(1 - \dfrac{k}{2N}\right)^2 \left[\dfrac{k^{1/3}}{N^{1/5}} - \dfrac{k'}{N^{1/5}k^{2/3}}\right]^2}{1 + \dfrac{a + k^{5/3}c}{6N}}. \tag{2.426}$$

Multiply (2.426) by $-\left(\dfrac{me^4}{2\hbar^2}\right)\dfrac{N^{7/5}}{\pi^4}$ and compare the result with (2.419), then we obtain

$$f(A_0) = -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{\pi^4}\left(\frac{16}{27}\right)\frac{1}{(c+3)^2}\,[\,\cdot\,]$$

$$\leqslant -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{(c+3)^2}\left(\frac{16}{\pi^4 27}\right)\frac{\left(1-\dfrac{k}{2N}\right)^2\left[\dfrac{k^{1/3}}{N^{1/5}}-\dfrac{k'}{N^{1/5}k^{2/3}}\right]^2}{1+\dfrac{1}{6}\left(\dfrac{a+k^{5/3}c}{N}\right)}. \qquad (2.427)$$

Substitute (2.427) in (2.408), we obtain the bound

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\left(\frac{16}{\pi^4 27}\right)\frac{N^{7/5}}{(c+3)^2}\frac{\left(1-\dfrac{k}{2N}\right)^2\left[\dfrac{k^{1/3}}{N^{1/5}}-\dfrac{k'}{N^{1/5}k^{2/3}}\right]^2}{1+\dfrac{1}{6}\left(\dfrac{a+k^{5/3}c}{N}\right)}. \qquad (2.428)$$

The $\dfrac{k^{1/3}}{N^{1/5}}$ term in the numerator and the term $\dfrac{k^{5/3}}{N}$ in the denominator dictate the choice $k \sim N^{3/5}$. More precisely, optimization of the coefficient of $N^{7/5}$ in (2.428) for $N \to \infty$, recalling that $k$ must be a positive integer, leads to the choice of $k$ as the largest positive integer such that

$$k \simeq (BN)^{3/5} \qquad (2.429)$$

where $B > 0$. Then consider the right-hand side of (2.428)

$$\frac{\left(1-\dfrac{k}{2N}\right)^2\left[\dfrac{k^{1/3}}{N^{1/5}}-\dfrac{k'}{N^{1/5}k^{2/3}}\right]^2}{1+\dfrac{1}{6}\left(\dfrac{a+k^{5/3}c}{N}\right)}$$

$$= \frac{\left(1-\dfrac{(BN)^{3/5}}{2N}\right)^2\left[\dfrac{\left((BN)^{3/5}\right)^{1/3}}{N^{1/5}}-\dfrac{k'}{N^{1/5}\left((BN)^{3/5}\right)^{2/3}}\right]^2}{1+\dfrac{1}{6}\left(\dfrac{a+\left((BN)^{3/5}\right)^{5/3}c}{N}\right)}$$

$$= \frac{\left(1 - \frac{B^{3/5}}{2N^{2/5}}\right)^2 \left[B^{1/5} - \frac{k'}{B^{2/5}N^{3/5}}\right]^2}{1 + \frac{a}{6N} + \frac{cB}{6}}$$

$$\equiv g(B). \tag{2.430}$$

Optimization of $g(B)$ over $B$ where $N \to \infty$ gives

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}B} g(B) = & \left(1 - \frac{B^{3/5}}{2N^{2/5}}\right)^2 \left[B^{1/5} - \frac{k'}{B^{2/5}N^{3/5}}\right]^2 \frac{\mathrm{d}}{\mathrm{d}B}\left(1 + \frac{a}{6N} + \frac{cB}{6}\right)^{-1} \\
& + \frac{\left(1 - \frac{B^{3/5}}{2N^{2/5}}\right)^2 \frac{\mathrm{d}}{\mathrm{d}B}\left[B^{1/5} - \frac{k'}{B^{2/5}N^{3/5}}\right]^2}{1 + \frac{a}{6N} + \frac{cB}{6}} \\
& + \frac{\frac{\mathrm{d}}{\mathrm{d}B}\left(1 - \frac{B^{3/5}}{2N^{2/5}}\right)^2 \left[B^{1/5} - \frac{k'}{B^{2/5}N^{3/5}}\right]^2}{1 + \frac{a}{6N} + \frac{cB}{6}} \\
= & \left(1 - \frac{B^{3/5}}{2N^{2/5}}\right)^2 \left[B^{1/5} - \frac{k'}{B^{2/5}N^{3/5}}\right]^2 (-1) \\
& \times \left(1 + \frac{a}{6N} + \frac{cB}{6}\right)^{-2} \frac{\mathrm{d}}{\mathrm{d}B}\left(1 + \frac{a}{6N} + \frac{cB}{6}\right) \\
& + \frac{\left(1 - \frac{B^{3/5}}{2N^{2/5}}\right)^2 (2) \left[B^{1/5} - \frac{k'}{B^{2/5}N^{3/5}}\right] \frac{\mathrm{d}}{\mathrm{d}B}\left[B^{1/5} - \frac{k'}{B^{2/5}N^{3/5}}\right]}{1 + \frac{a}{6N} + \frac{cB}{6}} \\
& + \frac{(2)\left(1 - \frac{B^{3/5}}{2N^{2/5}}\right) \frac{\mathrm{d}}{\mathrm{d}B}\left(1 - \frac{B^{3/5}}{2N^{2/5}}\right) \left[B^{1/5} - \frac{k'}{B^{2/5}N^{3/5}}\right]^2}{1 + \frac{a}{6N} + \frac{cB}{6}}
\end{aligned} \tag{2.431}$$

then

$$\lim_{N\to\infty}\frac{\mathrm{d}}{\mathrm{d}B}g(B) = -\frac{cB^{2/5}}{6\left(1+\dfrac{cB}{6}\right)^2} + \frac{2B^{1/5}B^{-4/5}}{5\left(1+\dfrac{cB}{6}\right)}$$

$$= \frac{B^{1/5}}{\left(1+\dfrac{cB}{6}\right)}\left\{\frac{2B^{-4/5}}{5} - \frac{cB^{1/5}}{6\left(1+\dfrac{cB}{6}\right)}\right\}. \tag{2.432}$$

$B$ will be obtained from

$$\lim_{N\to\infty}\frac{\mathrm{d}}{\mathrm{d}B}g(B) = 0,$$

then from (2.432), we have

$$\frac{2B^{-4/5}}{5} - \frac{cB^{1/5}}{6\left(1+\dfrac{cB}{6}\right)} = 0$$

$$\frac{2B^{-4/5}}{5} = \frac{cB^{1/5}}{6\left(1+\dfrac{cB}{6}\right)}$$

$$\frac{2}{5B^{4/5}} = \frac{cB^{1/5}}{6+cB}$$

$$12 + 2cB = 5Bc$$

$$B = \frac{4}{c}. \tag{2.433}$$

Substitute $B$ in (2.429) and because $k$ is the largest positive integer, then

$$k \leqslant \left(\frac{4N}{c}\right)^{3/5} \leqslant k+1 \tag{2.434}$$

then

$$k \leqslant \left(\frac{4N}{c}\right)^{3/5}, \tag{2.435}$$

$$k \geqslant \left(\frac{4N}{c}\right)^{3/5} - 1. \tag{2.436}$$

From (2.435), we obtain

$$-\frac{k}{2N} \geqslant -\frac{1}{2N}\left(\frac{4N}{c}\right)^{3/5}$$

which leads to

$$\left(1 - \frac{k}{2N}\right)^2 \geqslant \left[1 - \frac{1}{2N}\left(\frac{4N}{c}\right)^{3/5}\right]^2. \tag{2.437}$$

From (2.436), we have

$$k^{1/3} \geqslant \left[\left(\frac{4N}{c}\right)^{3/5} - 1\right]^{1/3}$$

multiply above inequality by $\frac{1}{N^{1/5}}$, we obtain

$$\frac{k^{1/3}}{N^{1/5}} \geqslant \frac{1}{N^{1/5}}\left[\left(\frac{4N}{c}\right)^{3/5} - 1\right]^{1/3}. \tag{2.438}$$

From (2.436), we have

$$k^{2/3} \geqslant \left[\left(\frac{4N}{c}\right)^{3/5} - 1\right]^{2/3}$$

which leads to

$$-\frac{k'}{k^{2/3}N^{1/5}} \geqslant -\frac{k'}{\left[\left(\frac{4N}{c}\right)^{3/5} - 1\right]^{2/3} N^{1/5}}. \tag{2.439}$$

From (2.434), we have

$$k^{5/3} \leqslant \left(\frac{4N}{c}\right)$$

then

$$\frac{a+ck^{5/3}}{6N} \leqslant \frac{a+c\left(\dfrac{4N}{c}\right)}{6N}.$$

Add above inequality by 1, we obtain

$$1+\frac{a+ck^{5/3}}{6N} \leqslant 1+\frac{a+4N}{6N}$$

then

$$\frac{1}{1+\dfrac{a+ck^{5/3}}{6N}} \geqslant \frac{1}{1+\dfrac{a+4N}{6N}}. \tag{2.440}$$

From (2.430) and by using (2.437)–(2.440), we obtain

$$\begin{aligned}
&\frac{\left(1-\dfrac{k}{2N}\right)^2\left[\dfrac{k^{1/3}}{N^{1/5}}-\dfrac{k'}{N^{1/5}k^{2/3}}\right]^2}{1+\dfrac{1}{6}\left(\dfrac{a+k^{5/3}c}{N}\right)} \\
&\quad\geqslant \left[1-\frac{1}{2N}\left(\frac{4N}{c}\right)^{3/5}\right]^2 \\
&\quad\quad\times\frac{\left\{\dfrac{1}{N^{1/5}}\left[\left(\dfrac{4N}{c}\right)^{3/5}-1\right]^{1/3}-\dfrac{k'}{N^{1/5}}\left[\left(\dfrac{4N}{c}\right)^{3/5}-1\right]^{-2/3}\right\}^2}{1+\dfrac{a+4N}{6N}}.
\end{aligned} \tag{2.441}$$

Consider the first term on the right-hand side of (2.441)

$$\begin{aligned}
\left[1-\frac{1}{2N}\left(\frac{4N}{c}\right)^{3/5}\right]^2 &= \left[1-\frac{1}{2}\left(\frac{4}{c}\right)^{1/5}\left(\frac{4}{c}\right)^{2/5}\frac{1}{N^{2/5}}\right]^2 \\
&= \left(1-\frac{2}{c}\frac{c^{2/5}}{4}\frac{4^{3/5}}{N^{2/5}}\right)^2 \\
&= \left[1-\frac{2}{c}\left(\frac{c}{4N}\right)^{2/5}\right]^2.
\end{aligned} \tag{2.442}$$

Consider the term in the square bracket on the right-hand side of (2.441)

$$\frac{1}{N^{1/5}}\left[\left(\frac{4N}{c}\right)^{3/5}-1\right]^{1/3}-\frac{k'}{N^{1/5}}\left[\left(\frac{4N}{c}\right)^{3/5}-1\right]^{-2/3}$$

$$=\left\{\frac{1}{N^{3/5}}\left[\left(\frac{4}{c}\right)^{3/5}N^{3/5}-1\right]\right\}^{1/3}-\frac{k'}{\left(\frac{4N}{c}\right)^{2/5}\left[1-\left(\frac{c}{4N}\right)^{3/5}\right]^{2/3}N^{1/5}}$$

$$=\left(\frac{4}{c}\right)^{1/5}\left[1-\left(\frac{c}{4N}\right)^{3/5}\right]^{1/3}-\left(\frac{4}{c}\right)^{1/5}\frac{k'}{\left(\frac{4N}{c}\right)^{3/5}\left[1-\left(\frac{c}{4N}\right)^{3/5}\right]^{2/3}}$$

$$=\left(\frac{4}{c}\right)^{1/5}\left\{\left[1-\left(\frac{c}{4N}\right)^{3/5}\right]^{1/3}-\left(\frac{c}{4N}\right)^{3/5}\frac{k'}{\left[1-\left(\frac{c}{4N}\right)^{3/5}\right]^{2/3}}\right\}. \tag{2.443}$$

Consider the denominator term on the right-hand side of (2.441)

$$1+\frac{a+4N}{6N}=1+\frac{a}{6N}+\frac{4}{6}$$

$$=\frac{5}{3}+\frac{a}{6N}. \tag{2.444}$$

Substitute the results from (2.442) and (2.444) in (2.441), then we obtain

$$\frac{\left(1-\frac{k}{2N}\right)^2\left[\frac{k^{1/3}}{N^{1/5}}-\frac{k'}{N^{1/5}k^{2/3}}\right]^2}{1+\frac{1}{6}\left(\frac{a+k^{5/3}c}{N}\right)}$$

$$\geqslant\left[1-\frac{2}{c}\left(\frac{c}{4N}\right)^{2/5}\right]^2\left(\frac{4}{c}\right)^{2/5}\frac{1}{\left(\frac{5}{3}+\frac{a}{6N}\right)}$$

$$\times \left\{ \left[ 1 - \left( \frac{c}{4N} \right)^{3/5} \right]^{1/3} - \frac{k' \left( \frac{c}{4N} \right)^{3/5}}{\left[ 1 - \left( \frac{c}{4N} \right)^{3/5} \right]^{2/3}} \right\}^2$$

$$\equiv \left( \frac{4}{c} \right)^{2/5} \{ \cdot\cdot \} \tag{2.445}$$

where

$$\{ \cdot\cdot \} = \frac{\left[ 1 - \frac{2}{c} \left( \frac{c}{4N} \right)^{2/5} \right]^2}{\left( \frac{5}{3} + \frac{a}{6N} \right)} \left\{ \left[ 1 - \left( \frac{c}{4N} \right)^{3/5} \right]^{1/3} - \frac{k' \left( \frac{c}{4N} \right)^{3/5}}{\left[ 1 - \left( \frac{c}{4N} \right)^{3/5} \right]^{2/3}} \right\}^2 . \tag{2.446}$$

Replace the result from (2.446) in (2.428), we obtain the upper bound for the ground-state energy of "bosonic matter"

$$E_{N,N} < - \left( \frac{me^4}{2\hbar^2} \right) \left( \frac{16}{\pi^4 27} \right) \frac{N^{7/5}}{(c+3)^2} \left( \frac{4}{c} \right)^{2/5} \{ \cdot\cdot \} . \tag{2.447}$$

For *all* allowed $n \geqslant n' = 100$, (up to infinity!), our estimate (2.377) gives $c = 2.25456$ as quoted earlier. On the other hand and elementary computer analysis (see Appendix A), involving a finite number of terms, yields the exact integer values:

$$k' = 511775, \quad a = 3081771357. \tag{2.448}$$

Hence, for realistic $N > 10^{15}$, (2.446) gives

$$\{ \cdot\cdot \} > \left[ 1 - \frac{2}{2.25456} \left( \frac{2.25456}{4 \times 10^{15}} \right)^{2/5} \right]^2 \frac{1}{\left( \frac{5}{3} + \frac{a}{6 \times 10^{15}} \right)}$$

$$\times\left\{\left[1-\left(\frac{2.25456}{4\times 10^{15}}\right)^{3/5}\right]^{1/3}-\frac{k'\left(\dfrac{2.25456}{4\times 10^{15}}\right)^{3/5}}{\left[1-\left(\dfrac{2.25456}{4\times 10^{15}}\right)^{3/5}\right]^{2/3}}\right\}^{2}. \qquad (2.449)$$

Multiply (2.449) by $\frac{1}{(c+3)^2}\left(\frac{16}{27}\right)\left(\frac{4}{c}\right)^{2/5}$, we obtain

$$\frac{1}{(c+3)^2}\left(\frac{16}{27}\right)\left(\frac{4}{c}\right)^{2/5}\{\cdot\cdot\}>\frac{1}{61.7838}>\frac{1}{62}. \qquad (2.450)$$

By using the result from (2.450), then (2.447) becomes

$$E_{N,N}<-\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{62\pi^4}. \qquad (2.451)$$

By comparing with Dyson bound (Dyson, 1967)

$$\begin{aligned} E_{\text{Dyson}} &< -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{1944\,\pi^4} \\ &= -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{62\,\pi^4}\frac{1}{(31.3548)} \\ &= E_{N,N}\frac{1}{(31.3548)}<E_{N,N}\frac{1}{(31)}. \end{aligned} \qquad (2.452)$$

Then, our bound improve the Dyson bound by a factor of 31. For a more conservative bound, elementary computer analysis shows that, at $n^2=6$, we have $k'\to 0$, then $a\to 0$ and we have $\alpha=1,2,3$ for $(1,1,2),(1,2,1),(2,1,1)$, respectively. Then for $\sqrt{6}\leqslant n^2\leqslant 100$ we have $\alpha\geqslant 1$, then

$$100\geqslant n^2\geqslant 6.$$

Multiply above inequality by $\frac{1}{c}$, we obtain

$$\frac{100}{c} \geqslant \frac{n^2}{c} \geqslant \frac{6}{c}$$

then

$$\frac{100^{3/2}}{c^{3/2}} \geqslant \frac{n^3}{c^{3/2}} \geqslant \frac{6^{3/2}}{c^{3/2}}. \tag{2.453}$$

Compare (2.453) with (2.377), then we obtain $c = 6$ for $\sqrt{6} \leqslant n^2 \leqslant 100$, $\alpha \geqslant 1$, and Eq. (2.447) becomes

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{7/5}}{267\,\pi^4} \tag{2.454}$$

improving the Dyson bound by a factor of 7.

# CHAPTER III

# IS 'BOSONIC MATTER' UNSTABLE IN $2D$?

## 3.1 Introduction and Orientation

With the mathematically rigorous analysis of the instability of the bosonic system carried out in the last chapter, it has become important for us to enquire whether the instability of bosonic system is a characteristic of the dimensionality of space, and if instability is tied up with the dimensionality of space. It is also an important question to investigate if the change of the dimensionality of space will change such matter from an "implosive" to a "stable" or to an "explosive" phase. Our analysis in this chapter and the remaining part of the thesis shows that this does not happen and instability happens in all dimensions. As a first step in investigating and answering this question, in this chapter, we have carried out an analysis of such systems in $2D$. In recent years there has been much interest in the physics of $2D$ and the connection of the Spin and Statistics (e.g., Geyer, 1995; Bhaduri, Murthy and Srivastava, 1996; Semenoff and Wijewardhana, 1987; Forte, 1992), and it is essential to investigate such bosonic systems, of central importance, in $2D$. One of our upper bounds for the ground-state energy in $2D$ is given by

$$E_{N,N} \leqslant -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{3/2}}{50\pi^2} \tag{3.1}$$

for large $N$ implying, in particular, collapse and, in general, a more 'violent' one for large $N$ than in $3D$. Such collapsing matter may be also considered as collapsing planar matter sheets set side by side in $3D$. Several other bounds are also derived for different range of values for $N$.

A general expression of the ground-state energy $E_{N,N}$ is derived in Sect. 3.1.

Surprisingly, the mathematical analysis turns out to be also complicated in $2D$ and several new Propositions and many more estimated are freshly derived in this case in Sect. 3.2. In Sect. 3.3, several upper bounds are obtained including the one in (3.1)

## 3.2 General Upper Bound Expression of $E_{N,N}$

The Hamiltonian in concerned is given by (2.1). Then we have the expectation value of above the Hamiltonian

$$\begin{aligned} \langle \Psi | H' | \Psi \rangle &= \sum_{i=1}^{2N} \left\langle \Psi \left| \frac{\mathbf{p}_i^2}{2m_i} \right| \Psi \right\rangle + \sum_{i<j}^{2N} \left\langle \Psi \left| \frac{e^2 \varepsilon_i \varepsilon_j}{|\mathbf{x}_i - \mathbf{x}_j|} \right| \Psi \right\rangle \\ &\equiv H'_{2N} \end{aligned} \tag{3.2}$$

where $\Psi$ is a trial function and will be defined later. Since $\left\langle \Psi \left| \frac{\mathbf{p}_i^2}{2m_i} \right| \Psi \right\rangle$ is positive, then

$$\left\langle \Psi \left| \frac{\mathbf{p}_i^2}{2m_i} \right| \Psi \right\rangle \leqslant \left\langle \Psi \left| \frac{\mathbf{p}_i^2}{2m} \right| \Psi \right\rangle \tag{3.3}$$

where $m$ is the smallest of the masses involves in (2.1). Let $H_{2N}$ is the expectation value of the Hamiltonian $H$

$$H_{2N} = \sum_{i=1}^{2N} \left\langle \Psi \left| \frac{\mathbf{p}_i^2}{2m_i} \right| \Psi \right\rangle + \sum_{i<j}^{2N} \left\langle \Psi \left| \frac{e^2 \varepsilon_i \varepsilon_j}{|\mathbf{x}_i - \mathbf{x}_j|} \right| \Psi \right\rangle \tag{3.4}$$

where

$$H = \sum_{i=1}^{2N} \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j}^{2N} \frac{e^2 \varepsilon_i \varepsilon_j}{|\mathbf{x}_i - \mathbf{x}_j|} \tag{3.5}$$

then from (3.2) and (3.3) we have

$$H'_{2N} \leqslant H_{2N} \tag{3.6}$$

and from Chapter II, $H_{2N}$ can not less than the ground-state energy $E_{2N,2N}$, i.e., that

$$E_{2N,2N} \leqslant H_{2N} \tag{3.7}$$

where $E_{N,N}$ denotes the ground-state energy $H'$ of $(N+N)$ particles.

We set $z = (\mathbf{x}, \varepsilon)$ and introduce trial two-particle states (Dyson, 1967)

$$G(z, z') = \sum_{\alpha=0}^{k} \lambda_\alpha c_\alpha(\varepsilon) c_\alpha(\varepsilon') \psi_\alpha(\mathbf{x}) \psi_\alpha(\mathbf{x}') \tag{3.8}$$

where $\psi_0(\mathbf{x}), \psi_1(\mathbf{x}), \ldots, \psi_k(\mathbf{x})$ are mutually orthonormal and the integer $k$ will be conveniently chosen later, with coefficients in (3.8) given by Dyson (Dyson, 1967)

$$\lambda_\alpha = \begin{cases} 1, & \alpha = 0 \\ -\dfrac{1}{2}, & \alpha = 1, \ldots, k \end{cases} \tag{3.9}$$

and

$$c_\alpha(\varepsilon) = \begin{cases} \dfrac{1}{\sqrt{2}}, & \alpha = 0 \\ \dfrac{\varepsilon}{\sqrt{2}}, & \alpha = 1, \ldots, k \end{cases} \tag{3.10}$$

One may then define a $2N$-particle wavefunction as follows:

$$\Psi_{2N}(z_1, \ldots, z_{2N}) = \sum_{\pi} G(z(\pi_1), z(\pi_2)) \cdots G(z(\pi_{2N-1}), z(\pi_{2N})). \tag{3.11}$$

The sum is over all permutations $(\pi_1, \ldots, \pi_{2N})$ of $(1, \ldots, 2N)$. The wavefunction $\Psi_{2N}$ is not yet normalized. Since $\Psi_{2N} / \|\Psi_{2N}\|$ does not necessarily coincide with the ground-state function of $H$, the expectation value of $H$ with respect to $\Psi_{2N} / \|\Psi_{2N}\|$ cannot be less than the corresponding ground-state energy. That is, the expression in (3.11) can only provide an upper bound for the ground-state energy.

Derivation of a general upper bound expression for $E_{N,N}$ by carrying out, in the process, the expectation value of $H$ with respect to $\Psi_{2N}/\left\|\Psi_{2N}\right\|$ turns out to be very tedious (Dyson, 1967; Manoukian and Muthaporn, 2002) as you have seen in Sect. 2.1. To give the general expression for this upper bound, we define the following expectation values with respect to single particle trial wavefunctions $\psi_\alpha(\mathbf{x})$ :

$$T_\alpha = \int \mathrm{d}^2\mathbf{x}\ \psi_\alpha^*(\mathbf{x}) \left(-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m}\right) \psi_\alpha(\mathbf{x}), \quad \alpha = 0, 1, \ldots, k, \tag{3.12}$$

$$I_{0\alpha} = \int \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}'\ \psi_0^*(\mathbf{x})\psi_\alpha^*(\mathbf{x}) \frac{e^2}{|\mathbf{x}-\mathbf{x}'|} \psi_0(\mathbf{x}')\psi_\alpha(\mathbf{x}'), \quad \alpha = 1, 2, \ldots, k. \tag{3.13}$$

We then have the following general expression-bound from (2.274) (Manoukian and Muthaporn, 2002, Eq. (2.18)):

$$E_{N,N} \leqslant \frac{1}{2}\sum_{\alpha=1}^{k} T_\alpha + \left(N - \frac{k}{3}\right) T_0 + \frac{1}{3}\left[N - \frac{(k-2)}{2}\right]\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right) \tag{3.14}$$

where $k < N$ and we note, in particular, that the coefficients of $T_0$ and $\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right)$ are strictly positive.

## 3.3 Basic Estimates

To derive the bound in (3.1), we need, in the process, to establish the bounds given, in turn, in (3.15), (3.38), (3.39) and (3.58).

To the above end, we consider the following construction. For each doublet $(n_1, n_2)$ of two natural numbers, we define a state specified by the tip of the vector $\mathbf{n} = (n_1, n_2)$. A non-trivial permutation of $(n_1, n_2)$ defines a different state. For example, $(1, 2)$, $(2, 1)$ define two distinct states satisfying, however, the constraint $n^2 = 5$.

For any given such an allowed $n^2$ (a natural number), let $k$ denote the number of distinct states, excluding the state $(1, 1)$, with the constraint that the length squared of each vector specifying such a state is less than or equal to $n^2$.

This is the total number of states, excluding the state $(1,1)$, lying within, or falling on, a quarter of a circle of radius $n$ in the so-called first quadrant, i.e., for $n_1 \geqslant 1$, $n_2 \geqslant 1$.

Since by definition the state $(1,1)$ is excluded, the lowest possible value of $n^2$ is 5. For $n^2 = 5$, we have $k = 2$ corresponding to the states $(1,2),(2,1)$. The next allowed value for $n^2$ is 8, with $k = 3$, corresponding to the states $(1,2),(2,1),(2,2)$, and so on for other values of $n^2 = 10, 13, 17, \ldots$. We now establish the following.

**Proposition 7**

*For any allowed $n^2$, as defined above, we have the following inequality for the number of states , also defined above, in relation to n :*

$$\frac{k}{n^2} \geqslant \sqrt{1 - \frac{1}{n^2}}\left(1 - \frac{3}{2n}\right) - \frac{1}{n} - \frac{1}{2} \tag{3.15}$$

*and the right-hand side of this inequality is strictly positive for allowed values of $n^2 \geqslant 29$.*

To establish (3.15), $s$ rectangles each of unit height and bases of sizes $N_1$, $N_2$,..., $N_s$, where the $N_i$ are positive integers defined below with $1 \leqslant N_s \leqslant \cdots \leqslant N_1$, are stacked on top of each other as shown in the Fig. 3.1 inside of a circle of radius $n$. Since the height of each rectangle is of one unit, we choose $N_1$, $N_2$,..., $N_s$ to be the largest positive integers such that

$$N_1^2 + 1^2 \leqslant n^2, \ldots, N_s^2 + s^2 \leqslant n^2 \tag{3.16}$$

to make sure that the rectangles fall within or just touch the circumference of a

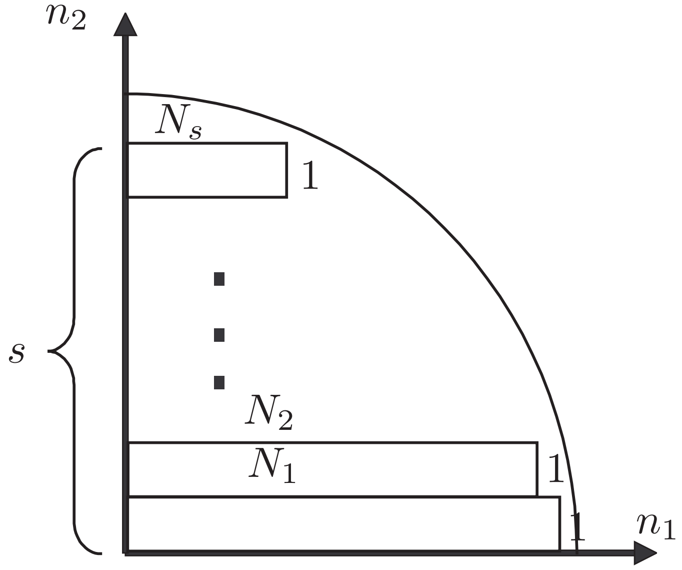


Figure 3.1: $s$ rectangles, each of unit height and bases of sizes $N_1,\ N_2,\ldots,N_s$, where the $N_i$ are positive integers, with $1 \leqslant N_s \leqslant \cdots \leqslant N_1$, are stacked on top of each other inside a quarter of a circle of radius $n$. Bounds are obtained on $N_1,\ N_2,\ldots,N_s$ such that the rectangles are within or just touch the circumference of a quarter of a circle.

quarter of the circle of radius $n$. That is, we take

$$N_1 \leqslant \sqrt{n^2-1} \leqslant N_1+1, \ldots, N_s \leqslant \sqrt{n^2-s^2} \leqslant N_s+1. \tag{3.17}$$

Then, from (3.17), we have

$$N_j \leqslant \sqrt{n^2-j^2} \leqslant N_j+1, \tag{3.18}$$

$$N_j \geqslant \sqrt{n^2-j^2}-1 \tag{3.19}$$

where $1 \leqslant j \leqslant s$. Also $N_s \geqslant 1$ requires that $1 \leqslant \sqrt{n^2-s^2} \leqslant N_s+1$. Then

$$1 \leqslant n^2 - s^2$$

or

$$s^2 \leqslant n^2 - 1.$$

Hence $s$ is taken to be the largest positive integer such that

$$s \leqslant \sqrt{n^2-1} \leqslant s+1. \tag{3.20}$$

From (3.20), we obtain

$$s \leq \sqrt{n^2-1}\,, \tag{3.21}$$

$$s \geqslant \sqrt{n^2-1}-1. \tag{3.22}$$

For any $N_j$, $1 \leqslant j \leqslant s$, we have the number of distinct states which lie within the rectangle of area $N_j \times 1$ such that

$$(j,1),(j,2),(j,3),\ldots,(j,N_j) \tag{3.23}$$

then we have the total number of distinct states $k$, for $1 \leqslant j \leqslant s$ such that, exclude state $(1,1)$,

$$k = \sum_{j=1}^{s} N_j - 1. \tag{3.24}$$

Because

$$n + j \geqslant n - j$$

multiply above inequality by $(n - j)$, then we obtain

$$(n - j)(n + j) \geqslant (n - j)^2$$

or

$$n^2 - j^2 \geqslant (n - j)^2$$

then

$$\sqrt{n^2 - j^2} \geqslant n - j$$

add above inequality by $(-1)$ we obtain

$$\sqrt{n^2 - j^2} - 1 \geqslant n - j - 1. \tag{3.25}$$

Compare the left-hand side of (3.25) with (3.19), then we obtain

$$N_j \geqslant n - j - 1. \tag{3.26}$$

Multiply above inequality by $\sum_{j=1}^{s}$ we obtain

$$\sum_{j=1}^{s} N_j \geqslant \sum_{j=1}^{s} \big(n - j - 1\big)$$

add above inequality by $(-1)$ we obtain

$$\sum_{j=1}^{s} N_j - 1 \geqslant \sum_{j=1}^{s} \big(n - j - 1\big) - 1. \tag{3.27}$$

Compare (3.27) with (3.24), we obtain

$$k \geqslant \sum_{j=1}^{s} \big(n - j - 1\big) - 1. \tag{3.28}$$

Consider the right-hand side of (3.28)

$$\begin{aligned} \sum_{j=1}^{s} \big(n - j - 1\big) - 1 &= \sum_{j=1}^{s} n - \sum_{j=1}^{s} j - \sum_{j=1}^{s} 1 - 1 \\ &= (n-1)s - \frac{s(s+1)}{2} - 1. \end{aligned} \tag{3.29}$$

Substitute (3.29) in (3.28), we obtain

$$\begin{aligned} k &\geqslant (n-1)s - \frac{s(s+1)}{2} - 1 \\ &= (n-1)s - \frac{s^2}{2} - \frac{s}{2} - 1. \end{aligned} \tag{3.30}$$

For $(n-1) \geqslant 0$, and from (3.21)–(3.22), we have

$$s \leqslant \sqrt{n^2 - 1}\,, \quad s^2 \leqslant n^2 - 1$$

then

$$\frac{s}{2} \leqslant \frac{\sqrt{n^2-1}}{2}\,, \quad \frac{s^2}{2} \leqslant \frac{n^2-1}{2}. \tag{3.31}$$

Multiply above inequalities by $(-1)$, we obtain

$$-\frac{s}{2} \geqslant -\frac{\sqrt{n^2-1}}{2}\,, \tag{3.32}$$

$$-\frac{s^2}{2} \geqslant -\frac{n^2-1}{2} \tag{3.33}$$

Also, for $s \geqslant \sqrt{n^2-1}\ -1$, we have

$$(n-1)s \geqslant (n-1)\left(\sqrt{n^2-1}\ -1\right). \tag{3.34}$$

The addition of (3.32)–(3.34) gives the right-hand side of (3.30) becomes

$$\begin{aligned}
(n-1)s-\frac{s^2}{2}-\frac{s}{2}-1 &\geqslant (n-1)\left(\sqrt{n^2-1}-1\right)-\frac{n^2-1}{2}-\frac{\sqrt{n^2-1}}{2}-1\\
&= \left(n-1-\frac{1}{2}\right)\sqrt{n^2-1}-\frac{n^2-1}{2}-1-(n-1)\\
&= \left(n-\frac{3}{2}\right)\sqrt{n^2-1}-\frac{n^2-1}{2}-n\\
&= n\left(1-\frac{3}{2n}\right)n\sqrt{1-\frac{1}{n^2}}-\frac{n^2}{2}\left(1-\frac{1}{n^2}\right)-n\\
&= n^2\sqrt{1-\frac{1}{n^2}}\ \left(1-\frac{3}{2n}\right)-\frac{n^2}{2}+\frac{1}{2}-n. \qquad (3.35)
\end{aligned}$$

Since $\dfrac{1}{2} > 0$, then (3.35) becomes

$$\begin{aligned}
(n-1)s-\frac{s^2}{2}-\frac{s}{2}-1 &\geqslant n^2\sqrt{1-\frac{1}{n^2}}\ \left(1-\frac{3}{2n}\right)-\frac{n^2}{2}-n\\
&= n^2\left[\sqrt{1-\frac{1}{n^2}}\ \left(1-\frac{3}{2n}\right)-\frac{1}{2}-\frac{1}{n}\right]. \qquad (3.36)
\end{aligned}$$

Substitute (3.36) in (3.30), we obtain

$$k \geqslant n^2\left[\sqrt{1-\frac{1}{n^2}}\left(1-\frac{3}{2n}\right)-\frac{1}{2}-\frac{1}{n}\right]. \tag{3.37}$$

Multiplying of (3.37) by $\dfrac{1}{n^2}$ leads to (3.15). □

Many estimates of the sort in (3.15), involving corrections, are available in the literature. A classic example of this is filling a sphere with smaller spheres (the so-called Swiss-Cheese Theorem) see, e.g., (Thirring, 1983; Fisher, 1964). The estimate in (3.15), as it stands, is not, however, what is ultimately needed. What we need is a more involved one which allows us to count $(k-k')$ states corresponding to two consecutive $n^2 > n'^2$ values which is of central importance in deriving the upper-bound for the ground-state energy in Sect. 3.4 This estimate is given in Proposition 9. We first establish the following result.

**Proposition 8**

*Let $n'^2 < n^2$ be consecutive allowed $n^2$ values, then*

$$n - n' \leqslant 1 + \frac{1}{n'} \tag{3.38}$$

*and*

$$n\left[1 - \frac{1}{n'}\left(1 + \frac{1}{n'}\right)\right] \leqslant n'. \tag{3.39}$$

To derive (3.38), note that although $n'^2$ is a natural number, $n'$ is not necessarily so. Accordingly, let $n'_0$ be the largest positive integer such that $n'_0 \leqslant n$. That is, we may write

$$n' = n'_0 + x, \qquad 0 \leqslant x < 1\ , \tag{3.40}$$

$$n' < n'_0 + 1. \tag{3.41}$$

Consider the state specified by the vector $\mathbf{n}''$ where

$$\mathbf{n}'' = (n'_0 + 1, 1), \tag{3.42}$$

the length squared of $\mathbf{n}''$ is given by

$$n''^2 = (n'_0 + 1)^2 + 1. \tag{3.43}$$

From (3.41), we have $(n'_0 + 1)^2 > n'^2$, then

$$(n'_0 + 1)^2 + 1 > n'^2 + 1. \tag{3.44}$$

Compare (3.44) with (3.43), clearly

$$n''^2 > n'^2 + 1 \tag{3.45}$$

or

$$n'' > n'. \tag{3.46}$$

Since $n^2$, $n'^2$ are consecutive with $n^2 > n'^2$, it follows that $n'' \geqslant n$.

By using (3.43) and (3.40), we obtain

$$\begin{aligned} n''^2 - n'^2 &= (n'_0 + 1)^2 + 1 - (n'_0 + x)^2 \\ &= n'^2_0 + 2n'_0 + 1 + 1 - n'^2_0 - 2n'_0 x - x^2 \\ &= n'^2_0 - n'^2_0 + 2n'_0 - 2n'_0 x - x^2 + 2 \\ &= 2n'_0(1 - x) + (2 - x^2). \end{aligned} \tag{3.47}$$

Also

$$(n'' - n')^2 = n''^2 + n'^2 - 2n'n'' \geqslant 0 \tag{3.48}$$

and from (3.48), we obtain

$$2n'n'' \leqslant n''^2 + n'^2.$$

Add above inequality by $(-2n'^2)$, we obtain

$$2n'n'' - 2n'^2 \leqslant \left(n''^2 + n'^2\right) - 2n'^2$$

then

$$2n'\left(n'' - n'\right) \leqslant n''^2 - n'^2. \tag{3.49}$$

Substitute (3.47) in (3.49), then we obtain

$$2n'\left(n'' - n'\right) \leqslant 2n'_0(1-x) + (2-x^2) \tag{3.50}$$

which is from $n \leqslant n'$ and $0 \leqslant x < 1$. The above inequality leads to

$$\begin{aligned}
n'' - n' &\leqslant \frac{2n'_0(1-x)}{2n'} + \frac{2-x^2}{2n'} \\
&= \frac{n'_0(1-x)}{n'_0 + x} + \frac{2-x^2}{2n'} \\
&= \frac{n'_0(1-x)}{n'_0\left(1 + \dfrac{x}{n'_0}\right)} + \frac{2-x^2}{2n'} \\
&= \frac{1-x}{1 + \dfrac{x}{n'_0}} + \frac{2-x^2}{2n'}.
\end{aligned} \tag{3.51}$$

Consider the right-hand side of (3.51), by using the fact that $0 \leqslant x < 1$, we obtain

$$\begin{aligned}
\frac{1-x}{1 + \dfrac{x}{n'_0}} + \frac{2-x^2}{2n'} &\leqslant \frac{1-0}{1 + \dfrac{0}{n'_0}} + \frac{2-0}{2n'} \\
&= 1 + \frac{1}{n'}
\end{aligned} \tag{3.52}$$

and compare (3.52) with (3.51), then we obtain

$$n'' - n' \leqslant 1 + \frac{1}{n'}. \tag{3.53}$$

By using the fact that $n'' \geqslant n$, we have

$$n \leqslant n'',$$

add above inequality by $(-n')$ and by using (3.52), we obtain

$$n - n' \leqslant n'' - n' \leqslant 1 + \frac{1}{n'}. \tag{3.54}$$

Then, Eq. (3.38) follows.

From (3.54), we have

$$\begin{aligned} n' &\geqslant n - \left(1 + \frac{1}{n'}\right) \\ &= n\left[1 - \frac{1}{n}\left(1 + \frac{1}{n'}\right)\right]. \end{aligned} \tag{3.55}$$

Because

$$n \geqslant n'$$

then

$$-\frac{1}{n} \geqslant -\frac{1}{n'}.$$

Multiply above inequality by $\left(1 + \frac{1}{n'}\right)$, we obtain

$$-\frac{1}{n}\left(1 + \frac{1}{n'}\right) \geqslant -\frac{1}{n'}\left(1 + \frac{1}{n'}\right),$$

add above inequality by 1 and multiply the result by $n$, we obtain

$$n\left[1-\frac{1}{n}\left(1+\frac{1}{n'}\right)\right] \geqslant n\left[1-\frac{1}{n'}\left(1+\frac{1}{n'}\right)\right]. \tag{3.56}$$

By comparing with (3.55), Eq. (3.39) follows. □

For any consecutive $n^2 > n'^2$, we label the $(k-k')$ states, specified by those vectors *all* of length squared equal precisely to $n^2$ in an arbitrary order, as $\alpha = k'+1, k'+2, \ldots, k$. Let

$$C(n') = \left[\sqrt{1-\frac{1}{n'^2}}\left(1-\frac{3}{2n'}\right)-\frac{1}{2}-\frac{1}{n'}\right] \tag{3.57}$$

which coincides with the right-hand side expression in (3.37) when $n$ is replaced by $n'$. We then have the following important result.

**Proposition 9**

$$\alpha \geqslant n^2\left[1-\frac{1}{n'}\left(1+\frac{1}{n'}\right)\right]^2 C(n') \tag{3.58}$$

*valid for* $n'^2 \geqslant 29$.

This inequality follows from that in (3.37) which leads, by using (3.57), to

$$k > \cdots > (k'+1) > k' \geqslant n'^2 C(n') \tag{3.59}$$

and the one in (3.39). The constraint $n'^2 \geqslant 29$ just ensures the positivity of $C(n')$. (For the state specified by the vector $\mathbf{n}' = (2,5)$, for example, $n'^2 = 29$.) □

Let

$$c = \left[1 - \frac{1}{n'}\left(1 + \frac{1}{n'}\right)\right]^{-2} C^{-1}(n'). \tag{3.60}$$

By using (3.58) and (3.60), we obtain

$$\alpha \geqslant \frac{n^2}{c}. \tag{3.61}$$

Consider the case of $5 \leqslant n^2 \leqslant 29$. For $n^2 = 5$, we have $k' = 0$, $\alpha = 1, 2$ for the states $(1, 2)$, $(2, 1)$, respectively. Then, we have the bound $\alpha \geqslant 1$. This case of $5 \leqslant n^2 \leqslant 29$ leads to $c = 5$ as given below

$$\alpha \geqslant \frac{n^2}{5}, \quad 5 \leqslant n^2 \leqslant 29. \tag{3.62}$$

Consider the case of $30 \leqslant n^2 \leqslant 109$, an elementary computer analysis shows that (see Appendix B)

$$\alpha \geqslant \frac{n^2}{5}, \quad 30 \leqslant n^2 \leqslant 109. \tag{3.63}$$

On the other hand, for $n^2 \geqslant 109$, we can use our explicit inequality in (3.58) (valid for $n^2$ up to infinity!) to conclude that

$$\alpha > \frac{n^2}{4.94894} > \frac{n^2}{5} \ ,$$

$$\alpha \geqslant \frac{n^2}{5}, \quad n^2 \geqslant 109. \tag{3.64}$$

That is, for all allowed $n^2$

$$\alpha \geqslant \frac{n^2}{5}. \tag{3.65}$$

## 3.4 Derivation of Upper Bounds

For orthonormal trial functions, we choose the Dyson ones (Dyson, 1967)

$$\phi_n(\mathbf{x}) = \frac{2}{L} \sin\left(\frac{n_1 \pi x_1}{L}\right) \sin\left(\frac{n_2 \pi x_2}{L}\right) \tag{3.66}$$

for $0 < x_i < L$, and vanishing outside this interval. We label the states as $\alpha = 0$ for $\mathbf{n}_0 = (1,1)$ and for $\alpha \geqslant 1$, $\alpha = 1,2,3$ for $\mathbf{n} = (1,1),(2,1),(2,2)$, respectively and so on.

With our effort in deriving the bound given below, we have found the Dyson trial functions most suitable for the problem at hand for the following reasons.

(1) We need an orthonormal set of functions, defined on a bounded interval, for each $x_i$, vanishing at its end points with the length of the interval, chosen optimally, becoming smaller and smaller as $N$ increases, implying the localization of the particles and eventual collapse for large $N$.

(2) The trial orthonormal functions in (3.66) are simple enough to make explicit sharp analytical estimates as is seen below.

(3) We have tried other orthonormal trial functions, such as the Hermite functions, with an arbitrary scale parameter, and in all cases analyzed, the negative interaction part becomes very small in comparison to the kinetic energy part for large $n$, and hence are not appropriate as trial functions. In particular, the normalization constant in (3.66) is independent of $n$ unlike the situation, for example, with Hermite functions.

(4) The trial functions in (3.66) overlap, which is what is needed for the interaction term in (3.68) below to be non-vanishing, and a choice of non-overlapping orthonormal states defined on sub-intervals of $(0, L)$, for each $x_i$, for example, is not useful.

Let

$$T^{(n)} = \left\langle \phi_n \left| -\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} \right| \phi_n \right\rangle$$

$$= \frac{\hbar^2}{2m} \int \mathrm{d}^2\mathbf{x} \; \left| \boldsymbol{\nabla} \phi_n(\mathbf{x}) \right|^2 , \tag{3.67}$$

$$I^{(n)} = \int \mathrm{d}^2\mathbf{x} \mathrm{d}^2\mathbf{x}' \; \phi_{n_0}(\mathbf{x}) \phi_n(\mathbf{x}) \frac{e^2}{|\mathbf{x} - \mathbf{x}'|} \phi_{n_0}(\mathbf{x}') \phi_n(\mathbf{x}') \tag{3.68}$$

where we note that the functions in (3.66) are real. The evaluation of the integral in (3.67) is given below.

For $\mathbf{x} = (x_1, x_2)$, we have

$$\boldsymbol{\nabla} = \frac{\partial}{\partial x_1} \hat{\mathbf{i}} + \frac{\partial}{\partial x_2} \hat{\mathbf{j}} \tag{3.69}$$

then

$$\boldsymbol{\nabla} \phi_n(\mathbf{x}) = \frac{\partial \phi_n(\mathbf{x})}{\partial x_1} \hat{\mathbf{i}} + \frac{\partial \phi_n(\mathbf{x})}{\partial x_2} \hat{\mathbf{j}}, \tag{3.70}$$

$$\left| \boldsymbol{\nabla} \phi_n(\mathbf{x}) \right|^2 = \left| \frac{\partial \phi_n(\mathbf{x})}{\partial x_1} \right|^2 + \left| \frac{\partial \phi_n(\mathbf{x})}{\partial x_2} \right|^2 . \tag{3.71}$$

Multiply above equation by $\int \mathrm{d}^2\mathbf{x}$, we obtain

$$\int \mathrm{d}^2\mathbf{x} \; \left| \boldsymbol{\nabla} \phi_n(\mathbf{x}) \right|^2 = \sum_{i=1}^{2} \int \mathrm{d}^2\mathbf{x} \left| \frac{\partial \phi_n(\mathbf{x})}{\partial x_i} \right|^2 . \tag{3.72}$$

Consider above equation only the case of $i = 1$, we have

$$\frac{\partial \phi_n(\mathbf{x})}{\partial x_1} = \left( \frac{2}{L} \right) \frac{\partial}{\partial x_1} \left[ \sin\left( \frac{n_1 \pi x_1}{L} \right) \sin\left( \frac{n_2 \pi x_2}{L} \right) \right]$$

$$= \left( \frac{2}{L} \right) \left( \frac{n_1 \pi}{L} \right) \cos\left( \frac{n_1 \pi x_1}{L} \right) \sin\left( \frac{n_2 \pi x_2}{L} \right) \tag{3.73}$$

then

$$\left|\frac{\partial\phi_n(\mathbf{x})}{\partial x_1}\right|^2 = \left(\frac{2}{L}\right)^2\left(\frac{n_1\pi}{L}\right)^2\cos^2\left(\frac{n_1\pi x_1}{L}\right)\sin^2\left(\frac{n_2\pi x_2}{L}\right). \tag{3.74}$$

Multiply above equation by $\int \mathrm{d}^2\mathbf{x}$, we obtain

$$\begin{aligned}\int \mathrm{d}^2\mathbf{x}\left|\frac{\partial\phi_n(\mathbf{x})}{\partial x_1}\right|^2 &= \left(\frac{2}{L}\right)^2\left(\frac{n_1\pi}{L}\right)^2\int_0^L \mathrm{d}x_1\,\cos^2\left(\frac{n_1\pi x_1}{L}\right)\int_0^L \mathrm{d}x_2\,\sin^2\left(\frac{n_2\pi x_2}{L}\right)\\ &= \left(\frac{2}{L}\right)^2\left(\frac{n_1\pi}{L}\right)^2\left(\frac{L}{2}\right)^2\\ &= \left(\frac{n_1\pi}{L}\right)^2.\end{aligned} \tag{3.75}$$

Eq. (3.75) leads to

$$\int \mathrm{d}^2\mathbf{x}\left|\frac{\partial\phi_n(\mathbf{x})}{\partial x_i}\right|^2 = \left(\frac{n_i\pi}{L}\right)^2. \tag{3.76}$$

Substitute (3.76) in (3.72), then we obtain

$$\begin{aligned}\int \mathrm{d}^2\mathbf{x}\,\left|\boldsymbol{\nabla}\phi_n(\mathbf{x})\right|^2 &= \left(\frac{n_1\pi}{L}\right)^2+\left(\frac{n_2\pi}{L}\right)^2\\ &= \left(\frac{n\pi}{L}\right)^2\end{aligned} \tag{3.77}$$

where $n^2 = n_1^2 + n_2^2$. By using (3.67), we obtain

$$\begin{aligned}T^{(n)} &= \frac{\pi^2\hbar^2 n^2}{2mL^2}\,,\\ T^{(n_0)} &= \frac{\pi^2\hbar^2}{mL^2}\end{aligned} \tag{3.78}$$

where $n_0^2 = 2$.

From (3.66), we have

$$\phi_n(\mathbf{x}) = \left(\frac{2}{L}\right)\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right), \tag{3.79}$$

$$\phi_m(\mathbf{x}) = \left(\frac{2}{L}\right) \sin\left(\frac{m_1 \pi x_1}{L}\right) \sin\left(\frac{m_2 \pi x_2}{L}\right) \tag{3.80}$$

then

$$\begin{aligned}\int \mathrm{d}^2\mathbf{x}\ \left|\phi_n(\mathbf{x})\phi_m(\mathbf{x})\right|^2 &= \left(\frac{2}{L}\right)^4 \left[\int_0^L \mathrm{d}x_1\ \sin^2\left(\frac{n_1 \pi x_1}{L}\right) \sin^2\left(\frac{m_1 \pi x_1}{L}\right)\right] \\ &\quad \times \left[\int_0^L \mathrm{d}x_2\ \sin^2\left(\frac{n_2 \pi x_2}{L}\right) \sin^2\left(\frac{m_2 \pi x_2}{L}\right)\right] \\ &= \left(\frac{2}{L}\right)^4 \prod_{i=1}^{2} \left[\int_0^L \mathrm{d}x_i\ \sin^2\left(\frac{n_i \pi x_i}{L}\right) \sin^2\left(\frac{m_i \pi x_i}{L}\right)\right] \end{aligned} \tag{3.81}$$

where

$$\int_0^L \mathrm{d}x_i\ \sin^2\left(\frac{n \pi x_i}{L}\right) \sin^2\left(\frac{m \pi x_i}{L}\right) = \frac{L}{4}.$$

Then (3.81) becomes

$$\int \mathrm{d}^2\mathbf{x}\ \left|\phi_n(\mathbf{x})\phi_m(\mathbf{x})\right|^2 = \left(\frac{2}{L}\right)^4 \left(\frac{L}{4}\right)^2 = \frac{1}{L^2}. \tag{3.82}$$

To obtain an appropriate bound for (3.68), we define

$$F(\mathbf{k}) = \int \mathrm{d}^2\mathbf{x}\ \phi_n(\mathbf{x})\phi_m(\mathbf{x})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{3.83}$$

and hence

$$\phi_n(\mathbf{x})\phi_m(\mathbf{x}) = \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2}\ F(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{3.84}$$

then

$$\boldsymbol{\nabla}\phi_n(\mathbf{x})\phi_m(\mathbf{x}) = \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2}\ F(\mathbf{k})(\mathrm{i}\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{3.85}$$

The square of above equation is given by

$$\left|\boldsymbol{\nabla}\phi_n(\mathbf{x})\phi_m(\mathbf{x})\right|^2 = \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \int \frac{\mathrm{d}^2\mathbf{k}'}{(2\pi)^2}\ (\mathrm{i}\mathbf{k}) \cdot (-\mathrm{i}\mathbf{k}')\ F(\mathbf{k})F^*(\mathbf{k}')\, \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \tag{3.86}$$

and multiply (3.86) by $\int d^2\mathbf{x}$, we obtain

$$\int d^2\mathbf{x} \left|\boldsymbol{\nabla}\phi_n(\mathbf{x})\phi_m(\mathbf{x})\right|^2 = \int \frac{d^2\mathbf{k}}{(2\pi)^2} \int \frac{d^2\mathbf{k}'}{(2\pi)^2}\, \mathbf{k}\cdot\mathbf{k}'\, F(\mathbf{k})F^*(\mathbf{k}') \int d^2\mathbf{x}\, e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}$$

$$= \int \frac{d^2\mathbf{k}}{(2\pi)^2} \int d^2\mathbf{k}'\, \mathbf{k}\cdot\mathbf{k}'\, F(\mathbf{k})F^*(\mathbf{k}') \left(\int \frac{d^2\mathbf{x}}{(2\pi)^2}\, e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}\right)$$

$$= \int \frac{d^2\mathbf{k}}{(2\pi)^2} \int d^2\mathbf{k}'\, \mathbf{k}\cdot\mathbf{k}'\, F(\mathbf{k})F^*(\mathbf{k}')\, \delta(\mathbf{k}-\mathbf{k}')$$

$$= \int \frac{d^2\mathbf{k}}{(2\pi)^2}\, \left|\mathbf{k}\right|^2\, \left|F(\mathbf{k})\right|^2. \tag{3.87}$$

From (3.84), we have

$$\left|\phi_n(\mathbf{x})\phi_m(\mathbf{x})\right|^2 = \int \frac{d^2\mathbf{k}}{(2\pi)^2} \int \frac{d^2\mathbf{k}'}{(2\pi)^2}\, F(\mathbf{k})F^*(\mathbf{k}')\, e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}. \tag{3.88}$$

Multiplying (3.88) by $\int d^2\mathbf{x}$ gives

$$\int d^2\mathbf{x}\, \left|\phi_n(\mathbf{x})\phi_m(\mathbf{x})\right|^2 = \int \frac{d^2\mathbf{k}}{(2\pi)^2} \int d^2\mathbf{k}'\, F(\mathbf{k})F^*(\mathbf{k}') \left(\int \frac{d^2\mathbf{x}}{(2\pi)^2}\, e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}\right)$$

$$= \int \frac{d^2\mathbf{k}}{(2\pi)^2} \int d^2\mathbf{k}'\, F(\mathbf{k})F^*(\mathbf{k}')\, \delta(\mathbf{k}-\mathbf{k}')$$

$$= \int \frac{d^2\mathbf{k}}{(2\pi)^2}\, \left|F(\mathbf{k})\right|^2. \tag{3.89}$$

From the elementary Schwarz inequality (Woan, 2000), we also have

$$\left(\int_a^b dx\; f(x)g(x)\right)^2 \leqslant \int_a^b dx\; \left[f(x)\right]^2 \int_a^b dx\, \left[g(x)\right]^2. \tag{3.90}$$

Eq. (3.89) can be rewritten as below

$$\int d^2\,\mathbf{x} \left|\phi_n(\mathbf{x})\phi_m(\mathbf{x})\right|^2 = \int \frac{d^2\mathbf{k}}{(2\pi)^2}\, \left|F(\mathbf{k})\right|^2$$

$$= \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \left|F(\mathbf{k})\right| \sqrt{|\mathbf{k}|} \frac{1}{\sqrt{|\mathbf{k}|}} \left|F(\mathbf{k})\right|. \tag{3.91}$$

By using (3.90), Eq. (3.91) becomes

$$\left(\int \mathrm{d}^2\mathbf{x} \left|\phi_n(\mathbf{x})\phi_m(\mathbf{x})\right|^2\right)^2 \leqslant \left(\int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \left|F(\mathbf{k})\right|^2 |\mathbf{k}|\right) \left(\int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \frac{\left|F(\mathbf{k})\right|^2}{|\mathbf{k}|}\right). \tag{3.92}$$

From (3.83), we have

$$\left|F(\mathbf{k})\right|^2 = \int \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}' \ \phi_n(\mathbf{x})\phi_m(\mathbf{x})\, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \ \phi_n(\mathbf{x}')\phi_m(\mathbf{x}'). \tag{3.93}$$

Multiplying of (3.93) by $\int \mathrm{d}^2\mathbf{k}\, |\mathbf{k}|^{-1}$ gives

$$\int \mathrm{d}^2\mathbf{k} \ \frac{\left|F(\mathbf{k})\right|^2}{|\mathbf{k}|} = \int \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}' \ \phi_n(\mathbf{x})\phi_m(\mathbf{x}) \left(\int \mathrm{d}^2\mathbf{k} \ \frac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}{|\mathbf{k}|}\right) \phi_n(\mathbf{x}')\phi_m(\mathbf{x}'). \tag{3.94}$$

Consider the integral of $\mathbf{k}$ on the right-hand side of (3.94)

$$\begin{aligned}
\int \mathrm{d}^2\mathbf{k} \ \frac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{|\mathbf{k}|} &= \int_0^\infty \int_0^{2\pi} k\mathrm{d}\theta\, \mathrm{d}k \ \frac{\mathrm{e}^{-\mathrm{i}kx\cos\theta}}{k} \\
&= \int_0^\infty \int_0^{2\pi} \mathrm{d}\theta \mathrm{d}k \ \mathrm{e}^{-\mathrm{i}kx\cos\theta} \\
&= \int_0^\infty \mathrm{d}k \ \int_0^{2\pi} \mathrm{d}\theta \ \mathrm{e}^{-\mathrm{i}kx\cos\theta}.
\end{aligned} \tag{3.95}$$

Because

$$\begin{aligned}
\mathrm{e}^{-\mathrm{i}kx\cos\theta} &= \sum_{n=0}^{\infty} \frac{(-\mathrm{i}kx\cos\theta)^n}{n!} \\
&= \sum_{n=0}^{\infty} \frac{(-\mathrm{i}kx)^n (\cos\theta)^n}{n!}
\end{aligned} \tag{3.96}$$

then

$$\int_0^{2\pi} \mathrm{d}\theta \; \mathrm{e}^{-\mathrm{i}kx\cos\theta} = \sum_{n=0}^{\infty} \int_0^{2\pi} \mathrm{d}\theta \; \frac{(-\mathrm{i}kx)^n \, (\cos\theta)^n}{n!}$$

$$= \sum_{n=0}^{\infty} \frac{(-\mathrm{i}kx)^n}{n!} \int_0^{2\pi} \mathrm{d}\theta \;\; (\cos\theta)^n. \tag{3.97}$$

Since

$$\cos^n\theta = \frac{\left(\mathrm{e}^{\mathrm{i}\theta} + \mathrm{e}^{-\mathrm{i}\theta}\right)^n}{2^n}$$

$$= 2^{-n} \left(\mathrm{e}^{-\mathrm{i}\theta} + \mathrm{e}^{\mathrm{i}\theta}\right)^n \tag{3.98}$$

and from the binomial expansion, we have

$$(a+b)^n = \sum_{k=0}^{n} \binom{n}{k} a^{n-k} \, b^k$$

$$= \sum_{k=0}^{n} \frac{n!}{k!(n-k)!} \; a^{n-k} \, b^k \tag{3.99}$$

then

$$\left(\mathrm{e}^{-\mathrm{i}\theta} + \mathrm{e}^{\mathrm{i}\theta}\right)^n = \sum_{k=0}^{n} \left[\frac{n!}{k!(n-k)!} \; \mathrm{e}^{-\mathrm{i}\theta(n-k)} \, \mathrm{e}^{\mathrm{i}\theta k}\right]$$

$$= \sum_{k=0}^{n} \left[\frac{n!}{k!(n-k)!} \; \mathrm{e}^{-\mathrm{i}\theta(n-2k)}\right]. \tag{3.100}$$

From (3.98)–(3.100), we obtain

$$\int_0^{2\pi} \mathrm{d}\theta \;\; \cos^n\theta = \int_0^{2\pi} \mathrm{d}\theta \; 2^{-n} \left(\mathrm{e}^{-\mathrm{i}\theta} + \mathrm{e}^{\mathrm{i}\theta}\right)^n$$

$$= \int_0^{2\pi} \mathrm{d}\theta \; 2^{-n} \sum_{k=0}^{n} \left[ \frac{n!}{k!(n-k)!} \, \mathrm{e}^{-\mathrm{i}\theta(n-2k)} \right]$$

$$= 2^{-n} \sum_{k=0}^{n} \left[ \frac{n!}{k!(n-k)!} \int_0^{2\pi} \mathrm{d}\theta \; \mathrm{e}^{-\mathrm{i}\theta(n-2k)} \right] \tag{3.101}$$

where the integral of $\theta$ on the right-hand side of (3.101) is

$$\int_0^{2\pi} \mathrm{d}\theta \; \mathrm{e}^{-\mathrm{i}\theta(n-2k)} = \int_0^{2\pi} \mathrm{d}\theta \; \left[ \cos\theta(n-2k) - \mathrm{i}\sin\theta(n-2k) \right]$$

$$= 2\pi \, \delta(n-2k). \tag{3.102}$$

Then $n$ should be even integer $(0, 2, 4, \ldots)$. Substitute (3.102) in (3.101), then we obtain

$$\int_0^{2\pi} \mathrm{d}\theta \; \cos^n\theta = 2^{-n} \sum_{k=0}^{n} \left[ \frac{n!}{k!(n-k)!} \; 2\pi \, \delta(n-2k) \right]$$

$$= \frac{2\pi}{2^n} \left[ \frac{n!}{\left(\frac{n}{2}\right)! \left(\frac{n}{2}\right)!} \right]. \tag{3.103}$$

For $j = 0, 1, 2, \ldots$, and $n = 2j$, substitute (3.103) in (3.97) we obtain

$$\int_0^{2\pi} \mathrm{d}\theta \; \mathrm{e}^{-\mathrm{i}kx\cos\theta} = 2\pi \sum_{n=\mathrm{even}}^{\infty} \frac{(-\mathrm{i}kx)^n \; (n!)}{2^n \, (n!) \left(\frac{n}{2}\right)! \left(\frac{n}{2}\right)!}$$

$$= 2\pi \sum_{n=\mathrm{even}}^{\infty} \frac{(-\mathrm{i}kx)^n}{2^n \left(\frac{n}{2}\right)! \left(\frac{n}{2}\right)!}$$

$$= 2\pi \sum_{j=0}^{\infty} \frac{(-\mathrm{i}kx)^{2j}}{(2)^{2j} \left(\frac{2j}{2}\right)! \left(\frac{2j}{2}\right)!}$$

$$= 2\pi \sum_{j=0}^{\infty} \frac{(-1)^{2j} \left[ \mathrm{i}^2 (kx)^2 \right]^j}{(2)^{2j} \left( \frac{2j}{2} \right)! \left( \frac{2j}{2} \right)!}$$

$$= 2\pi \sum_{j=0}^{\infty} \frac{\left[ - \left( k \frac{x}{2} \right)^2 \right]^j}{j!\, j!}$$

$$= 2\pi \sum_{j=0}^{\infty} \frac{\left[ - \frac{(kx)^2}{4} \right]^j}{j!\, \Gamma(j+1)}. \tag{3.104}$$

The expression of Bessel function is given by

$$J_\nu(z) = \left( \frac{z}{2} \right)^\nu \sum_{j=0}^{\infty} \frac{\left( -\frac{z^2}{4} \right)^j}{j!\, \Gamma(\nu + j + 1)}. \tag{3.105}$$

Compare (3.105) with (3.104), we obtain

$$\int_0^{2\pi} \mathrm{d}\theta \; \mathrm{e}^{-\mathrm{i}kx \cos\theta} = 2\pi \, J_0(kx). \tag{3.106}$$

Substitute (3.106) in (3.95), then we obtain

$$\int \mathrm{d}^2\mathbf{k} \; \frac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{|\mathbf{k}|} = 2\pi \int_0^\infty \mathrm{d}k \; J_0(kx). \tag{3.107}$$

It was shown by Lipschitz*) that

$$\int_0^\infty \mathrm{d}t \; \mathrm{e}^{-at} \, J_0(bt) = \frac{1}{\pi} \int_0^\infty \mathrm{d}t \; \mathrm{e}^{-at} \int_0^\pi \mathrm{d}\theta \; \mathrm{e}^{\mathrm{i}bt\cos\theta}$$

$$= \frac{1}{\pi} \int_0^\pi \frac{\mathrm{d}\theta}{a - \mathrm{i}b\cos\theta}$$

---

*) Watson, G. N. (1966). **A treatise on the theory of bessel functions** (Chap. XIII, p. 384, Section 13.2). New York: Cambridge University Press.

$$= \frac{1}{\sqrt{a^2 + b^2}} \tag{3.108}$$

then

$$\lim_{a \to 0} \int_0^\infty \mathrm{d}t \; \mathrm{e}^{-at} J_0(bt) = \int_0^\infty \mathrm{d}t \; J_0(bt)$$

$$= \frac{1}{|b|}. \tag{3.109}$$

Compare (3.107) with (3.109), we obtain

$$\int \mathrm{d}^2\mathbf{k} \; \frac{\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}{|\mathbf{k}|} = \frac{2\pi}{|\mathbf{x}-\mathbf{x}'|}. \tag{3.110}$$

Substitute (3.110) in (3.94), then we have

$$\int \mathrm{d}^2\mathbf{k} \; \frac{|F(\mathbf{k})|^2}{|\mathbf{k}|} = \int \mathrm{d}^2\mathbf{x} \, \mathrm{d}^2\mathbf{x}' \; \phi_n(\mathbf{x})\phi_m(\mathbf{x}) \, \frac{2\pi}{|\mathbf{x}-\mathbf{x}'|} \, \phi_n(\mathbf{x}')\phi_m(\mathbf{x}'). \tag{3.111}$$

Multiply (3.111) by $\dfrac{(2\pi)e^2}{(2\pi)^2}$ and let $\mathbf{m} = \mathbf{n}_0 = (1,1)$, then

$$(2\pi)\, e^2 \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \, \frac{|F(\mathbf{k})|^2}{|\mathbf{k}|} = \int \mathrm{d}^2\mathbf{x} \, \mathrm{d}^2\mathbf{x}' \; \phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x}) \, \frac{e^2}{|\mathbf{x}-\mathbf{x}'|} \, \phi_{n_0}(\mathbf{x}')\phi_n(\mathbf{x}')$$

$$\equiv I^{(n)}. \tag{3.112}$$

Multiply inequality (3.92) by $(2\pi)e^2$, by using (3.112), gives

$$(2\pi)\, e^2 \left( \int \mathrm{d}^2\mathbf{x} \; |\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})|^2 \right)^2$$

$$\leqslant \left( \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \; |F(\mathbf{k})|^2 \; |\mathbf{k}| \right) (2\pi)\, e^2 \left( \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \; \frac{|F(\mathbf{k})|^2}{|\mathbf{k}|} \right)$$

$$= \left( \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \; |F(\mathbf{k})|^2 \; |\mathbf{k}| \right) I^{(n)}. \tag{3.113}$$

Therefore

$$I^{(n)} \geqslant (2\pi)\, e^2 \; \frac{\left( \displaystyle\int \mathrm{d}^2\mathbf{x} \; |\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})|^2 \right)^2}{\displaystyle\int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \; |F(\mathbf{k})|^2 \; |\mathbf{k}|}. \tag{3.114}$$

Because

$$\sqrt{-\boldsymbol{\nabla}^2} \; \phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x}) = \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \; F(\mathbf{k}) \; |\mathbf{k}| \; \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{3.115}$$

By using (3.84) and the multiplying of (3.115) by $\int \mathrm{d}^2\mathbf{x} \; \phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})$, we obtain

$$\begin{aligned}
&\int \mathrm{d}^2\mathbf{x} \; \phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x}) \sqrt{-\boldsymbol{\nabla}^2} \; \phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x}) \\
&\quad = \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \; F(\mathbf{k}) \; |\mathbf{k}| \int \frac{\mathrm{d}^2\mathbf{k}'}{(2\pi)^2} \; F^*(\mathbf{k}') \int \mathrm{d}^2\mathbf{x} \; \mathrm{e}^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \\
&\quad = \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \; F(\mathbf{k}) \; |\mathbf{k}| \int \mathrm{d}^2\mathbf{k}' \; F^*(\mathbf{k}')\, \delta(\mathbf{k}-\mathbf{k}') \\
&\quad = \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \; |F(\mathbf{k})|^2 \; |\mathbf{k}|\,.
\end{aligned} \tag{3.116}$$

Substitute (3.116) in (3.114), we obtain

$$I^{(n)} \geqslant (2\pi)\, e^2 \frac{\left( \displaystyle\int \mathrm{d}^2\mathbf{x} \; |\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})|^2 \right)^2}{\displaystyle\int \mathrm{d}^2\mathbf{x} \; \phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x}) \sqrt{-\boldsymbol{\nabla}^2} \; \phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})}. \tag{3.117}$$

Let we define an operator, $G$, as

$$-\boldsymbol{\nabla}^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \equiv G$$

we have

$$\begin{aligned}
G\phi_n(\mathbf{x}) &= -\boldsymbol{\nabla}^2\phi_n(\mathbf{x}) \\
&= -\boldsymbol{\nabla}^2\left(\frac{2}{L}\right)\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right) \\
&= -\left(\frac{2}{L}\right)\left\{\frac{\partial^2}{\partial x_1^2}\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right)\right. \\
&\qquad \left.+\frac{\partial^2}{\partial x_2^2}\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right)\right\} \\
&= \left(\frac{2}{L}\right)\left\{\left(\frac{n_1\pi}{L}\right)^2\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right)\right. \\
&\qquad \left.+\left(\frac{n_2\pi}{L}\right)^2\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right)\right\} \\
&= \left(\frac{2}{L}\right)\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right)\left(n_1^2+n_2^2\right)\left(\frac{\pi}{L}\right)^2 \\
&= n^2\left(\frac{\pi}{L}\right)^2\left(\frac{2}{L}\right)\sin\left(\frac{n_1\pi x_1}{L}\right)\sin\left(\frac{n_2\pi x_2}{L}\right). \qquad (3.118)
\end{aligned}$$

Then from (3.118), we obtain “the eigenvalue equation”

$$\begin{aligned}
(-\boldsymbol{\nabla}^2)\phi_n(\mathbf{x}) &= -\boldsymbol{\nabla}^2\phi_n(\mathbf{x}) \\
&= \left(n^2\left(\frac{\pi}{L}\right)^2\right)\phi_n(\mathbf{x}) \\
&= g_n\phi_n(\mathbf{x}) \qquad (3.119)
\end{aligned}$$

where $g_n = n^2\left(\frac{\pi}{L}\right)^2$. For a function $f$ of $G$ defined by series

$$f(G) = \sum_{m=0}^{\infty} g_m G^m \qquad (3.120)$$

then we have

$$f(G)\phi_n(\mathbf{x}) = f\left(g_n\right)\phi_n(\mathbf{x}) \tag{3.121}$$

or

$$f(G)\phi_n(\mathbf{x})\phi_m(\mathbf{x}) = f\left(g_n + g_m\right)\phi_n(\mathbf{x})\phi_m(\mathbf{x}). \tag{3.122}$$

Then, by using (3.122), we have

$$\begin{aligned}\sqrt{-\boldsymbol{\nabla}^2}\;\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x}) &= \sqrt{n_0^2\left(\frac{\pi}{L}\right)^2 + n^2\left(\frac{\pi}{L}\right)^2}\;\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x}) \\ &= \left(\frac{\pi}{L}\right)\sqrt{(n_0^2+n^2)}\;\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x}).\end{aligned} \tag{3.123}$$

Multiplying of (3.123) by $\int \mathrm{d}^2\mathbf{x}\;\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})$, gives

$$\begin{aligned}&\int \mathrm{d}^2\mathbf{x}\;\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})\sqrt{-\boldsymbol{\nabla}^2}\;\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x}) \\ &\qquad= \left(\frac{\pi}{L}\right)\int \mathrm{d}^2\mathbf{x}\;\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})\sqrt{(n_0^2+n^2)}\;\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x}) \\ &\qquad= \left(\frac{\pi}{L}\right)\sqrt{n_0^2+n^2}\int \mathrm{d}^2\mathbf{x}\;\left|\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})\right|^2.\end{aligned} \tag{3.124}$$

Substitute (3.124) in (3.117), and by using (3.82), we obtain

$$\begin{aligned}I^{(n)} &\geqslant \frac{2\pi\, e^2\left(\int \mathrm{d}^2\mathbf{x}\;\left|\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})\right|^2\right)^2}{\left(\frac{\pi}{L}\right)\sqrt{n_0^2+n^2}\int \mathrm{d}^2\mathbf{x}\;\left|\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})\right|^2} \\ &= \frac{2L\, e^2}{\sqrt{n_0^2+n^2}}\int \mathrm{d}^2\mathbf{x}\;\left|\phi_{n_0}(\mathbf{x})\phi_n(\mathbf{x})\right|^2 \\ &= \frac{2L\, e^2}{\sqrt{n_0^2+n^2}}\frac{1}{L^2}\end{aligned}$$

$$= \frac{2e^2}{L\sqrt{n_0^2 + n^2}} \tag{3.125}$$

where $n_0^2 = 2$.

From the basic estimate in (3.65), we have $\alpha \geqslant \frac{n^2}{5}$, then

$$n^2 \leqslant 5\alpha. \tag{3.126}$$

Multiply (3.126) by $\frac{\hbar^2\pi^2}{2mL^2}$, and from (3.78), then we obtain

$$T_\alpha \leqslant 5\frac{\hbar^2\pi^2}{2mL^2}\,\alpha \tag{3.127}$$

with $T_\alpha$ defined in (3.12). From (3.126) we have

$$n^2 + 2 \leqslant 5\alpha + 2 \leqslant 5\alpha + 2\alpha$$

then

$$\sqrt{n^2+2} \leqslant \sqrt{5\alpha + 2\alpha}$$

or

$$\frac{1}{\sqrt{n^2+2}} \geqslant \frac{1}{\sqrt{7\alpha}}.$$

Multiply above inequality by $\frac{2\,e^2}{L}$ and compare the result with (3.125), then we obtain

$$I_{0\alpha} \geqslant \frac{2\,e^2}{L\sqrt{7\alpha}}. \tag{3.128}$$

Since $\alpha \leqslant k$, then

$$\sqrt{7\alpha} \leqslant \sqrt{7k}$$

then

$$\frac{1}{\sqrt{7\alpha}} \geqslant \frac{1}{\sqrt{7k}}. \tag{3.129}$$

Multiply (3.129) by $\dfrac{2\,e^2}{L}$, and compare the result with (3.128), we then obtain

$$I_{0\alpha} \geqslant \frac{2\,e^2}{L\sqrt{7k}} \tag{3.130}$$

with $I_{0\alpha}$ defined in (3.13).

For

$$\sum_n T^{(n)} = \sum_{\alpha=1}^{k} T_\alpha$$

and by using (3.127), we obtain

$$\begin{aligned}\sum_{\alpha=1}^{k} T_\alpha &\leqslant \left(\frac{5\hbar^2\pi^2}{2mL^2}\right)\sum_{\alpha=1}^{k}\alpha \\ &= \left(\frac{5\hbar^2\pi^2}{2mL^2}\right)\frac{k(k+1)}{2}.\end{aligned} \tag{3.131}$$

For

$$\sum_n I^{(n)} = \sum_{\alpha=1}^{k} I_{0\alpha}$$

and by using (3.130), we obtain

$$\begin{aligned}\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right) &\leqslant -\sum_{\alpha=1}^{k}\frac{2\,e^2}{L\sqrt{7k}} \\ &= -\frac{2\,e^2\sqrt{k}}{\sqrt{7}\,L}.\end{aligned} \tag{3.132}$$

The inequalities in (3.131) and (3.132) are needed in our upper bound in (3.14), which is given by

$$E_{N,N} < \frac{1}{2}\sum_{\alpha=1}^{k} T_\alpha + \left(N - \frac{k}{3}\right)T_0 + \frac{1}{3}\left[N - \frac{(k-2)}{2}\right]\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right).$$

Because $\left[N - \dfrac{(k-2)}{2}\right]$ is strictly positive, and by using (3.132)

$$\frac{1}{3}\left[N - \frac{(k-2)}{2}\right]\left(-\sum_{\alpha=1}^{k} I_{0\alpha}\right) \leqslant -\frac{1}{3}\left[N - \frac{(k-2)}{2}\right]\frac{2\,e^2\sqrt{k}}{\sqrt{7}\,L}. \tag{3.133}$$

From (3.78), we obtain

$$\left(N - \frac{k}{3}\right) T_0 = \frac{\hbar^2\pi^2}{mL^2}\left(N - \frac{k}{3}\right). \tag{3.134}$$

Multiplying of (3.131) by $\dfrac{1}{2}$, gives

$$\frac{1}{2}\sum_{\alpha=1}^{k} T_\alpha < \frac{5\,\hbar^2\pi^2}{2\,mL^2}\,\frac{k(k+1)}{4}. \tag{3.135}$$

The addition of (3.133), (3.134) and (3.135) gives

$$\begin{aligned} E_{N,N} &< \left(\frac{\hbar^2\pi^2}{2mL^2}\right)\frac{5k(k+1)}{4} + \frac{\hbar^2\pi^2}{mL^2}\left(N - \frac{k}{3}\right) - \frac{1}{3}\left[N - \frac{(k-2)}{2}\right]\frac{2e^2\sqrt{k}}{\sqrt{7}\,L} \\ &\equiv f(A). \end{aligned} \tag{3.136}$$

We want to find the minimum point of the right-hand side of (3.136), where

$$\begin{aligned} f(A) &= \left(\frac{\hbar^2\pi^2}{2mL^2}\right)\frac{5k(k+1)}{4} + \frac{\hbar^2\pi^2}{mL^2}\left(N - \frac{k}{3}\right) - \frac{1}{3}\left[N - \frac{(k-2)}{2}\right]\frac{2e^2\sqrt{k}}{\sqrt{7}\,L} \\ &\equiv pA^2 - qA. \end{aligned} \tag{3.137}$$

where $p$, $q > 0$ and $A$ will be optimally determined.

Let

$$\frac{\mathrm{d}f(A)}{\mathrm{d}A} = 2pA_0 - q = 0, \tag{3.138}$$

$$\frac{\mathrm{d}^2 f(A)}{\mathrm{d}A^2} = 2p \geqslant 0. \tag{3.139}$$

Then from (3.138), we have

$$A_0 = \frac{q}{2p} \tag{3.140}$$

which gives the minimum point $f(A_0)$ then

$$f(A) \geqslant f(A_0) \tag{3.141}$$

then

$$E_{N,N} < f(A_0) \tag{3.142}$$

where the minimum point of $f(A)$ is given by

$$\begin{aligned} f(A_0) &= pA_0^2 - qA_0 \\ &= p\left(\frac{q}{2p}\right)^2 - q\left(\frac{q}{2p}\right) \\ &= -\frac{q^2}{4p}. \end{aligned} \tag{3.143}$$

Let

$$\frac{1}{L} = \left(\frac{me^2}{\hbar^2\pi^2}\right) N^\alpha A \tag{3.144}$$

where $\alpha$ will be optimally determined. Substitute (3.144) in (3.137), we obtain

$$\begin{aligned} f(A) = &\left(\frac{\hbar^2\pi^2}{2m}\right)\left(\frac{m^2e^4N^{2\alpha}A^2}{\hbar^4\pi^4}\right)\left[\frac{5k(k+1)}{4}\right] \\ &+ \left(\frac{\hbar^2\pi^2}{m}\right)\left(\frac{m^2e^4N^{2\alpha}A^2}{\hbar^4\pi^4}\right)\left(N - \frac{k}{3}\right) \\ &- \frac{1}{3}\left[N - \frac{(k-2)}{2}\right]\left(\frac{2e^2\sqrt{k}}{\sqrt{7}}\right)\left(\frac{me^2}{\hbar^2\pi^2}\right) N^\alpha A \end{aligned}$$

$$= \left(\frac{me^4}{2\hbar^2}\right)\left[\frac{5k(k+1)}{4}\right]\left(\frac{N^{2\alpha}}{\pi^2}\right)A^2 + \left(\frac{me^4}{2\hbar^2}\right)2\left(N - \frac{k}{3}\right)\left(\frac{N^{2\alpha}}{\pi^2}\right)A^2$$

$$- \left(\frac{me^4}{2\hbar^2}\right)\frac{4}{3}\left[N - \frac{(k-2)}{2}\right]\left(\frac{\sqrt{k}}{\sqrt{7}}\frac{N^{2\alpha}}{\pi^2}\right)\frac{A}{N^\alpha}$$

$$= \left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{1+2\alpha}}{\pi^2}\right)\left[\frac{5k(k+1)}{4N}\right]A^2 + \left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{1+2\alpha}}{\pi^2}\right)2\left(1 - \frac{k}{3N}\right)A^2$$

$$- \left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{1+2\alpha}}{\pi^2}\right)\frac{4}{3}\left[1 - \frac{(k-2)}{2N}\right]\frac{\sqrt{k}}{\sqrt{7}}\frac{A}{N^\alpha}$$

$$= \left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{1+2\alpha}}{\pi^2}\right)\left\{A^2\left[2\left(1 - \frac{k}{3N}\right) + \frac{5k(k+1)}{4N}\right]\right.$$

$$\left. -\frac{4}{3}\left[1 - \frac{(k-2)}{2N}\right]\frac{k^{1/2}}{\sqrt{7}}\frac{A}{N^\alpha}\right\}$$

$$= \left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{1+2\alpha}}{\pi^2}\right)\{\,\cdot\,\} \tag{3.145}$$

where

$$\{\,\cdot\,\} = \left\{A^2\left[2\left(1 - \frac{k}{3N}\right) + \frac{5k(k+1)}{4N}\right] - \frac{4}{3}\left[1 - \frac{(k-2)}{2N}\right]\frac{k^{1/2}}{\sqrt{7}}\frac{A}{N^\alpha}\right\}. \tag{3.146}$$

Compare (3.145) with (3.137), we obtain

$$p = \left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{1+2\alpha}}{\pi^2}\right)\left[2\left(1 - \frac{k}{3N}\right) + \frac{5k(k+1)}{4N}\right], \tag{3.147}$$

$$q = \left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{1+2\alpha}}{\pi^2}\right)\frac{4}{3}\left[1 - \frac{(k-2)}{2N}\right]\frac{k^{1/2}}{\sqrt{7}}\frac{1}{N^\alpha} \tag{3.148}$$

where $\left[1-\dfrac{(k-2)}{2N}\right]$ is strictly positive. From (3.140), optimally we choose

$$A_0 = \frac{\left(\dfrac{me^4}{2\hbar^2}\right)\left(\dfrac{N^{1+2\alpha}}{\pi^2}\right)\dfrac{4}{3}\left[1-\dfrac{(k-2)}{2N}\right]\dfrac{k^{1/2}}{\sqrt{7}}\dfrac{1}{N^\alpha}}{2\left(\dfrac{me^4}{2\hbar^2}\right)\left(\dfrac{N^{1+2\alpha}}{\pi^2}\right)\left[2\left(1-\dfrac{k}{3N}\right)+\dfrac{5k(k+1)}{4N}\right]}$$

$$= \frac{\dfrac{4}{3}\left[1-\dfrac{(k-2)}{2N}\right]\dfrac{k^{1/2}}{\sqrt{7}}\dfrac{1}{N^\alpha}}{2\left[2\left(1-\dfrac{k}{3N}\right)+\dfrac{5k(k+1)}{4N}\right]}$$

$$= \frac{2}{3}\frac{\left[1-\dfrac{(k-2)}{2N}\right]\dfrac{k^{1/2}}{\sqrt{7}}\dfrac{1}{N^\alpha}}{\left[2\left(1-\dfrac{k}{3N}\right)+\dfrac{5k(k+1)}{4N}\right]}. \tag{3.149}$$

Substitute (3.154) in (3.143), we obtain

$$f(A_0) = -\frac{\left\{\left(\dfrac{me^4}{2\hbar^2}\right)\left(\dfrac{N^{1+2\alpha}}{\pi^2}\right)\dfrac{4}{3}\left[1-\dfrac{(k-2)}{2N}\right]\dfrac{k^{1/2}}{\sqrt{7}}\dfrac{1}{N^\alpha}\right\}^2}{4\left(\dfrac{me^4}{2\hbar^2}\right)\left(\dfrac{N^{1+2\alpha}}{\pi^2}\right)\left[2\left(1-\dfrac{k}{3N}\right)+\dfrac{5k(k+1)}{4N}\right]}$$

$$= -\left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{1+2\alpha}}{\pi^2}\right)\frac{\left\{\dfrac{4}{3}\left[1-\dfrac{(k-2)}{2N}\right]\dfrac{k^{1/2}}{\sqrt{7}}\dfrac{1}{N^\alpha}\right\}^2}{4\left[2\left(1-\dfrac{k}{3N}\right)+\dfrac{5k(k+1)}{4N}\right]}$$

$$= -\left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{1+2\alpha}}{\pi^2}\right)\left(\frac{2}{63}\right)\frac{\left[1-\dfrac{k}{2N}+\dfrac{1}{N}\right]^2\dfrac{k}{N^{2\alpha}}}{1-\dfrac{k}{3N}+\dfrac{5k(k+1)}{8N}}. \tag{3.150}$$

Since $N > 0$, then

$$\frac{1}{N} \geqslant 0$$

then

$$1-\frac{k}{2N}+\frac{1}{N} \geqslant 1-\frac{k}{2N}$$

which leads to

$$\left(1-\frac{k}{2N}+\frac{1}{N}\right)^2 \geqslant \left(1-\frac{k}{2N}\right)^2. \tag{3.151}$$

Since $\dfrac{k}{3N} \geqslant 0$, then

$$-\frac{k}{3N} \leqslant 0$$

then

$$1-\frac{k}{3N}+\frac{5k(k+1)}{8N} \leqslant 1+\frac{5k(k+1)}{8N}.$$

The inverse of above inequality gives

$$\frac{1}{1-\dfrac{k}{3N}+\dfrac{5k(k+1)}{8N}} \geqslant \frac{1}{1+\dfrac{5k(k+1)}{8N}}. \tag{3.152}$$

Multiplying of (3.151) by (3.152), gives

$$\begin{aligned}\frac{\left(1-\dfrac{k}{2N}+\dfrac{1}{N}\right)^2 \dfrac{k}{N^{2\alpha}}}{1-\dfrac{k}{3N}+\dfrac{5k(k+1)}{8N}} &\geqslant \frac{\left(1-\dfrac{k}{2N}\right)^2 \dfrac{k}{N^{2\alpha}}}{1+\dfrac{5k(k+1)}{8N}} \\ &= \frac{\left(1-\dfrac{k}{2N}\right)^2 \dfrac{k}{N^{2\alpha}}}{1+\dfrac{5k^2}{8N}+\dfrac{5k}{8N}}. \end{aligned} \tag{3.153}$$

The term on the right-hand side of (3.153) should finite when $N \to \infty$. Considering of $\dfrac{5k^2}{8N}$ in the denominator leads to

$$k \sim N^{1/2}$$

and the term $\dfrac{k}{N^{2\alpha}}$ in the numerator dictates the choice

$$\frac{k}{N^{2\alpha}} \equiv \text{ constant.}$$

Therefore, let

$$k = (BN)^{1/2}, \qquad B > 0 \tag{3.154}$$

then

$$\frac{k}{N^{2\alpha}} = \frac{(BN)^{1/2}}{N^{2\alpha}} = \text{constant}. \tag{3.155}$$

Eq. (3.155) leads to

$$N^{1/2} = N^{2\alpha}$$

then

$$N = N^{4\alpha}.$$

which gives

$$\alpha = \frac{1}{4}. \tag{3.156}$$

For $\alpha = \dfrac{1}{4}$, $k = (BN)^{1/2}$, Eq. (3.153) will be rewritten as below

$$\begin{aligned}
\frac{\left(1 - \dfrac{k}{2N} + \dfrac{1}{N}\right)^2 \dfrac{k}{N^{2\alpha}}}{1 - \dfrac{k}{3N} + \dfrac{5k(k+1)}{8N}} &\geqslant \frac{\left(1 - \dfrac{B^{1/2}N^{1/2}}{2N}\right)^2 \dfrac{B^{1/2}N^{1/2}}{N^{1/2}}}{1 + \dfrac{5BN}{8N} + \dfrac{5B^{1/2}N^{1/2}}{8N}} \\
&\geqslant \frac{\left(1 - \dfrac{B^{1/2}}{2N^{1/2}}\right)^2 B^{1/2}}{1 + \dfrac{5B}{8} + \dfrac{5B^{1/2}}{8N^{1/2}}} \\
&\equiv g(B)
\end{aligned} \tag{3.157}$$

where

$$g(B) = \frac{\left(1 - \dfrac{B^{1/2}}{2N^{1/2}}\right)^2 B^{1/2}}{1 + \dfrac{5B}{8} + \dfrac{5B^{1/2}}{8N^{1/2}}}. \tag{3.158}$$

Optimization of $g(B)$ with respect to $B$ where $N \to \infty$, is given by

$$\lim_{N\to\infty} \frac{\mathrm{d}g(B)}{\mathrm{d}B} = 0. \tag{3.159}$$

From (3.157), we obtain

$$\begin{aligned}
\lim_{N\to\infty} \frac{\mathrm{d}g(B)}{\mathrm{d}B} &= \lim_{N\to\infty} \frac{\mathrm{d}}{\mathrm{d}B} \frac{\left(1 - \dfrac{B^{1/2}}{2N^{1/2}}\right)^2 B^{1/2}}{1 + \dfrac{5B}{8} + \dfrac{5B^{1/2}}{8N^{1/2}}} \\
&= \lim_{N\to\infty} \left(1 - \frac{B^{1/2}}{2N^{1/2}}\right)^2 B^{1/2} \frac{\mathrm{d}}{\mathrm{d}B} \frac{1}{\left(1 + \dfrac{5B}{8} + \dfrac{5B^{1/2}}{8N^{1/2}}\right)} \\
&\quad + \lim_{N\to\infty} \frac{\left[\dfrac{\mathrm{d}}{\mathrm{d}B}\left(1 - \dfrac{B^{1/2}}{2N^{1/2}}\right)^2\right] B^{1/2} + \left[1 - \dfrac{B^{1/2}}{2N^{1/2}}\right]^2 \dfrac{\mathrm{d}}{\mathrm{d}B} B^{1/2}}{1 + \dfrac{5B}{8} + \dfrac{5B^{1/2}}{8N^{1/2}}} \\
&= -\frac{B^{1/2}}{\left(1 + \dfrac{5B}{8}\right)^2} \frac{\mathrm{d}}{\mathrm{d}B}\left(\frac{5B}{8}\right) + \frac{\dfrac{\mathrm{d}}{\mathrm{d}B} B^{1/2}}{1 + \dfrac{5B}{8}} \\
&= -\frac{5B^{1/2}}{8\left(1 + \dfrac{5B}{8}\right)^2} + \frac{1}{2B^{1/2}\left(1 + \dfrac{5B}{8}\right)} \\
&= \frac{1}{2\left(1 + \dfrac{5B}{8}\right)} \left[\frac{1}{B^{1/2}} - \frac{5B^{1/2}}{4\left(1 + \dfrac{5B}{8}\right)}\right].
\end{aligned} \tag{3.160}$$

Then from (3.159), we have

$$\frac{1}{B^{1/2}} - \frac{5B^{1/2}}{4\left(1 + \dfrac{5B}{8}\right)} = 0 \tag{3.161}$$

leads to

$$B = \frac{8}{5}. \tag{3.162}$$

Since $k$ is the largest integer, we substitute (3.162) in (3.154), then we obtain

$$k \leqslant \left(\frac{8N}{5}\right)^{1/2} \leqslant k+1 \tag{3.163}$$

or

$$k \leqslant \left(\frac{8N}{5}\right)^{1/2}, \tag{3.164}$$

$$k \geqslant \left(\frac{8N}{5}\right)^{1/2} - 1. \tag{3.165}$$

From (3.164), we obtain

$$\left[1 - \frac{k}{2N}\right]^2 \geqslant \left[1 - \frac{(8N)^{1/2}}{2N\sqrt{5}}\right]^2.$$

Multiplying above inequality by $\dfrac{k}{N^{1/2}}$ and by using (3.165), we obtain

$$\left(1 - \frac{k}{2N}\right)^2 \frac{k}{N^{1/2}} \geqslant \frac{1}{N^{1/2}} \left[1 - \frac{(8N)^{1/2}}{2N\sqrt{5}}\right]^2 \left[\left(\frac{8N}{5}\right)^{1/2} - 1\right]. \tag{3.166}$$

Also, (3.164) gives

$$k^2 \leqslant \left(\frac{8N}{5}\right)$$

then

$$\frac{5k^2}{8N} \leqslant 1 \tag{3.167}$$

and

$$\frac{5k}{8N} \leqslant \frac{5}{8N} \left(\frac{8N}{5}\right)^{1/2}$$

$$= \left(\frac{5}{8N}\right)^{1/2}. \tag{3.168}$$

The addition of the latter two inequalities, gives

$$1 + \frac{5k^2}{8N} + \frac{5k}{8N} \leqslant 2 + \left(\frac{5}{8N}\right)^{1/2}$$

or

$$\frac{1}{1 + \dfrac{5k^2}{8N} + \dfrac{5k}{8N}} \geqslant \frac{1}{2 + \left(\dfrac{5}{8N}\right)^{1/2}}. \tag{3.169}$$

Multiplying of (3.166) by (3.169), and compare the result with (3.157), gives

$$\begin{aligned}
\frac{\left(1 - \dfrac{k}{2N} + \dfrac{1}{N}\right)^2 \dfrac{k}{N^{1/2}}}{1 - \dfrac{k}{3N} + \dfrac{5k(k+1)}{8N}} &\geqslant \frac{\dfrac{1}{N^{1/2}} \left[1 - \dfrac{(8N)^{1/2}}{2N\sqrt{5}}\right]^2 \left[\left(\dfrac{8N}{5}\right)^{1/2} - 1\right]}{2 + \left(\dfrac{5}{8N}\right)^{1/2}} \\
&= \frac{\dfrac{1}{N^{1/2}} \left[1 - \dfrac{1}{2}\left(\dfrac{8}{5N}\right)^{1/2}\right]^2 \left[\left(\dfrac{8N}{5}\right)^{1/2} - 1\right]}{2 + \left(\dfrac{5}{8N}\right)^{1/2}} \\
&= \frac{\left[1 - \dfrac{1}{2}\left(\dfrac{8}{5N}\right)^{1/2}\right]^2 \left(\dfrac{8}{5}\right)^{1/2} \left[1 - \left(\dfrac{5}{8N}\right)^{1/2}\right]}{2 + \left(\dfrac{5}{8N}\right)^{1/2}}.
\end{aligned} \tag{3.170}$$

Substitute (3.170) in (3.150), we obtain

$$f(A_0) \leqslant -\left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{1+2\left(\frac{1}{4}\right)}}{\pi^2}\right)\left(\frac{2}{63}\right)\left(\frac{8}{5}\right)^{1/2}$$

$$\times \frac{\left[1 - \frac{1}{2}\left(\frac{8}{5N}\right)^{1/2}\right]^2 \left[1 - \left(\frac{5}{8N}\right)^{1/2}\right]}{2 + \left(\frac{5}{8N}\right)^{1/2}}$$

$$= -\left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{3/2}}{\pi^2}\right)\left(\frac{4}{63}\right)\left(\frac{2}{5}\right)^{1/2}$$

$$\times \frac{\left[1 - \left(\frac{2}{5N}\right)^{1/2}\right]^2 \left[1 - \frac{1}{2}\left(\frac{5}{2N}\right)^{1/2}\right]}{2 + \frac{1}{2}\left(\frac{5}{2N}\right)^{1/2}}$$

$$= -\left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{3/2}}{\pi^2}\right)\left(\frac{4}{63}\right)\left(\frac{2}{5}\right)^{1/2} \frac{1}{2} \frac{\left[1 - \left(\frac{2}{5N}\right)^{1/2}\right]^2 \left[1 - \frac{1}{2}\left(\frac{5}{2N}\right)^{1/2}\right]}{1 + \frac{1}{4}\left(\frac{5}{2N}\right)^{1/2}}$$

$$= -\left(\frac{me^4}{2\hbar^2}\right)\left(\frac{N^{3/2}}{\pi^2}\right)\{\cdot\cdot\} \tag{3.171}$$

where

$$\{\cdot\cdot\} = \left(\frac{4}{63}\right)\left(\frac{2}{5}\right)^{1/2} \frac{1}{2} \frac{\left[1 - \left(\frac{2}{5N}\right)^{1/2}\right]^2 \left[1 - \frac{1}{2}\left(\frac{5}{2N}\right)^{1/2}\right]}{1 + \frac{1}{4}\left(\frac{5}{2N}\right)^{1/2}}. \tag{3.172}$$

Consider the case of large $N$,

$$\lim_{N\to\infty}\{\cdot\cdot\} = \lim_{N\to\infty}\left(\frac{4}{63}\right)\left(\frac{2}{5}\right)^{1/2} \frac{1}{2} \frac{\left[1 - \left(\frac{2}{5N}\right)^{1/2}\right]^2 \left[1 - \frac{1}{2}\left(\frac{5}{2N}\right)^{1/2}\right]}{1 + \frac{1}{4}\left(\frac{5}{2N}\right)^{1/2}}$$

$$= \frac{1}{49.8059} > \frac{1}{50}. \tag{3.173}$$

Substitute (3.173) in (3.171), we obtain (3.142) as below

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{3/2}}{50\pi^2}. \tag{3.174}$$

# CHAPTER IV

# $N^{5/3}$ LAW FOR BOSONS FOR ARBITRARY LARGE $N$

## 4.1 Introduction

The rather complex problem involving the investigation of the collapse of "bosonic matter" in the bulk began in a classic paper by Dyson (Dyson, 1967) over three decades ago. This gave the famous $N^{7/5}$ law for the interaction of $(N+N)$ negatively and positively charged bosons via the Coulomb interaction. For a recent investigation of this law and of the improvement of Dyson's estimate, we refer the reader to our recent paper Manoukian and Muthaporn (2002) and elaborated upon in Chapter II. As mentioned in the introduction to the thesis, such a power law behaviour $N^{\alpha}$, with $\alpha > 1$, implies a collapse of "bosonic matter" since the formation of such matter consisting of $(2N+2N)$ particles will be favourable over two separate systems brought into contact, each consisting of $(N+N)$ particles, and the energy released upon collapse of two separate systems into a single system, being proportional to $[(2N)^{\alpha} - 2(N)^{\alpha}]$, will be overwhelmingly large for realistically large $N$, e.g., $N \sim 10^{23}$. One of the difficulties in such investigations, and the present one in the present chapter, is that both attractive and repulsive interactions occur, which are not necessarily globally attractive, in contrast to analyses involving only attractive, or globally attractive, ones (e.g., Hall, 2000; Perez, Malta and Coutinho, 1988). Also analyses dealing with instability problems, as necessary conditions, rather than stability ones (Weidl, 1996; Conlon, Lieb and Yan, 1988), as sufficiency conditions, turn out to be more complicated. Physically, what maybe more relevant to the problem of instability of "bosonic matter" is the Coulomb interaction of the negatively charged particles with fixed massive positively charged ones (Lieb, 1979). This is certainly non-academic. The reason for this is that by doing so, one does not dwell on the fate and dynamics of the so-called positive core which, undoubtedly, has a rather very complex dynamics at distances of nuclear dimensions. Such an investigation, by deriving an upper bound for the ground-state energy in question as a function of $N$, maybe then relevant to the collapse of "bosonic matter" down to the nuclear level beyond which some new physical insights may be needed. Unfortunately, the corresponding $N^{5/3}$ law (Lieb, 1979) for the upper bound has been given (Lieb, 1979) only for restrictive selected values for $N$ given for $N = 8, 64, 216, \ldots$. The purpose of this chapter is to complete this task and provide a complete and rigorous derivation for and upper bound of the ground-state energy for *arbitrary* $N \geqslant 8$. This is achieved by careful new methods of grouping of the particles in a non-trivial way.

The Hamiltonian under study is given by

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} - \sum_{j=1}^{N} \sum_{i=1}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{R}_j|} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{4.1}$$

where the $\mathbf{x}_i$ refer to the negatively charged particles, while the $\mathbf{R}_j$ refer to the positively charged ones. Here the masses $m_i$, as before, may be replaced by the smallest of the masses of the negatively charged bosons.

It is of some historical importance for us that we have initially tried to group the particles within spheres packed on various consecutive surfaces of larger spheres to obtain our bound. This turned out to be hopeless and we have soon realized that this is an *unsolved* problem in mathematics as announced in the Notices of the American Mathematical Society (Pfender and Ziegler, 2004; see also Croft, Falconer and Guy, 1991).

## 4.2 Derivation of Upper Bounds

With $N \geqslant 8$ denoting the number of negatively (or positively) charged particles, and $\left(\frac{N}{8}\right)^{1/3}$ being a real number, it may be written as

$$\left(\frac{N}{8}\right)^{1/3} = n + \varepsilon \tag{4.2}$$

where $n$ is a strictly positive integer and $0 \leqslant \varepsilon < 1$. Let

$$k = 8n^3. \tag{4.3}$$

From (4.2), we obtain

$$\frac{N}{8} = (n+\varepsilon)^3 = n^3\left(1+\frac{\varepsilon}{n}\right)^3,$$

$$N = 8n^3\left(1+\frac{\varepsilon}{n}\right)^3.$$

By using (4.3), we have

$$N = k\left(1+\frac{\varepsilon}{n}\right)^3. \tag{4.4}$$

Add (4.4) by $(-k)$, then

$$\begin{aligned}
N - k &= k\left(1+\frac{\varepsilon}{n}\right)^3 - k \\
&= k\left[\left(1+\frac{\varepsilon}{n}\right)^3 - 1\right] \\
&= k\left[\left(1+\frac{\varepsilon}{n}\right) - 1\right]\left[\left(1+\frac{\varepsilon}{n}\right)^2 + 1 + \left(1+\frac{\varepsilon}{n}\right)\right] \\
&= k\left(\frac{\varepsilon}{n}\right)\left[\left(1+\frac{\varepsilon}{n}\right)^2 + 1 + \left(1+\frac{\varepsilon}{n}\right)\right]
\end{aligned}$$

$$= k\left(\frac{\varepsilon}{n}\right)\left(1+\frac{\varepsilon}{n}\right)\left[\left(1+\frac{\varepsilon}{n}\right)+\frac{1}{\left(1+\frac{\varepsilon}{n}\right)}+1\right]. \tag{4.5}$$

Since $n \geqslant 1$, we have

$$\frac{1}{n} \leqslant 1 \tag{4.6}$$

then, for $0 \leqslant \varepsilon < 1$, the above inequality leads to

$$\frac{0}{n} \leqslant \frac{\varepsilon}{n} < \frac{1}{n} \leqslant 1. \tag{4.7}$$

By adding (4.7) by 1 gives

$$1 \leqslant 1+\frac{\varepsilon}{n} < 2 \tag{4.8}$$

then, we have

$$\left(1+\frac{\varepsilon}{n}\right) < 2. \tag{4.9}$$

The inverse of (4.9) leads to

$$\frac{1}{\left(1+\frac{\varepsilon}{n}\right)} > \frac{1}{2}. \tag{4.10}$$

From (4.8), we have

$$\left(1+\frac{\varepsilon}{n}\right) \geqslant 1. \tag{4.11}$$

The inverse of (4.11) leads to

$$\frac{1}{\left(1+\frac{\varepsilon}{n}\right)} \leqslant 1. \tag{4.12}$$

The addition of (4.9) and (4.12) gives

$$\left(1+\frac{\varepsilon}{n}\right)+\frac{1}{\left(1+\frac{\varepsilon}{n}\right)}+1 \leqslant 2+1+1$$

$$= 4 \tag{4.13}$$

and the addition of (4.10) and (4.11) gives

$$\left(1+\frac{\varepsilon}{n}\right)+\frac{1}{\left(1+\frac{\varepsilon}{n}\right)}+1>1+\frac{1}{2}+1$$

$$=\frac{5}{2}>2. \tag{4.14}$$

Substitute (4.13) and (4.14) in (4.5), we obtain

$$k\left(\frac{\varepsilon}{n}\right)\left(1+\frac{\varepsilon}{n}\right)\left[\left(1+\frac{\varepsilon}{n}\right)+\frac{1}{\left(1+\frac{\varepsilon}{n}\right)}+1\right]\geqslant 2k\left(\frac{\varepsilon}{n}\right)\left(1+\frac{\varepsilon}{n}\right) \tag{4.15}$$

and

$$k\left(\frac{\varepsilon}{n}\right)\left(1+\frac{\varepsilon}{n}\right)\left[\left(1+\frac{\varepsilon}{n}\right)+\frac{1}{\left(1+\frac{\varepsilon}{n}\right)}+1\right]\leqslant 4k\left(\frac{\varepsilon}{n}\right)\left(1+\frac{\varepsilon}{n}\right). \tag{4.16}$$

From (4.15) and (4.16), we have the useful bounds

$$2k\left(\frac{\varepsilon}{n}\right)\left(1+\frac{\varepsilon}{n}\right)\leqslant (N-k)\leqslant 4k\left(\frac{\varepsilon}{n}\right)\left(1+\frac{\varepsilon}{n}\right) \tag{4.17}$$

also $1\leqslant\left(1+\frac{\varepsilon}{N}\right)<2$. Our main result will apply for $\varepsilon=0$ as well.

We introduce an $N$-particle trial function

$$\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)=\frac{1}{\sqrt{N!k!}}\sum_{\pi}\phi\left(\mathbf{x}(\pi_1)\right)\ldots\phi\left(\mathbf{x}(\pi_k)\right)\psi_1\left(\mathbf{x}(\pi_{k+1})\right)\ldots\psi_{N-k}\left(\mathbf{x}(\pi_N)\right) \tag{4.18}$$

where the sum is over all permutations $\{\pi_1,\ldots,\pi_N\}$ of $\{1,\ldots,N\}$ such that

$$\int \mathrm{d}^3\mathbf{x}\;\psi_i^*(\mathbf{x})\psi_j(\mathbf{x})=\delta_{ij},$$

$$\int \mathrm{d}^3\mathbf{x}\;\phi^*(\mathbf{x})\psi_j(\mathbf{x})=0,$$

$$\int d^3\mathbf{x}\ |\phi(\mathbf{x})|^2 = 1. \tag{4.19}$$

Since $\Psi$ does not necessarily coincide with the ground-state wavefunction, we have for the ground-state energy $E_{N,N}$

$$E_{N,N} \leqslant \langle \Psi | H | \Psi \rangle\,. \tag{4.20}$$

## Example of Creation of $\Psi_4$

For case of $N = 4$, $k = 2$ ($N! = 24$, $k! = 2$), we will consider the sum of over all permutations $\{\pi_1, \pi_2, \pi_3, \pi_4\}$, let

$$\begin{aligned}\Lambda &= \sum_{\pi} \phi\left(\mathbf{x}(\pi_1)\right) \phi\left(\mathbf{x}(\pi_2)\right) \psi_1\left(\mathbf{x}(\pi_3)\right) \psi_2\left(\mathbf{x}(\pi_4)\right) \\ &= \sum_{n=1}^{N!=24} \Lambda_n.\end{aligned} \tag{4.21}$$

Let

$$\phi\left(\mathbf{x}(\pi_i)\right) \equiv (i), \tag{4.22}$$

$$\psi_q\left(\mathbf{x}(\pi_j)\right) \equiv [j]_q \tag{4.23}$$

where $\Lambda_n$ is the $n^{\text{th}}$ permutation term of $\{\pi_1, \ldots, \pi_4\}$, then we can choose

$$\Lambda_1 = (1)(2)[3]_1[4]_2, \quad \Lambda_2 = (3)(4)[1]_1[2]_2,$$

$$\Lambda_3 = (1)(3)[4]_1[2]_2, \quad \Lambda_4 = (3)(1)[2]_1[4]_2,$$

$$\Lambda_5 = (1)(4)[2]_1[3]_2, \quad \Lambda_6 = (3)(2)[4]_1[1]_2,$$

$$\Lambda_7 = (1)(2)[4]_1[3]_2, \quad \Lambda_8 = (3)(4)[2]_1[1]_2,$$

$$\Lambda_9 = (1)(3)[2]_1[4]_2, \quad \Lambda_{10} = (3)(1)[4]_1[2]_2,$$

$$\Lambda_{11} = (1)(4)[3]_1[2]_2, \quad \Lambda_{12} = (3)(2)[1]_1[4]_2,$$

$$\Lambda_{13} = (2)(3)[4]_1[1]_2, \quad \Lambda_{14} = (4)(1)[2]_1[3]_2,$$

$$\Lambda_{15} = (2)(4)[1]_1[3]_2, \quad \Lambda_{16} = (4)(2)[3]_1[1]_2,$$

$$\Lambda_{17} = (2)(1)[3]_1[4]_2, \quad \Lambda_{18} = (4)(3)[1]_1[2]_2,$$

$$\Lambda_{19} = (2)(3)[1]_1[4]_2, \quad \Lambda_{20} = (4)(1)[3]_1[2]_2,$$

$$\Lambda_{21} = (2)(4)[3]_1[1]_2, \quad \Lambda_{22} = (4)(2)[1]_1[3]_2,$$

$$\Lambda_{23} = (2)(1)[4]_1[3]_2, \quad \Lambda_{24} = (4)(3)[2]_1[1]_2. \tag{4.24}$$

Let

$$\sum_{\pi} = P_{N-1}P_{N-2}\dots P_2P_1 \tag{4.25}$$

where

$$P_M = 1 + \sum_{i=1}^{N-M} \left(\overline{P}_M\right)^i \tag{4.26}$$

for $1 \leqslant M \leqslant N-1$, and we have

$$\overline{P}_M\left\{\pi_1, \dots, \pi_M, \dots, \pi_N\right\} = \left\{\pi_1, \dots, \pi_{M-1}, \overline{P}_M\{\pi_M, \dots, \pi_N\}\right\} \tag{4.27}$$

where the definition of $\overline{P}_M$ is given by

$$\overline{P}_M\{\pi_M, \ldots, \pi_N\} = \{\pi_{M+1}, \pi_{M+2}, \ldots, \pi_N, \pi_M\}$$

$$\equiv \text{ the left-cyclic permutation of } \{\pi_M, \ldots, \pi_N\}. \qquad (4.28)$$

Example :

$$\overline{P}_1\{\pi_1, \ldots, \pi_N\} = \{\pi_2, \pi_3, \ldots, \pi_N, \pi_1\},$$

$$\overline{P}_2\overline{P}_1\{\pi_1, \ldots, \pi_N\} = \overline{P}_2\{\pi_2, \pi_3, \ldots, \pi_N, \pi_1\}$$

$$= \{\pi_2, \overline{P}_2\{\pi_3, \ldots, \pi_N, \pi_1\}\}$$

$$= \{\pi_2, \pi_4, \pi_5, \ldots, \pi_N, \pi_1, \pi_3\}. \qquad (4.29)$$

In case of $N = 4$, we have

$$P_1 = 1 + \sum_{i=1}^{3} \left(\overline{P}_M\right)^i. \qquad (4.30)$$

Then, the operation of $P_1$ on $\{\pi_1, \ldots, \pi_4\}$ gives

$$P_1\{\pi_1, \ldots, \pi_4\} = \left(1 + \overline{P}_1 + \overline{P}_1^2 + \overline{P}_1^3\right)\{\pi_1, \ldots, \pi_4\}$$

$$= \{\pi_1, \ldots, \pi_4\} + \overline{P}_1\{\pi_1, \ldots, \pi_4\} + \overline{P}_1^2\{\pi_1, \ldots, \pi_4\} + \overline{P}_1^3\{\pi_1, \ldots, \pi_4\}$$

$$= \{\pi_1, \ldots, \pi_4\} + \{\pi_2, \pi_3, \pi_4, \pi_1\} + \{\pi_3, \pi_4, \pi_1, \pi_2\} + \{\pi_4, \pi_1, \pi_2, \pi_3\}. \qquad (4.31)$$

Operate above equation by $P_2$, we obtain

$$P_2P_1\{\pi_1, \ldots, \pi_4\} = \left(1 + \overline{P}_2 + \overline{P}_2^2\right)$$

$$\times\ \big[\{\pi_1,\ldots,\pi_4\}+\{\pi_2,\pi_3,\pi_4,\pi_1\}+\{\pi_3,\pi_4,\pi_1,\pi_2\}+\{\pi_4,\pi_1,\pi_2,\pi_3\}\big]$$

$$\begin{aligned}
&= \big[\{\pi_1,\pi_2,\pi_3,\pi_4\}+\{\pi_2,\pi_3,\pi_4,\pi_1\}+\{\pi_3,\pi_4,\pi_1,\pi_2\}+\{\pi_4,\pi_1,\pi_2,\pi_3\}\big]\\
&+\overline{P}_2\big[\{\pi_1,\pi_2,\pi_3,\pi_4\}+\{\pi_2,\pi_3,\pi_4,\pi_1\}+\{\pi_3,\pi_4,\pi_1,\pi_2\}+\{\pi_4,\pi_1,\pi_2,\pi_3\}\big]\\
&+\overline{P}_2^2\big[\{\pi_1,\pi_2,\pi_3,\pi_4\}+\{\pi_2,\pi_3,\pi_4,\pi_1\}+\{\pi_3,\pi_4,\pi_1,\pi_2\}+\{\pi_4,\pi_1,\pi_2,\pi_3\}\big]\\
&= \big[\{\pi_1,\pi_2,\pi_3,\pi_4\}+\{\pi_2,\pi_3,\pi_4,\pi_1\}+\{\pi_3,\pi_4,\pi_1,\pi_2\}+\{\pi_4,\pi_1,\pi_2,\pi_3\}\big]\\
&+\ \big[\{\pi_1,\pi_3,\pi_4,\pi_2\}+\{\pi_2,\pi_4,\pi_1,\pi_3\}+\{\pi_3,\pi_1,\pi_2,\pi_4\}+\{\pi_4,\pi_2,\pi_3,\pi_1\}\big]\\
&+\overline{P}_2\big[\{\pi_1,\pi_3,\pi_4,\pi_2\}+\{\pi_2,\pi_4,\pi_1,\pi_3\}+\{\pi_3,\pi_1,\pi_2,\pi_4\}+\{\pi_4,\pi_2,\pi_3,\pi_1\}\big]\\
&= \big[\{\pi_1,\pi_2,\pi_3,\pi_4\}+\{\pi_2,\pi_3,\pi_4,\pi_1\}+\{\pi_3,\pi_4,\pi_1,\pi_2\}+\{\pi_4,\pi_1,\pi_2,\pi_3\}\big]\\
&+\ \big[\{\pi_1,\pi_3,\pi_4,\pi_2\}+\{\pi_2,\pi_4,\pi_1,\pi_3\}+\{\pi_3,\pi_1,\pi_2,\pi_4\}+\{\pi_4,\pi_2,\pi_3,\pi_1\}\big]\\
&+\ \big[\{\pi_1,\pi_4,\pi_2,\pi_3\}+\{\pi_2,\pi_1,\pi_3,\pi_4\}+\{\pi_3,\pi_2,\pi_4,\pi_1\}+\{\pi_4,\pi_3,\pi_1,\pi_2\}\big]\,.
\end{aligned} \tag{4.32}$$

Operate above equation by $P_3$, we obtain

$$\begin{aligned}
&P_3P_2P_1\{\pi_1,\ldots,\pi_4\}\\
&=\big(1+\overline{P}_3\big)\\
&\qquad\times\ \big[\{\pi_1,\pi_2,\pi_3,\pi_4\}+\{\pi_2,\pi_3,\pi_4,\pi_1\}+\{\pi_3,\pi_4,\pi_1,\pi_2\}+\{\pi_4,\pi_1,\pi_2,\pi_3\}\big]\\
&+\big(1+\overline{P}_3\big)\\
&\qquad\times\ \big[\{\pi_1,\pi_3,\pi_4,\pi_2\}+\{\pi_2,\pi_4,\pi_1,\pi_3\}+\{\pi_3,\pi_1,\pi_2,\pi_4\}+\{\pi_4,\pi_2,\pi_3,\pi_1\}\big]\\
&+\big(1+\overline{P}_3\big)\\
&\qquad\times\ \big[\{\pi_1,\pi_4,\pi_2,\pi_3\}+\{\pi_2,\pi_1,\pi_3,\pi_4\}+\{\pi_3,\pi_2,\pi_4,\pi_1\}+\{\pi_4,\pi_3,\pi_1,\pi_2\}\big]\\
&= \big[\{\pi_1,\pi_2,\pi_3,\pi_4\}+\{\pi_2,\pi_3,\pi_4,\pi_1\}+\{\pi_3,\pi_4,\pi_1,\pi_2\}+\{\pi_4,\pi_1,\pi_2,\pi_3\}\big]\\
&+\overline{P}_3\big[\{\pi_1,\pi_2,\pi_3,\pi_4\}+\{\pi_2,\pi_3,\pi_4,\pi_1\}+\{\pi_3,\pi_4,\pi_1,\pi_2\}+\{\pi_4,\pi_1,\pi_2,\pi_3\}\big]\\
&+\ \big[\{\pi_1,\pi_3,\pi_4,\pi_2\}+\{\pi_2,\pi_4,\pi_1,\pi_3\}+\{\pi_3,\pi_1,\pi_2,\pi_4\}+\{\pi_4,\pi_2,\pi_3,\pi_1\}\big]
\end{aligned}$$

$$+\overline{P}_3\left[\{\pi_1,\pi_3,\pi_4,\pi_2\}+\{\pi_2,\pi_4,\pi_1,\pi_3\}+\{\pi_3,\pi_1,\pi_2,\pi_4\}+\{\pi_4,\pi_2,\pi_3,\pi_1\}\right]$$
$$+\left[\{\pi_1,\pi_4,\pi_2,\pi_3\}+\{\pi_2,\pi_1,\pi_3,\pi_4\}+\{\pi_3,\pi_2,\pi_4,\pi_1\}+\{\pi_4,\pi_3,\pi_1,\pi_2\}\right]$$
$$+\overline{P}_3\left[\{\pi_1,\pi_4,\pi_2,\pi_3\}+\{\pi_2,\pi_1,\pi_3,\pi_4\}+\{\pi_3,\pi_2,\pi_4,\pi_1\}+\{\pi_4,\pi_3,\pi_1,\pi_2\}\right]$$

$$\begin{aligned}
&=\left[\{\pi_1,\pi_2,\pi_3,\pi_4\}+\{\pi_2,\pi_3,\pi_4,\pi_1\}+\{\pi_3,\pi_4,\pi_1,\pi_2\}+\{\pi_4,\pi_1,\pi_2,\pi_3\}\right]\\
&+\left[\{\pi_1,\pi_2,\pi_4,\pi_3\}+\{\pi_2,\pi_3,\pi_1,\pi_4\}+\{\pi_3,\pi_4,\pi_2,\pi_1\}+\{\pi_4,\pi_1,\pi_3,\pi_2\}\right]\\
&+\left[\{\pi_1,\pi_3,\pi_4,\pi_2\}+\{\pi_2,\pi_4,\pi_1,\pi_3\}+\{\pi_3,\pi_1,\pi_2,\pi_4\}+\{\pi_4,\pi_2,\pi_3,\pi_1\}\right]\\
&+\left[\{\pi_1,\pi_3,\pi_2,\pi_4\}+\{\pi_2,\pi_4,\pi_3,\pi_1\}+\{\pi_3,\pi_1,\pi_4,\pi_2\}+\{\pi_4,\pi_2,\pi_1,\pi_3\}\right]\\
&+\left[\{\pi_1,\pi_4,\pi_2,\pi_3\}+\{\pi_2,\pi_1,\pi_3,\pi_4\}+\{\pi_3,\pi_2,\pi_4,\pi_1\}+\{\pi_4,\pi_3,\pi_1,\pi_2\}\right]\\
&+\left[\{\pi_1,\pi_4,\pi_3,\pi_2\}+\{\pi_2,\pi_1,\pi_4,\pi_3\}+\{\pi_3,\pi_2,\pi_1,\pi_4\}+\{\pi_4,\pi_3,\pi_2,\pi_1\}\right]. \quad (4.33)
\end{aligned}$$

Then, compare (4.33) with (4.24), we obtain

$$\sum_{\pi}\{\pi_1,\pi_2,\pi_3,\pi_4\}=P_3P_2P_1\{\pi_1,\pi_2,\pi_3,\pi_4\}=\sum_{n=1}^{24}\Lambda_n.$$

Consider

$$\begin{aligned}
\Lambda^*\Lambda &= \left(\sum_{n=1}^{24}\Lambda_n^*\right)\left(\sum_{m=1}^{24}\Lambda_m\right)\\
&=(1)^*(2)^*[3]_1^*[4]_2^*\left(\sum_{m=1}^{24}\Lambda_m\right)+(1)^*(3)^*[4]_1^*[2]_2^*\left(\sum_{m=1}^{24}\Lambda_m\right)\\
&\qquad+\ldots+(4)^*(3)^*[2]_1^*[1]_2^*\left(\sum_{m=1}^{24}\Lambda_m\right)\\
&=(1)^*(2)^*[3]_1^*[4]_2^*\left\{(1)(2)[3]_1[4]_2+(1)(3)[4]_1[2]_2+\ldots+(4)(3)[2]_1[1]_2\right\}\\
&+(1)^*(3)^*[4]_1^*[2]_2^*\left\{(1)(2)[3]_1[4]_2+(1)(3)[4]_1[2]_2+\ldots+(4)(3)[2]_1[1]_2\right\}\\
&\quad+\\
&\quad\vdots
\end{aligned}$$

$$+$$

$$(4)^*(3)^*[2]_1^*[1]_2^* \left\{(1)(2)[3]_1[4]_2 + (1)(3)[4]_1[2]_2 + \ldots + (4)(3)[2]_1[1]_2\right\}$$

$$= (1)^*(2)^*[3]_1^*[4]_2^*$$

$$\times \left[\left\{\text{the sum of all permutations of } \{\pi_1, \pi_2\} \text{ of } \{(1)(2)\}\right\}[3]_1[4]_2 + \{\cdots\}\right]$$

$$+ (1)^*(3)^*[4]_1^*[2]_2^*$$

$$\times \left[\left\{\text{the sum of all permutations of } \{\pi_1, \pi_3\} \text{ of } \{(1)(3)\}\right\}[4]_1[2]_2 + \{\cdots\}\right]$$

$$+$$

$$\vdots$$

$$+$$

$$(4)^*(3)^*[2]_1^*[1]_2^*$$

$$\times \left[\left\{\text{the sum of all permutations of } \{\pi_4, \pi_3\} \text{ of } \{(4)(3)\}\right\}[2]_1[1]_2 + \{\cdots\}\right] \tag{4.34}$$

where $\{\cdots\}$ is the sum of other all possible permutations. Then

$$\Lambda^*\Lambda = \left(\sum_{n=1}^{24} \Lambda_n^*\right)\left(\sum_{m=1}^{24} \Lambda_m\right)$$

$$= (1)^*(2)^*[3]_1^*[4]_2^* \left[\left\{(1)(2) + (2)(1)\right\}[3]_1[4]_2 + \{\cdots\}\right]$$

$$+ (1)^*(3)^*[4]_1^*[2]_2^* \left[\left\{(1)(3) + (3)(1)\right\}[4]_1[2]_2 + \{\cdots\}\right]$$

$$+ \ldots +$$

$$(4)^*(3)^*[2]_1^*[1]_2^* \left[\left\{(4)(3) + (3)(4)\right\}[2]_1[1]_2 + \{\cdots\}\right]$$

$$= \left[\left\{|(1)|^2|(2)|^2 + |(2)|^2|(1)|^2\right\}|[3]_1|^2|[4]_2|^2 + (1)^*(2)^*\{\cdots\}[3]_1^*[4]_2^*\right]$$

$$+ \left[\left\{|(1)|^2|(3)|^2 + |(3)|^2|(1)|^2\right\}|[4]_1|^2|[2]_2|^2 + (1)^*(3)^*\{\cdots\}[4]_1^*[2]_2^*\right]$$

$$+$$

$$\vdots$$

$$+$$

$$\left[\,\left\{|(4)|^2\,|(3)|^2 + |(3)|^2\,|(4)|^2\right\}|[2]_1|^2\,|[1]_2|^2 + (4)^*(3)^*\,\{\cdots\}\,[2]_1^*[1]_2^*\right]$$

$$= \left\{2!\,|(1)|^2\,|(2)|^2\,|[3]_1|^2\,|[4]_2|^2 + (1)^*(2)^*\,\{\cdots\}\,[3]_1^*[4]_2^*\right\}$$

$$+ \left\{2!\,|(1)|^2\,|(3)|^2\,|[4]_1|^2\,|[2]_2|^2 + (1)^*(3)^*\,\{\cdots\}\,[4]_1^*[2]_2^*\right\}$$

$$+$$

$$\vdots$$

$$+$$

$$\left\{2!\,|(4)|^2\,|(3)|^2\,|[2]_1|^2\,|[1]_2|^2 + (4)^*(3)^*\,\{\cdots\}\,[2]_1^*[1]_2^*\right\}. \tag{4.35}$$

Then

$$\int d^3\mathbf{x}(\pi_1)\ldots d^3\mathbf{x}(\pi_4)\ \Lambda^*\Lambda = \int d^3\mathbf{x}(\pi_1)\ldots d^3\mathbf{x}(\pi_4)\ \left(\sum_{n=1}^{24}\Lambda_n^*\right)\left(\sum_{m=1}^{24}\Lambda_m\right)$$

$$= \int d^3\mathbf{x}(\pi_1)\ldots d^3\mathbf{x}(\pi_4)\left\{2!\,|(1)|^2\,|(2)|^2\,|[3]_1|^2\,|[4]_2|^2 + (1)^*(2)^*\,\{\cdots\}\,[3]_1^*[4]_2^*\right\}$$

$$+ \int d^3\mathbf{x}(\pi_1)\ldots d^3\mathbf{x}(\pi_4)\left\{2!\,|(1)|^2\,|(3)|^2\,|[4]_1|^2\,|[2]_2|^2 + (1)^*(3)^*\,\{\cdots\}\,[4]_1^*[2]_2^*\right\}$$

$$+\ldots+$$

$$\int d^3\mathbf{x}(\pi_1)\ldots d^3\mathbf{x}(\pi_4)\left\{2!\,|(4)|^2\,|(3)|^2\,|[2]_1|^2\,|[1]_2|^2 + (4)^*(3)^*\,\{\cdots\}\,[2]_1^*[1]_2^*\right\}$$

$$= \Bigg\{2!\int d^3\mathbf{x}(\pi_1)\,|(1)|^2\int d^3\mathbf{x}(\pi_2)\,|(2)|^2\int d^3\mathbf{x}(\pi_3)\,|[3]_1|^2\int d^3\mathbf{x}(\pi_4)\,|[4]_2|^2$$

$$+ \int d^3\mathbf{x}(\pi_1)\ldots d^3\mathbf{x}(\pi_4)(1)^*(2)^*\,\{\cdots\}\,[3]_1^*[4]_2^*\Bigg\}$$

$$+ \Bigg\{2!\int d^3\mathbf{x}(\pi_1)\,|(1)|^2\int d^3\mathbf{x}(\pi_3)\,|(3)|^2\int d^3\mathbf{x}(\pi_4)\,|[4]_1|^2\int d^3\mathbf{x}(\pi_2)\,|[2]_2|^2$$

$$+\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_4)(1)^*(3)^*\left\{\cdots\right\}[4]_1^*[2]_2^*\Big\}$$

$$+\ldots+$$

$$\Big\{2!\int \mathrm{d}^3\mathbf{x}(\pi_4)\,|(4)|^2\int \mathrm{d}^3\mathbf{x}(\pi_3)\,|(3)|^2\int \mathrm{d}^3\mathbf{x}(\pi_2)\,|[2]_1|^2\int \mathrm{d}^3\mathbf{x}(\pi_1)\,|[1]_2|^2$$

$$+\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_4)(4)^*(3)^*\left\{\cdots\right\}[2]_1^*[1]_2^*\Big\}$$

$$=\underbrace{\Big\{2!+0\Big\}+\Big\{2!+0\Big\}+\ldots+\Big\{2!+0\Big\}}_{4!\ \text{terms}}$$

$$=4!2!=N!k!. \tag{4.36}$$

Therefore, for any $N$, we define

$$\Lambda=\sum_{\pi}\phi\left(\mathbf{x}(\pi_1)\right)\phi\left(\mathbf{x}(\pi_2)\right)\ldots\left(\mathbf{x}(\pi_k)\right)\psi_1\left(\mathbf{x}(\pi_{k+1})\right)\ldots\psi_{N-k}\left(\mathbf{x}(\pi_N)\right)$$

$$=\sum_{n=1}^{N!}\Lambda_n \tag{4.37}$$

and from (4.36), we obtain

$$\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\;\Lambda^*\Lambda=\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\left(\sum_{n=1}^{N!}\Lambda_n^*\right)\left(\sum_{m=1}^{N!}\Lambda_m\right)$$

$$=N!k!. \tag{4.38}$$

Substitute (4.37) in (4.18), then we obtain

$$\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N)=\frac{1}{\sqrt{N!k!}}\;\sum_{n=1}^{N!}\Lambda_n. \tag{4.39}$$

By using (4.38), we obtain

$$\begin{aligned}
&\int d^3\mathbf{x}_1 \dots d^3\mathbf{x}_N \, |\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N)|^2 \\
&\quad = \frac{1}{N!k!} \int d^3\mathbf{x}(\pi_1) \dots d^3\mathbf{x}(\pi_N) \left( \sum_{n=1}^{N!} \Lambda_n^* \right) \left( \sum_{m=1}^{N!} \Lambda_m \right) \\
&\quad = \frac{1}{N!k!} N!k! \\
&\quad = 1.
\end{aligned} \tag{4.40}$$

We choose single-particle trial wavefunctions

$$\phi(\mathbf{x}) = \prod_{i=1}^{3} \left( \frac{1}{\sqrt{L}} \cos\left( \frac{\pi x_i}{2L} \right) \right) \equiv \phi_L(\mathbf{x}), \qquad |x_i| \leqslant L \tag{4.41}$$

and is zero otherwise, and for $j = 1, \dots, N - k$

$$\psi_j(\mathbf{x}) = \prod_{i=1}^{3} \left( \frac{1}{\sqrt{L_0}} \cos\left( \frac{\pi(x_i - L_{ji})}{2L_0} \right) \right) \equiv \phi_{L_0}(\mathbf{x} - \mathbf{L}_j), \qquad |x_i - Lji| \leqslant L_0 \tag{4.42}$$

and are zero otherwise, also

$$\mathbf{L}_j = jD(1, 1, 1) \tag{4.43}$$

$$|\mathbf{L}_j| = jD\sqrt{1^2 + 1^2 + 1^2} = jD\sqrt{3}. \tag{4.44}$$

From (4.44) and Fig. 4.2, we obtain

$$|\mathbf{L}_1| = \sqrt{3}D > \sqrt{3}L + \sqrt{3}L_0,$$

$$|\mathbf{L}_2| = 2\sqrt{3}D > \sqrt{3}L + 2\sqrt{3}L_0 + \sqrt{3}L_0 > \sqrt{3}L + 3\sqrt{3}L_0,$$

$$|\mathbf{L}_3| = 3\sqrt{3}D > \sqrt{3}L + 5\sqrt{3}L_0,$$

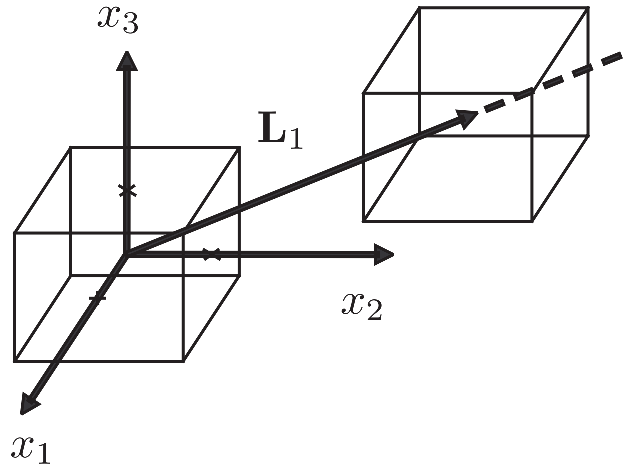


Figure 4.1: The figure shows the regions (non-overlapping boxes) where particles are localized. The centers of the boxes are situated at $0, \mathbf{L}_1, \ldots, \mathbf{L}_{N-k}$ with the latter $(N-k)$ vectors being along the vector $(1,1,1)$. The sides of the box at the origin are $2L, 2L, 2L$, while the ones of the other $(N-k)$ boxes are $2L_0, 2L_0, 2L_0$, where $L_0 \geqslant L$. The Coulomb potential being of long range, there are non-trivial interactions between particles in different boxes as well.

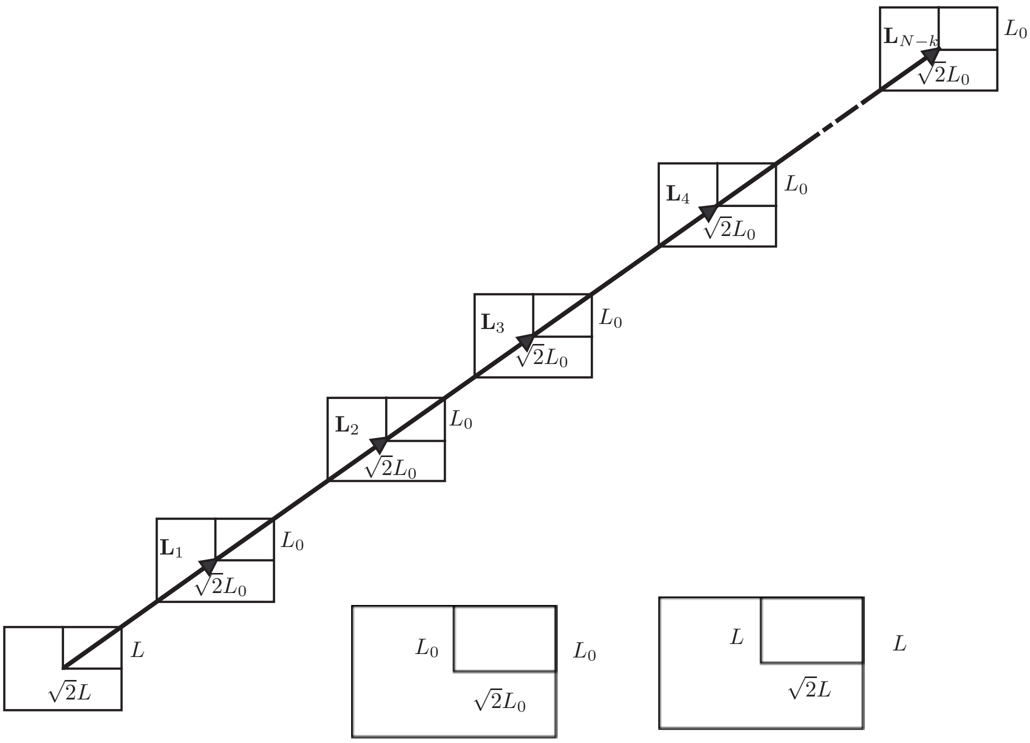


Figure 4.2: The figure displays the vectors $\mathbf{L}_1, \ldots, \mathbf{L}_{N-k}$

$$\vdots$$

$$|\mathbf{L}_j| = j\sqrt{3}D > \sqrt{3}L + (2j-1)\sqrt{3}L_0. \tag{4.45}$$

Then

$$jD > L + (2j-1)L_0 = (L - L_0) + 2jL_0. \tag{4.46}$$

Since $L_0 \geqslant L$, we have

$$L - L_0 \leqslant 0 \tag{4.47}$$

then (4.46) becomes

$$jD > 2jL_0$$

therefore

$$\frac{D}{2} > L_0. \tag{4.48}$$

Then, from (4.47), we obtain

$$L \leqslant L_0 < \frac{D}{2}. \tag{4.49}$$

Since $|x_i| \leqslant L$, then

$$-L \leqslant x_i \leqslant L \tag{4.50}$$

and since $|x_i - L_{ji}| \leqslant L_0$, then

$$-L_0 \leqslant x_i - L_{ji} \leqslant L_0. \tag{4.51}$$

Add (4.51) by $L_{ji}$, then we obtain

$$L_{ji} - L_0 \leqslant x_i \leqslant L_{ji} + L_0. \tag{4.52}$$

Since $\mathbf{L}_j = jD(1, 1, 1)$, then

$$L_{ji} = jD. \tag{4.53}$$

Substitute (4.53) in (4.52), we obtain

$$jD - L_0 \leqslant x_i \leqslant jD + L_0. \tag{4.54}$$

From (4.48), we may choose any $D$ such that

$$D \geqslant \chi L_0 \tag{4.55}$$

where $\chi > 2$, we choose

$$\chi \geqslant 6 \tag{4.56}$$

then, for $L_0 \geqslant L$, we have

$$D \geqslant 6L_0 \geqslant 6L. \tag{4.57}$$

With $L \leqslant L_0 < \dfrac{D}{2}$, the intervals $\{-L \leqslant x_i \leqslant L\}$, $\{jD - L_0 \leqslant x_i \leqslant jD + L_0\}$, for $j = 1, \ldots, N-k$, $(i = 1, 2, 3)$ are all disjoint and the wavefunctions $\phi(\mathbf{x}), \psi_j(\mathbf{x})$ are non-overlapping and automatically satisfy (4.19). Physically, they correspond, respectively, to particles localized in boxes of side $(2L, 2L, 2L)$ and $(2L_0, 2L_0, 2L_0)$ with the center of the first at the origin of the coordinate system and the centers of the other boxes for $\psi_1(\mathbf{x}), \ldots, \psi_{N-k}(\mathbf{x})$ defined by the tips of the vectors $\mathbf{L}_1, \ldots, \mathbf{L}_{N-k}$ (see the Fig. 4.1). We will actually choose $D \geqslant 6L_0 \geqslant 6L$.

The single-particle average kinetic energies are derived below

$$T = \frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{x}\ \left|\boldsymbol{\nabla}\phi(\mathbf{x})\right|^2 \tag{4.58}$$

and

$$T_j = \frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{x}\ \left|\boldsymbol{\nabla}\psi_j(\mathbf{x})\right|^2 . \tag{4.59}$$

From (4.41), with $\mathbf{x} = (x_1, x_2, x_3)$, we have

$$\begin{aligned}
\boldsymbol{\nabla}\phi(\mathbf{x}) = \frac{1}{L^{3/2}} \Big\{ & \hat{\mathbf{i}} \frac{\partial}{\partial x_1} \cos\left(\frac{\pi x_1}{2L}\right) \cos\left(\frac{\pi x_2}{2L}\right) \cos\left(\frac{\pi x_3}{2L}\right) \\
& + \hat{\mathbf{j}} \frac{\partial}{\partial x_2} \cos\left(\frac{\pi x_1}{2L}\right) \cos\left(\frac{\pi x_2}{2L}\right) \cos\left(\frac{\pi x_3}{2L}\right) \\
& + \hat{\mathbf{k}} \frac{\partial}{\partial x_3} \cos\left(\frac{\pi x_1}{2L}\right) \cos\left(\frac{\pi x_2}{2L}\right) \cos\left(\frac{\pi x_3}{2L}\right) \Big\} \\
= -\frac{\pi}{2L} \frac{1}{L^{3/2}} \Big\{ & \hat{\mathbf{i}} \sin\left(\frac{\pi x_1}{2L}\right) \cos\left(\frac{\pi x_2}{2L}\right) \cos\left(\frac{\pi x_3}{2L}\right) \\
& + \hat{\mathbf{j}} \cos\left(\frac{\pi x_1}{2L}\right) \sin\left(\frac{\pi x_2}{2L}\right) \cos\left(\frac{\pi x_3}{2L}\right) \\
& + \hat{\mathbf{k}} \cos\left(\frac{\pi x_1}{2L}\right) \cos\left(\frac{\pi x_2}{2L}\right) \sin\left(\frac{\pi x_3}{2L}\right) \Big\}
\end{aligned} \tag{4.60}$$

then

$$\begin{aligned}
|\boldsymbol{\nabla}\phi(\mathbf{x})|^2 = \frac{\pi^2}{4L^5} \Big\{ & \sin^2\left(\frac{\pi x_1}{2L}\right) \cos^2\left(\frac{\pi x_2}{2L}\right) \cos^2\left(\frac{\pi x_3}{2L}\right) \\
& + \cos^2\left(\frac{\pi x_1}{2L}\right) \sin^2\left(\frac{\pi x_2}{2L}\right) \cos^2\left(\frac{\pi x_3}{2L}\right) \\
& + \cos^2\left(\frac{\pi x_1}{2L}\right) \cos^2\left(\frac{\pi x_2}{2L}\right) \sin^2\left(\frac{\pi x_3}{2L}\right) \Big\} .
\end{aligned} \tag{4.61}$$

Multiply (4.61) by $\displaystyle\int \mathrm{d}^3\mathbf{x}$, we obtain

$$\begin{aligned}
& \int \mathrm{d}^3\mathbf{x}\ |\boldsymbol{\nabla}\phi(\mathbf{x})|^2 \\
& = \frac{\pi^2}{4L^5} \Big\{ \int_{-L}^{L} \mathrm{d}x_1\ \sin^2\left(\frac{\pi x_1}{2L}\right) \int_{-L}^{L} \mathrm{d}x_2\ \cos^2\left(\frac{\pi x_2}{2L}\right) \int_{-L}^{L} \mathrm{d}x_3\ \cos^2\left(\frac{\pi x_3}{2L}\right) \\
& + \int_{-L}^{L} \mathrm{d}x_1\ \cos^2\left(\frac{\pi x_1}{2L}\right) \int_{-L}^{L} \mathrm{d}x_2\ \sin^2\left(\frac{\pi x_2}{2L}\right) \int_{-L}^{L} \mathrm{d}x_3\ \cos^2\left(\frac{\pi x_3}{2L}\right)
\end{aligned}$$

$$+\int_{-L}^{L}\mathrm{d}x_1\ \cos^2\left(\frac{\pi x_1}{2L}\right)\int_{-L}^{L}\mathrm{d}x_2\ \cos^2\left(\frac{\pi x_2}{2L}\right)\int_{-L}^{L}\mathrm{d}x_3\ \sin^2\left(\frac{\pi x_3}{2L}\right)\Bigg\}$$

$$=\frac{3\pi^2}{4L^5}\left\{\int_{-L}^{L}\mathrm{d}x_1\ \sin^2\left(\frac{\pi x_1}{2L}\right)\int_{-L}^{L}\mathrm{d}x_2\ \cos^2\left(\frac{\pi x_2}{2L}\right)\int_{-L}^{L}\mathrm{d}x_3\ \cos^2\left(\frac{\pi x_3}{2L}\right)\right\}$$

$$=\frac{3\pi^2}{4L^5}L^3=\frac{3\pi^2}{4L^2}. \tag{4.62}$$

Substitute (4.62) in (4.58), we obtain

$$T=\frac{3\pi^2\hbar^2}{8mL^2}. \tag{4.63}$$

From (4.42), we have

$$\begin{aligned}\boldsymbol{\nabla}\psi_j(\mathbf{x}) &= \frac{1}{L_0^{3/2}}\left\{\hat{\mathbf{i}}\frac{\partial}{\partial x_1}\cos\left(\frac{\pi(x_1-L_{j1})}{2L_0}\right)\cos\left(\frac{\pi(x_2-L_{j2})}{2L_0}\right)\cos\left(\frac{\pi(x_3-L_{j3})}{2L_0}\right)\right.\\
&\quad+\hat{\mathbf{j}}\frac{\partial}{\partial x_2}\cos\left(\frac{\pi(x_1-L_{j1})}{2L_0}\right)\cos\left(\frac{\pi(x_2-L_{j2})}{2L_0}\right)\cos\left(\frac{\pi(x_3-L_{j3})}{2L_0}\right)\\
&\quad\left.+\hat{\mathbf{k}}\frac{\partial}{\partial x_3}\cos\left(\frac{\pi(x_1-L_{j1})}{2L_0}\right)\cos\left(\frac{\pi(x_2-L_{j2})}{2L_0}\right)\cos\left(\frac{\pi(x_3-L_{j3})}{2L_0}\right)\right\}\\
&= -\frac{\pi}{2L_0}\frac{1}{L_0^{3/2}}\\
&\quad\times\left\{\hat{\mathbf{i}}\sin\left(\frac{\pi(x_1-L_{j1})}{2L_0}\right)\cos\left(\frac{\pi(x_2-L_{j2})}{2L_0}\right)\cos\left(\frac{\pi(x_3-L_{j3})}{2L_0}\right)\right.\\
&\quad+\hat{\mathbf{j}}\cos\left(\frac{\pi(x_1-L_{j1})}{2L_0}\right)\sin\left(\frac{\pi(x_2-L_{j2})}{2L_0}\right)\cos\left(\frac{\pi(x_3-L_{j3})}{2L_0}\right)\\
&\quad\left.+\hat{\mathbf{k}}\cos\left(\frac{\pi(x_1-L_{j1})}{2L_0}\right)\cos\left(\frac{\pi(x_2-L_{j2})}{2L_0}\right)\sin\left(\frac{\pi(x_3-L_{j3})}{2L_0}\right)\right\}\end{aligned} \tag{4.64}$$

then

$$|\boldsymbol{\nabla}\psi_j(\mathbf{x})|^2 = \frac{\pi^2}{4L_0^5}$$
$$\times \left\{\sin^2\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right)\cos^2\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right)\cos^2\left(\frac{\pi(x_3 - L_{j3})}{2L_0}\right)\right.$$
$$+\cos^2\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right)\sin^2\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right)\cos^2\left(\frac{\pi(x_3 - L_{j3})}{2L_0}\right)$$
$$\left.+\cos^2\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right)\cos^2\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right)\sin^2\left(\frac{\pi(x_3 - L_{j3})}{2L_0}\right)\right\}. \tag{4.65}$$

Let

$$a_i = L_{ji} - L_0, \tag{4.66a}$$

$$b_i = L_{ji} + L_0. \tag{4.66b}$$

Multiply (4.65) by $\int \mathrm{d}^3\mathbf{x}$, and by using (4.66), we obtain

$$\int \mathrm{d}^3\mathbf{x}\ |\boldsymbol{\nabla}\psi_j(\mathbf{x})|^2$$
$$= \frac{\pi^2}{4L_0^5}\left\{\int_{a_1}^{b_1}\mathrm{d}x_1\ \sin^2\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right)\int_{a_2}^{b_2}\mathrm{d}x_2\ \cos^2\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right)\right.$$
$$\times \int_{a_3}^{b_3}\mathrm{d}x_3\ \cos^2\left(\frac{\pi(x_3 - L_{j3})}{2L_0}\right)$$
$$+\int_{a_1}^{b_1}\mathrm{d}x_1\ \cos^2\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right)\int_{a_2}^{b_2}\mathrm{d}x_2\ \sin^2\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right)$$
$$\times \int_{a_3}^{b_3}\mathrm{d}x_3\ \cos^2\left(\frac{\pi(x_3 - L_{j3})}{2L_0}\right)$$

$$+\int_{a_1}^{b_1}\mathrm{d}x_1\ \cos^2\left(\frac{\pi(x_1-L_{j1})}{2L_0}\right)\int_{a_2}^{b_2}\mathrm{d}x_2\ \cos^2\left(\frac{\pi(x_2-L_{j2})}{2L_0}\right)$$

$$\times\int_{a_3}^{b_3}\mathrm{d}x_3\ \sin^2\left(\frac{\pi(x_3-L_{j3})}{2L_0}\right)\Bigg\} \tag{4.67}$$

where

$$\int_{a_i}^{b_i}\mathrm{d}x_i\ \sin^2\left(\frac{\pi(x_i-L_{ji})}{2L_0}\right)=L_0 \tag{4.68}$$

and

$$\int_{a_i}^{b_i}\mathrm{d}x_i\ \cos^2\left(\frac{\pi(x_i-L_{ji})}{2L_0}\right)=L_0. \tag{4.69}$$

Substitute (4.68) and (4.69) in (4.67), we obtain

$$\int\mathrm{d}^3\mathbf{x}\ |\boldsymbol{\nabla}\psi_j(\mathbf{x})|^2=\frac{\pi^2}{4L_0^5}\left\{L_0^3+L_0^3+L_0^3\right\}$$

$$=\frac{3\pi^2}{4L_0^2}. \tag{4.70}$$

Substitute (4.70) in (4.59), we obtain

$$T_j=\frac{3\pi^2\hbar^2}{8mL_0^2}\equiv T_0. \tag{4.71}$$

If $\sum'$ is over all the permutations $\{\pi_1,\pi_2,\ldots,\pi_N\}$ of $\{2,\ldots,N\}$ and $\pi_1$ is fixed. Example, for $N=4$, we have

$$\sum{}'\{\pi_1,\pi_2,\pi_3,\pi_4\}=\{\pi_1,\pi_2,\pi_3,\pi_4\}+\{\pi_1,\pi_2,\pi_4,\pi_3\}$$

$$+\{\pi_1,\pi_3,\pi_4,\pi_2\}+\{\pi_1,\pi_3,\pi_2,\pi_4\}$$

$$+\{\pi_1,\pi_4,\pi_2,\pi_3\}+\{\pi_1,\pi_4,\pi_3,\pi_2\},$$

$$\sum{}'\{\pi_2,\pi_1,\pi_3,\pi_4\}=\{\pi_2,\pi_1,\pi_3,\pi_4\}+\{\pi_2,\pi_1,\pi_4,\pi_3\}$$

$$+ \{\pi_3, \pi_1, \pi_4, \pi_2\} + \{\pi_3, \pi_1, \pi_2, \pi_4\}$$

$$+ \{\pi_4, \pi_1, \pi_2, \pi_3\} + \{\pi_4, \pi_1, \pi_3, \pi_2\} \qquad (4.72)$$

we can see from above equations that there are 3! terms for each sum of permutation $\sum'$. Thus, in case of $N$, we will have $(N-1)!$ terms for all of the sum in $\sum' \{\pi_1, \pi_2, \ldots, \pi_N\}$.

Therefore, by using the method of permutations from (4.72), we can write $\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N)$ in the way such that

$$\begin{aligned}
&\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N) \\
&= \frac{1}{\sqrt{N!k!}} \Big\{ \sum{}' \Big[ \phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3)) \ldots \phi(\mathbf{x}(\pi_k)) \\
&\qquad \times\ \psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2})) \ldots \psi_{N-k}(\mathbf{x}(\pi_N)) \Big] \\
&\quad + \sum{}' \Big[ \phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_3)) \ldots \phi(\mathbf{x}(\pi_k)) \\
&\qquad \times\ \psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2})) \ldots \psi_{N-k}(\mathbf{x}(\pi_N)) \Big] \\
&\quad + \sum{}' \Big[ \phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\phi(\mathbf{x}(\pi_1)) \ldots \phi(\mathbf{x}(\pi_k)) \\
&\qquad \times\ \psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2})) \ldots \psi_{N-k}(\mathbf{x}(\pi_N)) \Big] \\
&\qquad + \\
&\qquad \vdots \\
&\qquad + \\
&\quad \sum{}' \Big[ \phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3)) \ldots \phi(\mathbf{x}(\pi_k))\phi(\mathbf{x}(\pi_1)) \\
&\qquad \times\ \psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2})) \ldots \psi_{N-k}(\mathbf{x}(\pi_N)) \Big]
\end{aligned}$$

$$+ \sum{}' \Big[\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3)) \ldots \phi(\mathbf{x}(\pi_k))\phi(\mathbf{x}(\pi_{k+1}))$$

$$\times\ \psi_1(\mathbf{x}(\pi_1))\psi_2(\mathbf{x}(\pi_{k+2})) \ldots \psi_{N-k}(\mathbf{x}(\pi_N))\Big]$$

$$+ \sum{}' \Big[\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3)) \ldots \phi(\mathbf{x}(\pi_k))\phi(\mathbf{x}(\pi_{k+1}))$$

$$\times\ \psi_1(\mathbf{x}(\pi_{k+2}))\psi_2(\mathbf{x}(\pi_1)) \ldots \psi_{N-k}(\mathbf{x}(\pi_N))\Big]$$

$$+$$

$$\vdots$$

$$+ \sum{}' \Big[\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3)) \ldots \phi(\mathbf{x}(\pi_k))\phi(\mathbf{x}(\pi_{k+1}))$$

$$\times\ \psi_1(\mathbf{x}(\pi_{k+2}))\psi_2(\mathbf{x}(\pi_{k+3})) \ldots \psi_{N-k-1}(\mathbf{x}(\pi_N))\psi_{N-k}(\mathbf{x}(\pi_1))\Big]\ \Bigg\}$$

$$= \frac{1}{\sqrt{N!k!}} \Bigg\{ \sum{}'[1] + \sum{}'[2] + \ldots + \sum{}'[k] + \sum{}'[k+1] + \ldots + \sum{}'[N] \Bigg\} \tag{4.73}$$

where we denote

$$[1] = \Big[\phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3)) \ldots \phi(\mathbf{x}(\pi_k))$$

$$\times\ \psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2})) \ldots \psi_{N-k}(\mathbf{x}(\pi_N))\Big],$$

$$[2] = \Big[\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_3)) \ldots \phi(\mathbf{x}(\pi_k))$$

$$\times\ \psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2})) \ldots \psi_{N-k}(\mathbf{x}(\pi_N))\Big],$$

$$[3] = \Big[\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\phi(\mathbf{x}(\pi_1)) \ldots \phi(\mathbf{x}(\pi_k))$$

$$\times\ \psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2})) \ldots \psi_{N-k}(\mathbf{x}(\pi_N))\Big],$$

$$\vdots$$

$$[k] = \Big[\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\dots\phi(\mathbf{x}(\pi_k))\phi(\mathbf{x}(\pi_1))$$

$$\times\ \psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\dots\psi_{N-k}(\mathbf{x}(\pi_N))\Big],$$

$$[k+1] = \Big[\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\dots\phi(\mathbf{x}(\pi_k))\phi(\mathbf{x}(\pi_{k+1}))$$

$$\times\ \psi_1(\mathbf{x}(\pi_1))\psi_2(\mathbf{x}(\pi_{k+2}))\dots\psi_{N-k}(\mathbf{x}(\pi_N))\Big],$$

$$[k+2] = \Big[\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\dots\phi(\mathbf{x}(\pi_k))\phi(\mathbf{x}(\pi_{k+1}))$$

$$\times\ \psi_1(\mathbf{x}(\pi_{k+2}))\psi_2(\mathbf{x}(\pi_1))\dots\psi_{N-k}(\mathbf{x}(\pi_N))\Big],$$

$$\vdots$$

$$[N] = \Big[\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\dots\phi(\mathbf{x}(\pi_k))\phi(\mathbf{x}(\pi_{k+1}))$$

$$\times\ \psi_1(\mathbf{x}(\pi_{k+2}))\psi_2(\mathbf{x}(\pi_{k+3}))\dots\psi_{N-k-1}(\mathbf{x}(\pi_N))\psi_{N-k}(\mathbf{x}(\pi_1))\Big] \tag{4.74}$$

and

$$\sum{}'[n] = \sum_{j=1}^{(N-1)!}[n]_j \tag{4.75}$$

where $[n]_j$ is the $j^{\text{th}}$ term in the $\sum{}'[n]$, $1 \leqslant j \leqslant (N-1)!$ and $1 \leqslant n \leqslant N$. Then we can rewrite (4.73) as

$$\Psi(\mathbf{x}_1,\dots,\mathbf{x}_N)$$

$$= \frac{1}{\sqrt{N!k!}}\Big\{\sum{}'[1] + \sum{}'[2] + \dots + \sum{}'[k] + \sum{}'[k+1] + \dots + \sum{}'[N]\Big\}$$

$$= \frac{1}{\sqrt{N!k!}} \sum_{n=1}^{N} \sum_{j=1}^{(N-1)!} [n]_j. \tag{4.76}$$

Consider the kinetic energy

$$\left\langle \Psi \left| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \right| \Psi \right\rangle = \frac{\hbar^2}{2m} \sum_{i=1}^{N} \int \mathrm{d}^3\mathbf{x}_1 \ldots \mathrm{d}^3\mathbf{x}_N \ \ |\boldsymbol{\nabla}_i \Psi|^2$$

$$= \frac{\hbar^2}{2m} \sum_{i=1}^{N} \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \ \ |\boldsymbol{\nabla}_{\pi_i} \Psi|^2 \tag{4.77}$$

where $\mathbf{x} = (x_1, x_2, x_3)$ and

$$\boldsymbol{\nabla}_{\pi_i} = \hat{\mathbf{i}} \frac{\partial}{\partial x_1(\pi_i)} + \hat{\mathbf{j}} \frac{\partial}{\partial x_2(\pi_i)} + \hat{\mathbf{k}} \frac{\partial}{\partial x_3(\pi_i)}. \tag{4.78}$$

From (4.76), we obtain

$$\int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \ \ |\boldsymbol{\nabla}_{\pi_i} \Psi|^2$$

$$= \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \ \ \left(\boldsymbol{\nabla}_{\pi_i} \Psi\right)^* \cdot \boldsymbol{\nabla}_{\pi_i} \Psi$$

$$= \frac{1}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \ \ \left( \boldsymbol{\nabla}_{\pi_i} \sum_{n=1}^{N} \sum_{j=1}^{(N-1)!} [n]_j \right)^* \cdot \boldsymbol{\nabla}_{\pi_i} \Psi$$

$$= \frac{1}{\sqrt{N!k!}} \sum_{n=1}^{N} \sum_{j=1}^{(N-1)!} \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \ \ \left(\boldsymbol{\nabla}_{\pi_i} [n]_j\right)^* \cdot \boldsymbol{\nabla}_{\pi_i} \Psi. \tag{4.79}$$

Since, for any $[n]_j, [m]_k$,

$$\int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \ \ \left(\boldsymbol{\nabla}_{\pi_i} [n]_j\right)^* \cdot \boldsymbol{\nabla}_{\pi_i} \Psi$$

$$= \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ \left(\boldsymbol{\nabla}_{\pi_i}[m]_k\right)^* \cdot \boldsymbol{\nabla}_{\pi_i}\Psi \tag{4.80}$$

then, we can choose any $[n]_j$. Let we choose

$$[0] = [n]_j = \Big[\phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\ldots\phi(\mathbf{x}(\pi_k))$$

$$\times\ \psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}(\mathbf{x}(\pi_N))\Big]. \tag{4.81}$$

Substitute (4.81) in (4.79), we obtain

$$\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ |\boldsymbol{\nabla}_{\pi_i}\Psi|^2$$

$$= \frac{1}{\sqrt{N!k!}}\sum_{n=1}^{N}\sum_{j=1}^{(N-1)!}\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ \left(\boldsymbol{\nabla}_{\pi_i}[0]\right)^* \cdot \boldsymbol{\nabla}_{\pi_i}\Psi$$

$$= \frac{N!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ \left(\boldsymbol{\nabla}_{\pi_i}[0]\right)^* \cdot \boldsymbol{\nabla}_{\pi_i}\Psi. \tag{4.82}$$

Consider $\boldsymbol{\nabla}_{\pi_i}[0]$,

$$\boldsymbol{\nabla}_{\pi_i}[0] = \boldsymbol{\nabla}_{\pi_i}\big[\phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\ldots\phi(\mathbf{x}(\pi_k))$$

$$\times\ \psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}(\mathbf{x}(\pi_N))\big]$$

$$= \left(\boldsymbol{\nabla}_{\pi_i}\phi(\mathbf{x}(\pi_1))\right)\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\ldots\phi(\mathbf{x}(\pi_k))$$

$$\times\psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}(\mathbf{x}(\pi_N))$$

$$+\ \phi(\mathbf{x}(\pi_1))\left(\boldsymbol{\nabla}_{\pi_i}\phi(\mathbf{x}(\pi_2))\right)\phi(\mathbf{x}(\pi_3))\ldots\phi(\mathbf{x}(\pi_k))$$

$$\times\psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}(\mathbf{x}(\pi_N))$$

$$+\ \phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_2))\left(\boldsymbol{\nabla}_{\pi_i}\phi(\mathbf{x}(\pi_3))\right)\ldots\phi(\mathbf{x}(\pi_k))$$

$$\times\psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}(\mathbf{x}(\pi_N))$$

$$+$$
$$\vdots$$
$$+$$
$$\phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\ldots\phi(\mathbf{x}(\pi_k))$$
$$\times\,\psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\ldots\,\big(\boldsymbol{\nabla}_{\pi_i}\psi_{N-k}(\mathbf{x}(\pi_N))\big)$$
$$=\sum_{\ell=1}^{N}\mathbf{G}_{i\ell} \tag{4.83}$$

where

$$\begin{aligned}
\mathbf{G}_{i1} =&\ \big(\boldsymbol{\nabla}_{\pi_i}\phi(\mathbf{x}(\pi_1))\big)\,\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\ldots\phi(\mathbf{x}(\pi_k))\\
&\times\,\psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}(\mathbf{x}(\pi_N)),\\
\mathbf{G}_{i2} =&\ \phi(\mathbf{x}(\pi_1))\,\big(\boldsymbol{\nabla}_{\pi_i}\phi(\mathbf{x}(\pi_2))\big)\,\phi(\mathbf{x}(\pi_3))\ldots\phi(\mathbf{x}(\pi_k))\\
&\times\,\psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}(\mathbf{x}(\pi_N)),\\
\mathbf{G}_{i3} =&\ \phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_2))\,\big(\boldsymbol{\nabla}_{\pi_i}\phi(\mathbf{x}(\pi_3))\big)\ldots\phi(\mathbf{x}(\pi_k))\\
&\times\,\psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}(\mathbf{x}(\pi_N)),\\
&+\\
&\vdots\\
&+\\
\mathbf{G}_{iN} =&\ \phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_2))\phi(\mathbf{x}(\pi_3))\ldots\phi(\mathbf{x}(\pi_k))\\
&\times\,\psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\ldots(\boldsymbol{\nabla}_{\pi_i}\psi_{N-k}(\mathbf{x}(\pi_N)))\,.
\end{aligned} \tag{4.84}$$

Substitute (4.83) in (4.82), we obtain

$$\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ \left|\boldsymbol{\nabla}_{\pi_i}\Psi\right|^2$$

$$= \frac{N!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N) \ \left(\sum_{\ell=1}^{N} \mathbf{G}_{i\ell}\right)^* \cdot \boldsymbol{\nabla}_{\pi_i}\Psi. \tag{4.85}$$

Multiply (4.85) by $\dfrac{\hbar^2}{2m}$, we have

$$\frac{\hbar^2}{2m}\sum_{i=1}^{N}\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N) \ |\boldsymbol{\nabla}_{\pi_i}\Psi|^2$$

$$= \frac{\hbar^2}{2m}\sum_{i=1}^{N}\sum_{\ell=1}^{N}\frac{N!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N) \ \mathbf{G}_{i\ell}^* \cdot \boldsymbol{\nabla}_{\pi_i}\Psi. \tag{4.86}$$

We have 2 cases; $1 \leqslant \ell \leqslant k$ and $k+1 \leqslant \ell \leqslant N$,

**1. For** $1 \leqslant \ell \leqslant k$ :

$$\frac{\hbar^2}{2m}\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N) \ \mathbf{G}_{i\ell}^* \cdot \boldsymbol{\nabla}_{\pi_i}\Psi$$

$$= \frac{\hbar^2}{2m}\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N) \ \phi^*(\mathbf{x}(\pi_1))\phi^*(\mathbf{x}(\pi_2))\ldots[\boldsymbol{\nabla}_{\pi_i}\phi(\mathbf{x}(\pi_\ell))]^*\ldots$$
$$\times\ \phi^*(\mathbf{x}(\pi_k))\psi_1^*(\mathbf{x}(\pi_{k+1}))\psi_2^*(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}^*(\mathbf{x}(\pi_N)) \cdot \boldsymbol{\nabla}_{\pi_i}\Psi$$

$$= \frac{1}{\sqrt{N!k!}}\frac{\hbar^2}{2m}\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N) \ \phi^*(\mathbf{x}(\pi_1))\phi^*(\mathbf{x}(\pi_2))\ldots$$
$$\times\ [\boldsymbol{\nabla}_{\pi_i}\phi(\mathbf{x}(\pi_\ell))]^*\ldots\phi^*(\mathbf{x}(\pi_k))\psi_1^*(\mathbf{x}(\pi_{k+1}))\psi_2^*(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}^*(\mathbf{x}(\pi_N))$$

$$\times\ k!\Big\{\phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_2))\ldots[\boldsymbol{\nabla}_{\pi_i}\phi(\mathbf{x}(\pi_\ell))]\ldots\phi^*(\mathbf{x}(\pi_k))$$
$$\times\ \ \psi_1^*(\mathbf{x}(\pi_{k+1}))\psi_2^*(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}^*(\mathbf{x}(\pi_N))\Big\}$$

$$= \frac{k!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}(\pi_1) \ |\phi(\mathbf{x}(\pi_1))|^2\int \mathrm{d}^3\mathbf{x}(\pi_2) \ |\phi(\mathbf{x}(\pi_2))|^2\ldots$$

$$\times\ \frac{\hbar^2}{2m}\int \mathrm{d}^3\mathbf{x}(\pi_\ell) \ |\boldsymbol{\nabla}_{\pi_i}\phi(\mathbf{x}(\pi_\ell))|^2\ldots\int \mathrm{d}^3\mathbf{x}(\pi_k) \ |\phi(\mathbf{x}(\pi_k))|^2$$

$$\times \int \mathrm{d}^3\mathbf{x}(\pi_{k+1})\ \left|\psi_1(\mathbf{x}(\pi_{k+1}))\right|^2 \int \mathrm{d}^3\mathbf{x}(\pi_{k+2})\ \left|\psi_2(\mathbf{x}(\pi_{k+2}))\right|^2 \ldots$$

$$\times \int \mathrm{d}^3\mathbf{x}(\pi_N)\ \left|\psi_{N-k}(\mathbf{x}(\pi_N))\right|^2$$

$$= \frac{k!}{\sqrt{N!k!}} \frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{x}(\pi_\ell)\ \left|\boldsymbol{\nabla}_{\pi_i}\phi(\mathbf{x}(\pi_\ell))\right|^2 . \tag{4.87}$$

By using (4.58), Eq. (4.87) becomes

$$\frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ \mathbf{G}^*_{i\ell}\cdot\boldsymbol{\nabla}_{\pi_i}\Psi = \frac{k!}{\sqrt{N!k!}} T\delta_{i\ell}. \tag{4.88}$$

**2. For $k+1 \leqslant \ell \leqslant N$ :**

$$\frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ \mathbf{G}^*_{i\ell}\cdot\boldsymbol{\nabla}_{\pi_i}\Psi$$

$$= \frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ \phi^*(\mathbf{x}(\pi_1))\phi^*(\mathbf{x}(\pi_2))\ldots\phi^*(\mathbf{x}(\pi_k))$$
$$\times\ \psi_1^*(\mathbf{x}(\pi_{k+1}))\psi_2^*(\mathbf{x}(\pi_{k+2}))\ldots[\boldsymbol{\nabla}_{\pi_i}\psi_{\ell-k}(\mathbf{x}(\pi_\ell))]^*\ldots\psi^*_{N-k}(\mathbf{x}(\pi_N))\cdot\boldsymbol{\nabla}_{\pi_i}\Psi$$

$$= \frac{1}{\sqrt{N!k!}} \frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ \phi^*(\mathbf{x}(\pi_1))\phi^*(\mathbf{x}(\pi_2))\ldots\phi^*(\mathbf{x}(\pi_k))$$
$$\times\ \psi_1^*(\mathbf{x}(\pi_{k+1}))\psi_2^*(\mathbf{x}(\pi_{k+2}))\ldots[\boldsymbol{\nabla}_{\pi_i}\psi_{\ell-k}(\mathbf{x}(\pi_\ell))]^*\ldots\psi^*_{N-k}(\mathbf{x}(\pi_N))$$

$$\times\ k!\Big\{\phi(\mathbf{x}(\pi_1))\phi(\mathbf{x}(\pi_2))\ldots\phi(\mathbf{x}(\pi_k))$$
$$\times\ \ \psi_1(\mathbf{x}(\pi_{k+1}))\psi_2(\mathbf{x}(\pi_{k+2}))\ldots[\boldsymbol{\nabla}_{\pi_i}\psi_{\ell-k}(\mathbf{x}(\pi_\ell))]\ldots\psi_{N-k}(\mathbf{x}(\pi_N))\Big\}$$

$$= \frac{k!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}(\pi_1)\left|\phi(\mathbf{x}(\pi_1))\right|^2 \int \mathrm{d}^3\mathbf{x}(\pi_2)\left|\phi(\mathbf{x}(\pi_2))\right|^2 \ldots \int \mathrm{d}^3\mathbf{x}(\pi_k)\left|\phi(\mathbf{x}(\pi_k))\right|^2$$

$$\times \int \mathrm{d}^3\mathbf{x}(\pi_{k+1})\ \left|\psi_1(\mathbf{x}(\pi_{k+1}))\right|^2 \int \mathrm{d}^3\mathbf{x}(\pi_{k+2})\ \left|\psi_2(\mathbf{x}(\pi_{k+2}))\right|^2 \ldots$$

$$\times \frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{x}(\pi_\ell) \ |\boldsymbol{\nabla}_{\pi_i}\psi_{\ell-k}(\mathbf{x}(\pi_\ell))|^2 \ldots \int \mathrm{d}^3\mathbf{x}(\pi_N) \ |\psi_{N-k}(\mathbf{x}(\pi_N))|^2$$

$$= \frac{k!}{\sqrt{N!k!}} \frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{x}(\pi_\ell) \ |\boldsymbol{\nabla}_{\pi_i}\psi_{\ell-k}(\mathbf{x}(\pi_\ell))|^2 . \tag{4.89}$$

By using (4.59), Eq. (4.89) becomes

$$\frac{\hbar^2}{2m} \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \ \mathbf{G}^*_{i\ell} \cdot \boldsymbol{\nabla}_{\pi_i}\Psi = \frac{k!}{\sqrt{N!k!}} T_0 \delta_{i\ell}. \tag{4.90}$$

Substitute (4.88) and (4.90) in (4.86) we obtain the kinetic energy part,

$$\frac{\hbar^2}{2m} \sum_{i=1}^{N} \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \ |\boldsymbol{\nabla}_{\pi_i}\Psi|^2$$

$$= \frac{N!}{\sqrt{N!k!}} \frac{k!}{\sqrt{N!k!}} \sum_{i=1}^{N} \left\{ \sum_{\ell=1}^{k} T\delta_{i\ell} + \sum_{\ell=k+1}^{N} T_0\delta_{i\ell} \right\}$$

$$= kT + (N-k)T_0. \tag{4.91}$$

Consider the interaction term,

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

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

$$= \frac{e^2}{\sqrt{N!k!}} \sum_{j=1}^{N} \sum_{i=1}^{N} \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N)$$

$$\times \sum_{\pi} \phi\left(\mathbf{x}(\pi_1)\right) \ldots \phi\left(\mathbf{x}(\pi_k)\right) \psi_1\left(\mathbf{x}(\pi_{k+1})\right) \ldots \psi_{N-k}\left(\mathbf{x}(\pi_N)\right) \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \Psi$$

$$= \frac{e^2}{\sqrt{N!k!}} \sum_{j=1}^{N} \sum_{i=1}^{N} \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \ \sum_{n=1}^{N} \sum_{m=1}^{(N-1)!} [n]^*_m \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \Psi \tag{4.92}$$

where, for any $[n]_m, [p]_k$,

$$\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N) \sum_{n=1}^{N} \sum_{m=1}^{(N-1)!} [n]_m^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \Psi$$

$$= \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N) \sum_{p=1}^{N} \sum_{k=1}^{(N-1)!} [p]_k^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \Psi$$

$$= \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N) \sum_{p=1}^{N} \sum_{k=1}^{(N-1)!} [0]^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \Psi$$

$$= N! \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \Psi \tag{4.93}$$

where [0] is defined in (4.81). Substitute (4.93) in (4.92), we obtain

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

$$= \frac{e^2 N!}{\sqrt{N!k!}} \sum_{j=1}^{N} \sum_{i=1}^{N} \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \Psi. \tag{4.94}$$

Consider the integral on the right-hand side of (4.94),

$$\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \Psi$$

$$= \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ \phi^*(\mathbf{x}(\pi_1))\phi^*(\mathbf{x}(\pi_2))\phi^*(\mathbf{x}(\pi_3))\ldots\phi^*(\mathbf{x}(\pi_k))$$

$$\times\ \psi_1^*(\mathbf{x}(\pi_{k+1}))\psi_2^*(\mathbf{x}(\pi_{k+2}))\ldots\psi_{N-k}^*(\mathbf{x}(\pi_N)) \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \Psi. \tag{4.95}$$

For $1 \leqslant i \leqslant k$ and $|x_i| \leqslant L$, we have

$$\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \Psi$$

$$= \frac{k!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_i) \ldots \mathrm{d}^3\mathbf{x}(\pi_N)$$

$$\times\, \phi^2(\mathbf{x}(\pi_1))\phi^2(\mathbf{x}(\pi_2)) \ldots \phi^2(\mathbf{x}(\pi_i)) \ldots \phi^2(\mathbf{x}(\pi_k))$$

$$\times\, \psi_1^2(\mathbf{x}(\pi_{k+1}))\psi_2^2(\mathbf{x}(\pi_{k+2})) \ldots \psi_{N-k}^2(\mathbf{x}(\pi_N)) \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|}$$

$$= \frac{k!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}(\pi_i) \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \phi^2(\mathbf{x}(\pi_i))$$

$$= \frac{k!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x} \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi^2(\mathbf{x}). \tag{4.96}$$

For $k+1 \leqslant i \leqslant N$ and $|x_i - L_{ji}| \leqslant L_0$,

$$\int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N)\; [0]^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \Psi$$

$$= \frac{k!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_i) \ldots \mathrm{d}^3\mathbf{x}(\pi_N)$$

$$\times\, \phi^2(\mathbf{x}(\pi_1))\phi^2(\mathbf{x}(\pi_2))\phi^2(\mathbf{x}(\pi_3)) \ldots \phi^2(\mathbf{x}(\pi_k))$$

$$\times\, \psi_1^2(\mathbf{x}(\pi_{k+1})) \ldots \psi_{i-k}^2(\mathbf{x}(\pi_i)) \ldots \psi_{N-k}^2(\mathbf{x}(\pi_N)) \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|}$$

$$= \frac{k!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}(\pi_i)\; \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \psi_{i-k}^2(\mathbf{x}(\pi_i))$$

$$= \frac{k!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}(\pi_i)\; \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|} \phi_{L_0}^2(\mathbf{x}(\pi_i) - \mathbf{L}_{i-k}). \tag{4.97}$$

We define

$$\mathbf{x} = \mathbf{x}(\pi_i) - \mathbf{L}_{i-k}, \tag{4.98a}$$

$$\mathbf{x}(\pi_i) = \mathbf{x} + \mathbf{L}_{i-k}, \tag{4.98b}$$

$$\mathrm{d}^3\mathbf{x}(\pi_i) = \mathrm{d}^3\mathbf{x}. \tag{4.98c}$$

Substitute (4.98) in (4.97), we obtain

$$\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{R}_j|}\Psi = \frac{k!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}\ \frac{1}{|\mathbf{x} + \mathbf{L}_{i-k} - \mathbf{R}_j|}\phi^2_{L_0}(\mathbf{x}). \tag{4.99}$$

Substitute (4.96) and (4.99) in (4.94), we obtain

$$\begin{aligned}\left\langle \Psi \left| \sum_{j=1}^{N}\sum_{i=1}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \right| \Psi \right\rangle &= \frac{e^2 N!}{\sqrt{N!k!}}\frac{k!}{\sqrt{N!k!}} \sum_{j=1}^{N} \left\{ \sum_{i=1}^{k} \int \mathrm{d}^3\mathbf{x} \frac{1}{|\mathbf{x} - \mathbf{R}_j|}\phi^2_L(\mathbf{x}) \right. \\ &\quad \left. + \sum_{i=k+1}^{N} \int \mathrm{d}^3\mathbf{x} \frac{1}{|\mathbf{x} + \mathbf{L}_{i-k} - \mathbf{R}_j|}\phi^2_{L_0}(\mathbf{x}) \right\} \\ &= e^2 \sum_{j=1}^{N} \left\{ k \int \mathrm{d}^3\mathbf{x} \frac{1}{|\mathbf{x} - \mathbf{R}_j|}\phi^2_L(\mathbf{x}) \right. \\ &\quad \left. + \sum_{i=1}^{N-k} \int \mathrm{d}^3\mathbf{x} \frac{1}{|\mathbf{x} + \mathbf{L}_i - \mathbf{R}_j|}\phi^2_{L_0}(\mathbf{x}) \right\}. \end{aligned} \tag{4.100}$$

Multiply (4.100) by $(-1)$, we obtain

$$\begin{aligned} -\left\langle \Psi \left| \sum_{j=1}^{N}\sum_{i=1}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{R}_j|} \right| \Psi \right\rangle &= -e^2 k \sum_{j=1}^{N} \int \mathrm{d}^3\mathbf{x}\ \frac{1}{|\mathbf{x} - \mathbf{R}_j|}\phi^2_L(\mathbf{x}) \\ &\quad - e^2 \sum_{j=1}^{N}\sum_{i=1}^{N-k} \int \mathrm{d}^3\mathbf{x}\ \frac{1}{|\mathbf{x} + \mathbf{L}_i - \mathbf{R}_j|}\phi^2_{L_0}(\mathbf{x}) \\ &\equiv \langle V_1 \rangle . \end{aligned} \tag{4.101}$$

Consider the interaction term,

$$\left\langle \Psi \left| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \right| \Psi \right\rangle$$

$$= e^2 \sum_{j=2}^{N} \sum_{i=1}^{j-1} \left\langle \Psi \left| \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} \right| \Psi \right\rangle$$

$$= \frac{e^2}{\sqrt{N!k!}} \sum_{j=2}^{N} \sum_{i=1}^{j-1} \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \sum_{n=1}^{N} \sum_{m=1}^{(N-1)!} [n]_m^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{x}(\pi_j)|} \Psi \tag{4.102}$$

where, for any $[n]_m, [p]_k$,

$$\int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \sum_{n=1}^{N} \sum_{m=1}^{(N-1)!} [n]_m^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{x}(\pi_j)|} \Psi$$

$$= \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \sum_{p=1}^{N} \sum_{k=1}^{(N-1)!} [p]_k^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{x}(\pi_j)|} \Psi$$

$$= \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N) \sum_{p=1}^{N} \sum_{k=1}^{(N-1)!} [0]^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{x}(\pi_j)|} \Psi$$

$$= N! \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{x}(\pi_j)|} \Psi. \tag{4.103}$$

Then Eq. (4.102) becomes

$$\left\langle \Psi \left| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} \right| \Psi \right\rangle$$

$$= \frac{e^2 N!}{\sqrt{N!k!}} \sum_{j=2}^{N} \sum_{i=1}^{j-1} \int \mathrm{d}^3\mathbf{x}(\pi_1) \ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^* \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{x}(\pi_j)|} \Psi. \tag{4.104}$$

We consider 3 cases of $i < j$:

- $1 \leqslant i < k,\ 2 \leqslant j \leqslant k,$
- $1 \leqslant i \leqslant k,\ k+1 \leqslant j \leqslant N$
- $k+1 \leqslant i < N,\ k+2 \leqslant j \leqslant N.$

**1. For** $1 \leqslant i < k,\ 2 \leqslant j \leqslant k$

$$\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^* \frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\Psi$$

$$= \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ \phi^*\left(\mathbf{x}(\pi_1)\right)\ldots\phi^*\left(\mathbf{x}(\pi_i)\right)\ldots\phi^*\left(\mathbf{x}(\pi_j)\right)\ldots\phi^*\left(\mathbf{x}(\pi_k)\right)$$

$$\times\ \psi_1^*\left(\mathbf{x}(\pi_{k+1})\right)\ldots\psi_{N-k}^*\left(\mathbf{x}(\pi_N)\right)\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\Psi$$

$$= \frac{k!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_i)\ldots \mathrm{d}^3\mathbf{x}(\pi_j)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)$$

$$\times\ \phi^2\left(\mathbf{x}(\pi_1)\right)\ldots\phi^2\left(\mathbf{x}(\pi_i)\right)\ldots\phi^2\left(\mathbf{x}(\pi_j)\right)\ldots\phi^2\left(\mathbf{x}(\pi_k)\right)$$

$$\times\ \psi_1^2\left(\mathbf{x}(\pi_{k+1})\right)\ldots\psi_{N-k}^2\left(\mathbf{x}(\pi_N)\right)\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}$$

$$= \frac{k!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}(\pi_i)\,\mathrm{d}^3\mathbf{x}(\pi_j)\ \phi^2\left(\mathbf{x}(\pi_i)\right)\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\phi^2\left(\mathbf{x}(\pi_j)\right)$$

$$= \frac{k!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\ \phi_L^2\left(\mathbf{x}\right)\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2\left(\mathbf{x}'\right). \tag{4.105}$$

**2. For** $1 \leqslant i \leqslant k,\ k+1 \leqslant j \leqslant N$

$$\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^* \frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\Psi$$

$$= \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)\ \phi^*\left(\mathbf{x}(\pi_1)\right)\ldots\phi^*\left(\mathbf{x}(\pi_i)\right)\ldots\phi^*\left(\mathbf{x}(\pi_k)\right)$$

$$\times\ \psi_1^*\left(\mathbf{x}(\pi_{k+1})\right)\ldots\psi_{j-k}^*\left(\mathbf{x}(\pi_j)\right)\ldots\psi_{N-k}^*\left(\mathbf{x}(\pi_N)\right)\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\Psi$$

$$= \frac{k!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_i)\ldots \mathrm{d}^3\mathbf{x}(\pi_j)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)$$

$$\times\ \phi^2\left(\mathbf{x}(\pi_1)\right)\ldots\phi^2\left(\mathbf{x}(\pi_i)\right)\ldots\phi^2\left(\mathbf{x}(\pi_k)\right)$$

$$\times\ \psi_1^2\left(\mathbf{x}(\pi_{k+1})\right)\ldots\psi_{j-k}^2\left(\mathbf{x}(\pi_j)\right)\ldots\psi_{N-k}^2\left(\mathbf{x}(\pi_N)\right)\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}$$

$$=\frac{k!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}(\pi_i)\,\mathrm{d}^3\mathbf{x}(\pi_j)\ \phi^2\left(\mathbf{x}(\pi_i)\right)\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\psi_{j-k}^2\left(\mathbf{x}(\pi_j)\right)$$

$$=\frac{k!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}(\pi_i)\,\mathrm{d}^3\mathbf{x}(\pi_j)\ \phi_L^2\left(\mathbf{x}(\pi_i)\right)$$

$$\times\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\phi_{L_0}^2(\mathbf{x}(\pi_j)-\mathbf{L}_{j-k}). \tag{4.106}$$

Let

$$\mathbf{x}(\pi_j)-\mathbf{L}_{j-k}=\mathbf{x}', \tag{4.107a}$$

$$\mathbf{x}(\pi_j)=\mathbf{x}'+\mathbf{L}_{j-k}, \tag{4.107b}$$

$$\mathrm{d}^3\mathbf{x}(\pi_j)=\mathrm{d}^3\mathbf{x}'. \tag{4.107c}$$

Substitute (4.107) in (4.106) we obtain

$$\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^*\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\Psi$$

$$=\frac{k!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\ \phi_L^2\left(\mathbf{x}\right)\frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_{j-k}|}\phi_{L_0}^2(\mathbf{x}'). \tag{4.108}$$

**3. For** $k+1\leqslant i<N,\ k+2\leqslant j\leqslant N$

$$\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^*\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\Psi$$

$$=\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_i)\ldots\mathrm{d}^3\mathbf{x}(\pi_j)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)$$

$$\times\ \phi^*\left(\mathbf{x}(\pi_1)\right)\ldots\phi^*\left(\mathbf{x}(\pi_k)\right)$$

$$\times\ \psi_1^*\left(\mathbf{x}(\pi_{k+1})\right)\ldots\psi_{i-k}^*\left(\mathbf{x}(\pi_i)\right)\ldots\psi_{j-k}^*\left(\mathbf{x}(\pi_j)\right)\ldots\psi_{N-k}^*\left(\mathbf{x}(\pi_N)\right)$$

$$\times \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{x}(\pi_j)|}\Psi$$

$$= \frac{k!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots \mathrm{d}^3\mathbf{x}(\pi_i)\ldots \mathrm{d}^3\mathbf{x}(\pi_j)\ldots \mathrm{d}^3\mathbf{x}(\pi_N)$$

$$\times \phi^2\left(\mathbf{x}(\pi_1)\right)\ldots \phi^2\left(\mathbf{x}(\pi_k)\right)$$

$$\times \psi_1^2\left(\mathbf{x}(\pi_{k+1})\right)\ldots \psi_{i-k}^2\left(\mathbf{x}(\pi_i)\right)\ldots \psi_{j-k}^2\left(\mathbf{x}(\pi_j)\right)\ldots \psi_{N-k}^2\left(\mathbf{x}(\pi_N)\right)$$

$$\times \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{x}(\pi_j)|}$$

$$= \frac{k!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}(\pi_i)\,\mathrm{d}^3\mathbf{x}(\pi_j)\ \psi_{i-k}^2\left(\mathbf{x}(\pi_i)\right) \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{x}(\pi_j)|}\psi_{j-k}^2\left(\mathbf{x}(\pi_j)\right)$$

$$= \frac{k!}{\sqrt{N!k!}} \int \mathrm{d}^3\mathbf{x}(\pi_i)\,\mathrm{d}^3\mathbf{x}(\pi_j)\ \phi_{L_0}^2\left(\mathbf{x}(\pi_i) - \mathbf{L}_{i-k}\right)$$

$$\times \frac{1}{|\mathbf{x}(\pi_i) - \mathbf{x}(\pi_j)|}\phi_{L_0}^2(\mathbf{x}(\pi_j) - \mathbf{L}_{j-k}). \tag{4.109}$$

Let

$$\mathbf{x}(\pi_i) - \mathbf{L}_{i-k} = \mathbf{x}, \tag{4.110a}$$

$$\mathbf{x}(\pi_i) = \mathbf{x} + \mathbf{L}_{i-k}, \tag{4.110b}$$

$$\mathrm{d}^3\mathbf{x}(\pi_i) = \mathrm{d}^3\mathbf{x} \tag{4.110c}$$

and

$$\mathbf{x}(\pi_j) - \mathbf{L}_{j-k} = \mathbf{x}', \tag{4.110d}$$

$$\mathbf{x}(\pi_j) = \mathbf{x}' + \mathbf{L}_{j-k}, \tag{4.110e}$$

$$\mathrm{d}^3\mathbf{x}(\pi_j) = \mathrm{d}^3\mathbf{x}'. \tag{4.110f}$$

Substitute (4.110) in (4.109), we obtain

$$\begin{aligned}
&\int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^*\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\Psi \\
&\qquad = \frac{k!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi^2_{L_0}(\mathbf{x})\frac{1}{|\mathbf{x}+\mathbf{L}_{i-k}-\mathbf{x}'-\mathbf{L}_{j-k}|}\phi^2_{L_0}(\mathbf{x}') \\
&\qquad = \frac{k!}{\sqrt{N!k!}}\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi^2_{L_0}(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_{i-k}-\mathbf{L}_{j-k}|}\phi^2_{L_0}(\mathbf{x}'). \qquad (4.111)
\end{aligned}$$

By using (4.105), (4.108) and (4.111), Eq. (4.104) becomes

$$\begin{aligned}
&\left\langle \Psi \middle| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i-\mathbf{x}_j|} \middle| \Psi \right\rangle \\
&= e^2 \sum_{j=2}^{N}\sum_{i=1}^{j-1} \left\langle \Psi \middle| \frac{1}{|\mathbf{x}_i-\mathbf{x}_j|} \middle| \Psi \right\rangle \\
&= \frac{e^2 N!}{\sqrt{N!k!}}\left\{ \sum_{j=2}^{k}\sum_{i=1}^{j-1} \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^*\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\Psi \right. \\
&\quad + \sum_{j=k+1}^{N}\sum_{i=1}^{k} \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^*\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\Psi \\
&\quad \left. + \sum_{j=k+2}^{N}\sum_{i=k+1}^{j-1} \int \mathrm{d}^3\mathbf{x}(\pi_1)\ldots\mathrm{d}^3\mathbf{x}(\pi_N)\ [0]^*\frac{1}{|\mathbf{x}(\pi_i)-\mathbf{x}(\pi_j)|}\Psi \right\} \\
&= \frac{e^2 N!}{\sqrt{N!k!}}\frac{k!}{\sqrt{N!k!}}\left\{ \sum_{j=2}^{k}\sum_{i=1}^{j-1} \int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi^2_L(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi^2_L(\mathbf{x}') \right. \\
&\quad + \sum_{j=k+1}^{N}\sum_{i=1}^{k} \int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi^2_L(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_{j-k}|}\phi^2_{L_0}(\mathbf{x}')
\end{aligned}$$

$$+\sum_{j=k+2}^{N}\sum_{i=k+1}^{j-1}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_{L_0}^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_{i-k}-\mathbf{L}_{j-k}|}\phi_{L_0}^2(\mathbf{x}')\Bigg\}$$

$$=e^2\Bigg\{\sum_{j=2}^{k}\sum_{i=1}^{j-1}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_L^2\,(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2\,(\mathbf{x}')$$

$$+\sum_{j=k+1}^{N}\sum_{i=1}^{k}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_L^2\,(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_{j-k}|}\phi_{L_0}^2(\mathbf{x}')$$

$$+\sum_{j=k+2}^{N}\sum_{i=k+1}^{j-1}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_{L_0}^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_{i-k}-\mathbf{L}_{j-k}|}\phi_{L_0}^2(\mathbf{x}')\Bigg\}$$

$$=e^2\frac{k(k-1)}{2}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_L^2\,(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2\,(\mathbf{x}')$$

$$+e^2k\sum_{j=k+1}^{N}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_L^2\,(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_{j-k}|}\phi_{L_0}^2(\mathbf{x}')$$

$$+e^2\sum_{j=k+2}^{N}\sum_{i=k+1}^{j-1}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_{L_0}^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_{i-k}-\mathbf{L}_{j-k}|}\phi_{L_0}^2(\mathbf{x}')$$

$$=e^2\frac{k(k-1)}{2}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_L^2\,(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2\,(\mathbf{x}')$$

$$+e^2k\sum_{j=1}^{N-k}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_L^2\,(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_{j}|}\phi_{L_0}^2(\mathbf{x}')$$

$$+e^2\sum_{j=2}^{N-k}\sum_{i=1}^{j-1}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_{L_0}^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_{i}-\mathbf{L}_{j}|}\phi_{L_0}^2(\mathbf{x}')$$

$$=e^2\frac{k(k-1)}{2}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_L^2\,(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2\,(\mathbf{x}')$$

$$+e^2k\sum_{j=1}^{N-k}\int d^3\mathbf{x}d^3\mathbf{x}'\ \phi_L^2\,(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_{j}|}\phi_{L_0}^2(\mathbf{x}')$$

$$+\, e^2 \sum_{i<j}^{N-k} \int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi_{L_0}^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|} \phi_{L_0}^2(\mathbf{x}')$$

$$\equiv \langle V_2 \rangle\,. \tag{4.112}$$

Consider the interaction term,

$$\left\langle \Psi \left| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|} \right| \Psi \right\rangle = \left\langle \Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) \left| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|} \right| \Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) \right\rangle$$

$$= \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|} \left\langle \Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) \,|\, \Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) \right\rangle$$

$$= \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}. \tag{4.113}$$

The addition of (4.91), (4.101), (4.112) and (4.113) leads to

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

$$+ \sum_{i<j}^{N} \left\langle \Psi \left| \frac{e^2}{|\mathbf{x}_i-\mathbf{x}_j|} \right| \Psi \right\rangle + \sum_{i<j}^{N} \left\langle \Psi \left| \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|} \right| \Psi \right\rangle$$

$$= [kT + (N-k)T_0] + \langle V_1 \rangle + \langle V_2 \rangle + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}. \tag{4.114}$$

We set $\mathbf{R}_{k+j} = \mathbf{L}_j$, from (4.101), we obtain

$$\langle V_1 \rangle = -e^2 k \sum_{j=1}^{N} \int \mathrm{d}^3\mathbf{x} \frac{1}{|\mathbf{x}-\mathbf{R}_j|} \phi_L^2(\mathbf{x})$$

$$-\, e^2 \sum_{j=1}^{N} \int \mathrm{d}^3\mathbf{x} \left( \frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|} \right) \phi_{L_0}^2(\mathbf{x})$$

$$= -e^2 k \sum_{j=1}^{k} \int d^3\mathbf{x} \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x}) - e^2 k \sum_{j=k+1}^{N} \int d^3\mathbf{x} \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x})$$
$$- e^2 \sum_{j=1}^{k} \int d^3\mathbf{x} \left( \frac{1}{|\mathbf{x} + \mathbf{L}_1 - \mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x} + \mathbf{L}_{N-k} - \mathbf{R}_j|} \right) \phi_{L_0}^2(\mathbf{x})$$
$$- e^2 \sum_{j=k+1}^{N} \int d^3\mathbf{x} \left( \frac{1}{|\mathbf{x} + \mathbf{L}_1 - \mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x} + \mathbf{L}_{N-k} - \mathbf{R}_j|} \right) \phi_{L_0}^2(\mathbf{x}). \tag{4.115}$$

Because

$$e^2 k \sum_{j=k+1}^{N} \int d^3\mathbf{x} \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x}) \geqslant 0 \tag{4.116}$$

and

$$e^2 \sum_{j=1}^{k} \int d^3\mathbf{x} \left( \frac{1}{|\mathbf{x} + \mathbf{L}_1 - \mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x} + \mathbf{L}_{N-k} - \mathbf{R}_j|} \right) \phi_{L_0}^2(\mathbf{x}) \geqslant 0 \tag{4.117}$$

then, the addition of (4.116) and (4.117) gives

$$\langle V_1 \rangle \leqslant -e^2 k \sum_{j=1}^{k} \int d^3\mathbf{x} \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x})$$
$$- e^2 \sum_{j=k+1}^{N} \int d^3\mathbf{x} \left( \frac{1}{|\mathbf{x} + \mathbf{L}_1 - \mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x} + \mathbf{L}_{N-k} - \mathbf{R}_j|} \right) \phi_{L_0}^2(\mathbf{x}). \tag{4.118}$$

For $1 \leqslant i \leqslant N - k$, we have

$$\sum_{j=k+1}^{N} \frac{1}{|\mathbf{x} + \mathbf{L}_i - \mathbf{R}_j|} = \frac{1}{|\mathbf{x} + \mathbf{L}_i - \mathbf{R}_{k+1}|} + \ldots + \frac{1}{|\mathbf{x} + \mathbf{L}_i - \mathbf{R}_{k+i}|}$$
$$+ \ldots + \frac{1}{|\mathbf{x} + \mathbf{L}_i - \mathbf{R}_N|}$$

$$= \frac{1}{|\mathbf{x}+\mathbf{L}_i-\mathbf{R}_{k+1}|}+\ldots+\frac{1}{|\mathbf{x}+\mathbf{L}_i-\mathbf{L}_i|}+\ldots+\frac{1}{|\mathbf{x}+\mathbf{L}_i-\mathbf{R}_N|}$$

$$= \frac{1}{|\mathbf{x}+\mathbf{L}_i-\mathbf{R}_{k+1}|}+\ldots+\frac{1}{|\mathbf{x}|}+\ldots+\frac{1}{|\mathbf{x}+\mathbf{L}_i-\mathbf{R}_N|}$$

$$\geqslant \frac{1}{|\mathbf{x}|}. \tag{4.119}$$

Then, by using (4.119), we obtain

$$\sum_{j=k+1}^{N}\left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|}+\ldots+\frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\geqslant\sum_{j=k+1}^{N}\frac{1}{|\mathbf{x}|}$$

$$= \frac{(N-k)}{|\mathbf{x}|}. \tag{4.120}$$

Therefore

$$-e^2\sum_{j=k+1}^{N}\int \mathrm{d}^3\mathbf{x}\left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|}+\ldots+\frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\phi_{L_0}^2(\mathbf{x})$$

$$\leqslant -e^2\int \mathrm{d}^3\mathbf{x}\,\frac{(N-k)}{|\mathbf{x}|}\phi_{L_0}^2(\mathbf{x})$$

$$= -e^2(N-k)\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\phi_{L_0}^2(\mathbf{x}). \tag{4.121}$$

Substitute (4.121) in (4.118), we obtain

$$\langle V_1\rangle \leqslant -e^2k\sum_{j=1}^{k}\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x}) - e^2(N-k)\int \mathrm{d}^3\mathbf{x}\,\frac{1}{|\mathbf{x}|}\phi_{L_0}^2(\mathbf{x}). \tag{4.122}$$

Consider the second integral in (4.122), where $|x_i| \leqslant L_0$,

$$|\mathbf{x}|^2 = x_1^2+x_2^2+x_3^2 \leqslant L_0^2+L_0^2+L_0^2,$$

$$|\mathbf{x}|^2 \leqslant 3L_0^2,$$

$$|\mathbf{x}| \leqslant \sqrt{3}L_0 \tag{4.123}$$

then

$$\frac{1}{|\mathbf{x}|} \geqslant \frac{1}{\sqrt{3}\,L_0}. \tag{4.124}$$

Multiply (4.124) by $\int \mathrm{d}^3\mathbf{x}\, \phi_{L_0}^2(\mathbf{x})$, then we obtain

$$\int \mathrm{d}^3\mathbf{x}\, \frac{\phi_{L_0}^2(\mathbf{x})}{|\mathbf{x}|} \geqslant \frac{1}{\sqrt{3}\,L_0} \int \mathrm{d}^3\mathbf{x}\, \phi_{L_0}^2(\mathbf{x})$$

$$= \frac{1}{\sqrt{3}\,L_0}. \tag{4.125}$$

By using (4.125), we have

$$-e^2(N-k)\int \mathrm{d}^3\mathbf{x}\, \frac{1}{|\mathbf{x}|}\phi_{L_0}^2(\mathbf{x}) \leqslant -\frac{e^2(N-k)}{\sqrt{3}\,L_0}. \tag{4.126}$$

Substitute (4.126) in (4.122), we obtain

$$\langle V_1 \rangle \leqslant -e^2 k \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x}\, \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x}) - \frac{e^2(N-k)}{\sqrt{3}\,L_0}. \tag{4.127}$$

For $j \geqslant 1$, $|\mathbf{L}_j| = j\sqrt{3}\,D$, then

$$|\mathbf{L}_j| \geqslant \sqrt{3}D \tag{4.128}$$

and, for $i > j$, $i - j \geqslant 1$,

$$\mathbf{L}_i - \mathbf{L}_j = iD(1,1,1) - jD(1,1,1)$$

$$= (i-j)D(1,1,1)$$

then

$$
\begin{aligned}
|\mathbf{L}_i - \mathbf{L}_j| &= \sqrt{(i-j)^2}\sqrt{3}\,D \\
&\geqslant \sqrt{3}\,D.
\end{aligned}
\tag{4.129}
$$

For $\mathbf{x} - \mathbf{x}' - \mathbf{L}_j = (\mathbf{x} - \mathbf{x}') - \mathbf{L}_j$, we have

$$
\begin{aligned}
|\mathbf{x} - \mathbf{x}' - \mathbf{L}_j|^2 &= |\mathbf{x} - \mathbf{x}'|^2 + |\mathbf{L}_j|^2 - 2(\mathbf{x} - \mathbf{x}') \cdot \mathbf{L}_j \\
&\geqslant |\mathbf{x} - \mathbf{x}'|^2 + |\mathbf{L}_j|^2 - 2\,|\mathbf{x} - \mathbf{x}'|\,|\mathbf{L}_j| \\
&\geqslant |\mathbf{L}_j|^2 - 2\,|\mathbf{x} - \mathbf{x}'|\,|\mathbf{L}_j| \\
&= |\mathbf{L}_j|^2 \left(1 - 2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_j|}\right).
\end{aligned}
\tag{4.130}
$$

For $L \leqslant L_0$, we have

$$
|\mathbf{x} - \mathbf{x}'| \leqslant \sqrt{3}L + \sqrt{3}L_0 = \sqrt{3}(L + L_0) \leqslant \sqrt{3}(L_0 + L_0) = 2\sqrt{3}L_0
$$

then

$$
\begin{aligned}
2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_j|} &\leqslant 2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_j|}, \\
-2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_j|} &\geqslant -2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_j|}, \\
1 - 2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_j|} &\geqslant 1 - 2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_j|}, \\
|\mathbf{L}_j|^2 \left(1 - 2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_j|}\right) &\geqslant |\mathbf{L}_j|^2 \left(1 - 2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_j|}\right).
\end{aligned}
\tag{4.131}
$$

Substitute (4.131) in (4.130) we obtain

$$|\mathbf{x} - \mathbf{x}' - \mathbf{L}_j| \geqslant |\mathbf{L}_j| \left(1 - 2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_j|}\right)^{1/2}. \tag{4.132}$$

From (4.128) and (4.57), $|\mathbf{L}_j| \geqslant \sqrt{3}\,D$, then

$$\frac{1}{|\mathbf{L}_j|} \leqslant \frac{1}{\sqrt{3}D},$$

$$L_0 \leqslant \frac{D}{6}.$$

The multiplication of the latter two inequalities, gives

$$\frac{L_0}{|\mathbf{L}_j|} \leqslant \frac{D}{6}\frac{1}{\sqrt{3}D}$$

then

$$2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_j|} \leqslant 2 \cdot \frac{2\sqrt{3}D}{6}\frac{1}{\sqrt{3}D}$$

or

$$-2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_j|} \geqslant -\frac{2}{3}.$$

By adding above inequality by 1, leads to

$$\left(1 - 2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_j|}\right)^{1/2} \geqslant \left(\frac{1}{3}\right)^{1/2}$$

then

$$|\mathbf{L}_j| \left(1 - 2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_j|}\right)^{1/2} \geqslant |\mathbf{L}_j| \frac{1}{\sqrt{3}} \geqslant \sqrt{3}D\frac{1}{\sqrt{3}}$$

$$= D. \tag{4.133}$$

Substitute (4.133) in (4.132), we obtain

$$|\mathbf{x} - \mathbf{x}' - \mathbf{L}_j| \geqslant D \tag{4.134}$$

Now, we will consider $|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j|$, we have

$$\begin{aligned} |\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j|^2 &= |\mathbf{x} - \mathbf{x}'|^2 + |\mathbf{L}_i - \mathbf{L}_j|^2 - 2(\mathbf{x} - \mathbf{x}') \cdot (\mathbf{L}_i - \mathbf{L}_j) \\ &\geqslant |\mathbf{x} - \mathbf{x}'|^2 + |\mathbf{L}_i - \mathbf{L}_j|^2 - 2\,|\mathbf{x} - \mathbf{x}'|\,|\mathbf{L}_i - \mathbf{L}_j| \\ &\geqslant |\mathbf{L}_i - \mathbf{L}_j|^2 - 2\,|\mathbf{x} - \mathbf{x}'|\,|\mathbf{L}_i - \mathbf{L}_j| \\ &= |\mathbf{L}_i - \mathbf{L}_j|^2 \left(1 - 2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_i - \mathbf{L}_j|}\right) \end{aligned} \tag{4.135}$$

then

$$|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j| \geqslant |\mathbf{L}_i - \mathbf{L}_j| \left(1 - 2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_i - \mathbf{L}_j|}\right)^{1/2}. \tag{4.136}$$

For

$$\begin{aligned} |\mathbf{x} - \mathbf{x}'| &\leqslant \sqrt{3}L_0 + \sqrt{3}L_0 \\ &= 2\sqrt{3}L_0. \end{aligned} \tag{4.137}$$

and multiplying (4.137) by $-\dfrac{2}{|\mathbf{L}_i - \mathbf{L}_j|}$ leads to

$$-2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_i - \mathbf{L}_j|} \geqslant -2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_i - \mathbf{L}_j|}.$$

By adding above inequality by 1 gives

$$|\mathbf{L}_i - \mathbf{L}_j| \left(1 - 2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_i - \mathbf{L}_j|}\right)^{1/2} \geqslant |\mathbf{L}_i - \mathbf{L}_j| \left(1 - 2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_i - \mathbf{L}_j|}\right)^{1/2}. \tag{4.138}$$

Since, $|\mathbf{L}_i - \mathbf{L}_j| \geqslant \sqrt{3}D$, then

$$\frac{1}{|\mathbf{L}_i - \mathbf{L}_j|} \leqslant \frac{1}{\sqrt{3}D}$$

and we have

$$L_0 \leqslant \frac{D}{6}.$$

The multiplication of the latter two inequalities, gives

$$\frac{L_0}{|\mathbf{L}_i - \mathbf{L}_j|} \leqslant \frac{D}{6}\frac{1}{\sqrt{3}D}.$$

Multiplying above inequality by $-4\sqrt{3}$, leads to

$$-2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_i - \mathbf{L}_j|} \geqslant -\frac{2}{3}$$

then

$$1 - 2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_i - \mathbf{L}_j|} \geqslant 1 - \frac{2}{3}$$

or

$$\left(1 - 2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_i - \mathbf{L}_j|}\right)^{1/2} \geqslant \left(\frac{1}{3}\right)^{1/2},$$

$$\begin{aligned} |\mathbf{L}_i - \mathbf{L}_j| \left(1 - 2 \cdot \frac{2\sqrt{3}L_0}{|\mathbf{L}_i - \mathbf{L}_j|}\right)^{1/2} &\geqslant |\mathbf{L}_i - \mathbf{L}_j| \frac{1}{\sqrt{3}} \\ &\geqslant \sqrt{3}D\frac{1}{\sqrt{3}} \\ &= D. \end{aligned} \tag{4.139}$$

Then, with $i < j$, substitute (4.139) in (4.136), we obtain

$$|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j| \geqslant D. \tag{4.140}$$

From (4.134), we obtain

$$\frac{1}{|\mathbf{x} - \mathbf{x}' - \mathbf{L}_j|} \leqslant \frac{1}{D}$$

then multiply above inequality by $\phi_L^2(\mathbf{x})\,\phi_{L_0}^2(\mathbf{x}')$, we obtain

$$\phi_L^2(\mathbf{x})\,\frac{1}{|\mathbf{x} - \mathbf{x}' - \mathbf{L}_j|}\phi_{L_0}^2(\mathbf{x}') \leqslant \phi_L^2(\mathbf{x})\,\frac{1}{D}\phi_{L_0}^2(\mathbf{x}').$$

Then

$$\begin{aligned}
&e^2 k \sum_{j=1}^{N-k} \int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi_L^2(\mathbf{x})\,\frac{1}{|\mathbf{x} - \mathbf{x}' - \mathbf{L}_j|}\phi_{L_0}^2(\mathbf{x}') \\
&\qquad \leqslant e^2 k \sum_{j=1}^{N-k} \int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi_L^2(\mathbf{x})\,\frac{1}{D}\phi_{L_0}^2(\mathbf{x}') \\
&\qquad = \frac{e^2 k}{D} \sum_{j=1}^{N-k} \int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi_L^2(\mathbf{x})\,\phi_{L_0}^2(\mathbf{x}') \\
&\qquad = \frac{e^2 k}{D} \sum_{j=1}^{N-k} 1 \\
&\qquad = \frac{e^2 k}{D}(N-k).
\end{aligned} \tag{4.141}$$

From (4.140), we obtain

$$\frac{1}{|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j|} \leqslant \frac{1}{D}$$

then multiply above inequality by $\phi^2_{L_0}(\mathbf{x})\phi^2_{L_0}(\mathbf{x}')$, we obtain

$$\phi^2_{L_0}(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|}\phi^2_{L_0}(\mathbf{x}') \leqslant \phi^2_{L_0}(\mathbf{x})\frac{1}{D}\phi^2_{L_0}(\mathbf{x}').$$

Then

$$\begin{aligned}
e^2\sum_{i<j}^{N-k}\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi^2_{L_0}(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|}\phi^2_{L_0}(\mathbf{x}')& \\
\leqslant e^2\sum_{i<j}^{N-k}\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi^2_{L_0}(\mathbf{x})\frac{1}{D}\phi^2_{L_0}(\mathbf{x}')& \\
=\frac{e^2}{D}\sum_{i<j}^{N-k}\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi^2_{L_0}(\mathbf{x})\phi^2_{L_0}(\mathbf{x}')& \\
=\frac{e^2}{D}\sum_{i<j}^{N-k}1 & \qquad (4.142)
\end{aligned}$$

where we have

$$\frac{e^2}{D}\sum_{i<j}^{N-k}1=\frac{e^2(N-k)(N-k-1)}{2D}. \qquad (4.143)$$

Substitute (4.143) in (4.142), we obtain

$$e^2\sum_{i<j}^{N-k}\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi^2_{L_0}(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|}\phi^2_{L_0}(\mathbf{x}') \leqslant \frac{e^2(N-k)(N-k-1)}{2D}. \qquad (4.144)$$

The addition of (4.141) and (4.144), gives

$$\begin{aligned}
\langle V_2\rangle = e^2\frac{k(k-1)}{2}\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi^2_L(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi^2_L(\mathbf{x}')& \\
+e^2k\sum_{j=1}^{N-k}\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi^2_L(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_j|}\phi^2_{L_0}(\mathbf{x}')&
\end{aligned}$$

$$+ e^2 \sum_{i<j}^{N-k} \int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}' \; \phi_{L_0}^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|} \phi_{L_0}^2(\mathbf{x}')$$

$$\leqslant e^2 \frac{k(k-1)}{2} \int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}' \; \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}')$$

$$+ \frac{e^2 k}{D}(N-k) + \frac{e^2(N-k)(N-k-1)}{2D} \tag{4.145}$$

where we have

$$\frac{e^2 k}{D}(N-k) + \frac{e^2(N-k)(N-k-1)}{2D} = \frac{e^2}{D}(N-k)\left(k + \frac{N-k-1}{2}\right)$$

$$= \frac{e^2(N-k)(N+k-1)}{2D}. \tag{4.146}$$

Substitute (4.146) in (4.145), we obtain

$$\langle V_2 \rangle \leqslant e^2 \frac{k(k-1)}{2} \int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}' \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}')$$

$$+ \frac{e^2(N-k)(N+k-1)}{2D}. \tag{4.147}$$

Now, we will consider the repulsive term

$$\sum_{i<j}^{N} \frac{1}{|\mathbf{R}_i-\mathbf{R}_j|} = \sum_{j=2}^{N}\sum_{i=1}^{j-1} \frac{1}{|\mathbf{R}_i-\mathbf{R}_j|}$$

$$= \sum_{j=2}^{k}\sum_{i=1}^{j-1} \frac{1}{|\mathbf{R}_i-\mathbf{R}_j|} + \sum_{j=k+1}^{N}\sum_{i=1}^{j-1} \frac{1}{|\mathbf{R}_i-\mathbf{R}_j|}. \tag{4.148}$$

We set $\mathbf{R}_j = \mathbf{L}_{j-k}$, for $j = k+1, \ldots, N$, then for $j \geqslant k+1$, we have

$$|\mathbf{R}_j| = |\mathbf{L}_{j-k}| \geqslant \sqrt{3}D. \tag{4.149}$$

And for $j \leqslant k$, we have

$$\begin{aligned}|\mathbf{R}_j| &\leqslant \sqrt{3}L \\ &\leqslant \sqrt{3}\frac{D}{6} < \frac{\sqrt{3}D}{3}.\end{aligned} \tag{4.150}$$

Since

$$|\mathbf{R}_i - \mathbf{R}_j|^2 = |\mathbf{R}_i|^2 + |\mathbf{R}_j|^2 - 2\mathbf{R}_i \cdot \mathbf{R}_j$$

then

$$\begin{aligned}|\mathbf{R}_i - \mathbf{R}_j|^2 &\geqslant |\mathbf{R}_i|^2 + |\mathbf{R}_j|^2 - 2\,|\mathbf{R}_i|\,|\mathbf{R}_j| \\ &\geqslant |\mathbf{R}_j|^2 - 2\,|\mathbf{R}_i|\,|\mathbf{R}_j| \\ &= |\mathbf{R}_j|^2\left(1 - 2\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|}\right)\end{aligned} \tag{4.151}$$

or

$$|\mathbf{R}_i - \mathbf{R}_j| \geqslant |\mathbf{R}_j|\left(1 - 2\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|}\right)^{1/2}. \tag{4.152}$$

By considering the case of $1 \leqslant i \leqslant k$, $k+1 \leqslant j \leqslant N$, $i < j$, we have

$$\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|} \leqslant \frac{\sqrt{3}L}{\sqrt{3}D} \leqslant \frac{D}{3}\frac{1}{D} = \frac{1}{3}$$

then

$$-2\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|} \geqslant -\frac{2}{3}$$

then we obtain

$$1 - 2\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|} \geqslant 1 - \frac{2}{3}. \tag{4.153}$$

By using (4.149) and compare (4.153) with (4.152), we obtain

$$\begin{aligned}|\mathbf{R}_j|\left(1-2\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|}\right)^{1/2} &\geqslant |\mathbf{R}_j|\left(\frac{1}{3}\right)^{1/2}\\ &\geqslant \sqrt{3}D\frac{1}{\sqrt{3}}\\ &= D \end{aligned}\tag{4.154}$$

then we have

$$|\mathbf{R}_i-\mathbf{R}_j|\geqslant D,\quad \text{for } 1\leqslant i\leqslant k,\quad k+1\leqslant j\leqslant N,\quad i<j. \tag{4.155}$$

Consider the case $k+1\leqslant i<N$, $k+2\leqslant j\leqslant N$, $i<j$, we have

$$\begin{aligned}|\mathbf{R}_i-\mathbf{R}_j| &= |\mathbf{L}_{i-k}-\mathbf{L}_{j-k}|\\ &\geqslant \sqrt{3}D\\ &\geqslant D. \end{aligned}\tag{4.156}$$

Then, from (4.155) and (4.156), we conclude that

$$|\mathbf{R}_i-\mathbf{R}_j|\geqslant D. \tag{4.157}$$

The inverse of (4.157) gives

$$\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|}\leqslant\frac{1}{D}$$

then we have

$$\sum_{j=k+1}^{N}\sum_{i=1}^{j-1}\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|}\leqslant\sum_{j=k+1}^{N}\sum_{i=1}^{j-1}\frac{1}{D}$$

$$= \frac{1}{D} \sum_{j=k+1}^{N} \sum_{i=1}^{j-1} 1$$

$$= \frac{1}{D} \frac{(N-k)(N+k-1)}{2}. \tag{4.158}$$

Substitute (4.158) in (4.148) we obtain

$$\sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \leqslant \sum_{i<j}^{k} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} + \frac{e^2(N-k)(N+k-1)}{2D}. \tag{4.159}$$

The addition of (4.127), (4.147) and (4.159) and by using (4.114), lead to

$$\langle \Psi | H | \Psi \rangle = [kT + (N-k)T_0] + \langle V_1 \rangle + \langle V_2 \rangle + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|}$$

$$\leqslant [kT + (N-k)T_0]$$

$$- e^2 k \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x} \, \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x}) - \frac{e^2(N-k)}{\sqrt{3}L_0}$$

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

$$+ \frac{e^2(N-k)(N+k-1)}{2D}$$

$$+ \sum_{i<j}^{k} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} + \frac{e^2(N-k)(N+k-1)}{2D}$$

$$= kT - ke^2 \sum_{j=1}^{k} \int \mathrm{d}^3\mathbf{x} \, \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x})$$

$$+\frac{k(k-1)e^2}{2}\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')+\sum_{i<j}^{k}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}$$

$$+(N-k)T_0+\frac{e^2(N-k)(N+k-1)}{D}-\frac{e^2(N-k)}{\sqrt{3}L_0}. \tag{4.160}$$

Therefore

$$\langle\Psi|H|\Psi\rangle\leqslant kT+\langle H_1\rangle+(N-k)\left[T_0+\frac{e^2(N+k-1)}{D}-\frac{e^2}{\sqrt{3}L_0}\right] \tag{4.161}$$

where, for $|x_i|\leqslant L$,

$$\langle H_1\rangle=-ke^2\sum_{j=1}^{k}\int \mathrm{d}^3\mathbf{x}\ \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x})$$

$$+\frac{k(k-1)e^2}{2}\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')+\sum_{i<j}^{k}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}. \tag{4.162}$$

Because $k(k-1)<k^2$, then

$$\langle H_1\rangle\leqslant -ke^2\sum_{j=1}^{k}\int \mathrm{d}^3\mathbf{x}\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x})$$

$$+\frac{e^2}{2}k^2\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')+\sum_{i<j}^{k}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}$$

$$\equiv H_1(k,\mathbf{R}) \tag{4.163}$$

where we set $\mathbf{R}=\{\mathbf{R}_1,\ldots,\mathbf{R}_k\}$ and

$$H_1(k,\mathbf{R})=-ke^2\sum_{j=1}^{k}\int \mathrm{d}^3\mathbf{x}\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x})$$

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

$$+\sum_{i<j}^{k} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|}. \tag{4.164}$$

We define

$$A_1(k, \mathbf{R}) = -ke^2 \sum_{j=1}^{k} \int d^3\mathbf{x} \; \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x}), \tag{4.165a}$$

$$A_2(k) = \frac{e^2}{2} k^2 \int d^3\mathbf{x} d^3\mathbf{x}' \; \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \phi_L^2(\mathbf{x}'), \tag{4.165b}$$

$$A_3(k, \mathbf{R}) = \sum_{i<j}^{k} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{4.165c}$$

then

$$\langle H_1 \rangle \leqslant H_1(k, \mathbf{R}) = A_1(k, \mathbf{R}) + A_2(k) + A_3(k, \mathbf{R}). \tag{4.166}$$

Therefore, to derive the upper bound of $\langle H_1 \rangle$, we partition the interval $[0, L]$ into $n$ subintervals: $0 = a'_0 < a'_1 < a'_2 < \ldots < a'_n = L$ and we choose $a'_j$, $a'_{j-1}$ such that

$$\frac{1}{L} \int_{a'_{j-1}}^{a'_j} dx_i \; \cos^2\left(\frac{\pi x_i}{2L}\right) \equiv \int_{a'_{j-1}}^{a'_j} dx_i \; g^2(x_i) = \frac{1}{2n} \tag{4.167}$$

where

$$g(x_i) = \frac{1}{\sqrt{L}} \cos\left(\frac{\pi x_i}{2L}\right) \tag{4.168}$$

for $j = 1, \ldots, n$. By doing so, we divide the box of side $2L, 2L, 2L$ into $(2n)^3 = 8n^3 = k$ smaller boxes which labeled $B'(m)$.

Let

$$0 = a'_0 < a'_1 < a'_2 < \cdots < a'_n = L, \tag{4.169}$$

$$\alpha'_j = a'_j - a'_{j-1}, \qquad j = 1, \ldots, n \tag{4.170}$$

where

$$\sum_{j=1}^{n} \alpha'_j = L. \tag{4.171}$$

Let $m = (j_1, j_2, j_3)$, then

$$B'(m) \text{ is equivalent to box of sides } \alpha'_{j_1} \times \alpha'_{j_2} \times \alpha'_{j_3} \tag{4.172}$$

where we have the normalization condition that

$$\left(\frac{1}{L}\right)^3 \int_{a'_{j_1-1}}^{a'_{j_1}} \mathrm{d}x_1 \; \cos^2\left(\frac{\pi x_1}{2L}\right) \int_{a'_{j_2-1}}^{a'_{j_2}} \mathrm{d}x_2 \; \cos^2\left(\frac{\pi x_2}{2L}\right) \int_{a'_{j_3-1}}^{a'_{j_3}} \mathrm{d}x_3 \; \cos^2\left(\frac{\pi x_3}{2L}\right)$$

$$= \int_{a'_{j_1-1}}^{a'_{j_1}} \mathrm{d}x_1 \; g^2(x_1) \int_{a'_{j_2-1}}^{a'_{j_2}} \mathrm{d}x_2 \; g^2(x_2) \int_{a'_{j_3-1}}^{a'_{j_3}} \mathrm{d}x_3 \; g^2(x_3)$$

$$= \int_{B'(m)} \mathrm{d}^3\mathbf{x} \; \phi_L^2(\mathbf{x})$$

$$= \frac{1}{(2n)^3} = \frac{1}{k}. \tag{4.173}$$

Therefore

$$\int \mathrm{d}^3\mathbf{x} \; \phi_L^2(\mathbf{x}) = (2)^3 \sum_{B'(m)=1}^{k/(2)^3} \int_{B'(m)} \mathrm{d}^3\mathbf{x} \; \phi_L^2(\mathbf{x})$$

$$= (2)^3 \sum_{B'(m)=1}^{k/(2)^3} \left(\frac{1}{k}\right)$$

$$= (2)^3 \frac{k}{(2)^3} \frac{1}{k}$$

$$= 1. \tag{4.174}$$

Now we place $\mathbf{R}_1$ in box $B'(m) = 1$, $\mathbf{R}_2$ in box $B'(m) = 2, \ldots, \mathbf{R}_k$ in box

$B'(m) = k$, and then we average $H_1(k, \mathbf{R})$ over the positions, $\mathbf{R}_1, \ldots, \mathbf{R}_k$, of the positive particles within the boxes with a relative weight $\phi_L^2(\mathbf{R}_1), \ldots, \phi_L^2(\mathbf{R}_k)$ in box $B'(m) = 1, \ldots, B'(m) = k$, respectively.

## The Average of $A_1(k, \mathbf{R})$:

The term $A_1(k, \mathbf{R})$ may be rewritten as sums of integrals over such boxes as follows:

$$\begin{aligned} A_1(k, \mathbf{R}) &= -(2)^3 k e^2 \sum_{B'(m)=1}^{k/2^3} \sum_{j=1}^{k/2^3} \int_{B'(m)} \mathrm{d}^3\mathbf{x}\, \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x}) \\ &= -(2)^3 k e^2 \sum_{B'(m)=1}^{n^3} \sum_{j=1}^{n^3} \int_{B'(m)} \mathrm{d}^3\mathbf{x}\, \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x}) \\ &= -(2)^3 k e^2 \sum_{B'(m)=1}^{n^3} \int_{B'(m)} \mathrm{d}^3\mathbf{x}\, \phi_L^2(\mathbf{x}) \sum_{j=1}^{n^3} \frac{1}{|\mathbf{x} - \mathbf{R}_j|}. \end{aligned} \tag{4.175}$$

Then $\langle A_1(k, \mathbf{R}) \rangle$ will be derived below. Since

$$\sum_{j=1}^{n^3} \frac{1}{|\mathbf{x} - \mathbf{R}_j|} = \frac{1}{|\mathbf{x} - \mathbf{R}_1|} + \ldots + \frac{1}{|\mathbf{x} - \mathbf{R}_{n^3}|}$$

then we have

$$\begin{aligned} \left( \sum_{j=1}^{n^3} \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \right) \Bigg|_{\text{average}} &= \frac{\displaystyle\int_{B'(j)=1} \mathrm{d}^3\mathbf{x}' \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}}{\displaystyle\int_{B'(j)=1} \mathrm{d}^3\mathbf{x}' \phi_L^2(\mathbf{x}')} + \ldots + \frac{\displaystyle\int_{B'(j)=n^3} \mathrm{d}^3\mathbf{x}' \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}}{\displaystyle\int_{B'(j)=n^3} \mathrm{d}^3\mathbf{x}' \phi_L^2(\mathbf{x}')} \\ &= \frac{\displaystyle\int_{B'(j)=1} \mathrm{d}^3\mathbf{x}' \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}}{\frac{1}{k}} + \ldots + \frac{\displaystyle\int_{B'(j)=n^3} \mathrm{d}^3\mathbf{x}' \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}}{\frac{1}{k}} \end{aligned}$$

$$= k \int\limits_{B'(j)=1} \mathrm{d}^3\mathbf{x}' \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} + \ldots + k \int\limits_{B'(j)=n^3} \mathrm{d}^3\mathbf{x}' \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

$$= k \sum_{B'(q)=1}^{n^3} \int\limits_{B'(q)} \mathrm{d}^3\mathbf{x}' \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}. \tag{4.176}$$

Then

$$\langle A_1(k,\mathbf{R})\rangle = -(2)^3 k e^2 \sum_{B'(m)=1}^{n^3} \int\limits_{B'(m)} \mathrm{d}^3\mathbf{x}\ \phi_L^2(\mathbf{x}) k \sum_{B'(q)=1}^{n^3} \int\limits_{B'(q)} \mathrm{d}^3\mathbf{x}'\ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

$$= -(2)^3 k^2 e^2 \sum_{B'(m)=1}^{n^3} \sum_{B'(q)=1}^{n^3} \int\limits_{B'(m)} \mathrm{d}^3\mathbf{x} \int\limits_{B'(q)} \mathrm{d}^3\mathbf{x}'\ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}'). \tag{4.177}$$

## The Average of $A_2(k)$:

The term $A_2(k)$ may be rewritten as sums of integrals over such boxes directly as follows:

$$A_2(k) = \frac{e^2}{2} k^2 \int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}')$$

$$= (2)^3 \frac{e^2}{2} k^2 \sum_{B'(m)=1}^{n^3} \sum_{B'(q)=1}^{n^3} \int\limits_{B'(m)} \mathrm{d}^3\mathbf{x} \int\limits_{B'(q)} \mathrm{d}^3\mathbf{x}'\ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}'). \tag{4.178}$$

## The Average of $A_3(k, \mathbf{R})$:

Since

$$A_3(k,\mathbf{R}) = \frac{1}{2}\sum_{i\neq j}^{k}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|} = \frac{(2)^3}{2}\sum_{i\neq j}^{n^3}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|} \tag{4.179}$$

then we have

$$\left.\left(\sum_{i\neq j}^{n^3}\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|}\right)\right|_{\text{average over }\mathbf{R}_j}$$

$$= \sum_{i=1}^{n^3}\sum_{j(\neq i)=1}^{n^3}\left.\left(\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|}\right)\right|_{\text{average over }\mathbf{R}_j}$$

$$= \sum_{i(\neq j)=1}^{n^3}\left\{\frac{\int\limits_{B'(j)=1} \mathrm{d}^3\mathbf{x}'\frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i-\mathbf{x}'|}}{\int\limits_{B'(j)=1}\mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x}')} + \ldots + \frac{\int\limits_{B'(j)=n^3} \mathrm{d}^3\mathbf{x}'\frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i-\mathbf{x}'|}}{\int\limits_{B'(j)=n^3}\mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x}')}\right\}$$

$$= \sum_{i(\neq j)=1}^{n^3}\left\{\frac{\int\limits_{B'(j)=1} \mathrm{d}^3\mathbf{x}'\frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i-\mathbf{x}'|}}{\frac{1}{k}} + \ldots + \frac{\int\limits_{B'(j)=n^3} \mathrm{d}^3\mathbf{x}'\frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i-\mathbf{x}'|}}{\frac{1}{k}}\right\}$$

$$= \sum_{i(\neq j)=1}^{n^3}\left\{k\int\limits_{B'(j)=1} \mathrm{d}^3\mathbf{x}'\frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i-\mathbf{x}'|} + \ldots + k\int\limits_{B'(j)=n^3} \mathrm{d}^3\mathbf{x}'\frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i-\mathbf{x}'|}\right\}$$

$$= k\sum_{i(\neq j)=1}^{n^3}\sum_{B'(j)=1}^{n^3}\int_{B'(j)}\mathrm{d}^3\mathbf{x}'\;\frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i-\mathbf{x}'|} \tag{4.180}$$

and

$$\left.\left(\sum_{i\neq j}^{n^3}\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|}\right)\right|_{\text{average}}$$

$$= k \sum_{B'(j(\neq i))=1}^{n^3} \int_{B'(j)} \mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x}') \left\{ \frac{\int\limits_{B'(i)=1} \mathrm{d}^3\mathbf{x} \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x}-\mathbf{x}'|}}{\int\limits_{B'(i)=1} \mathrm{d}^3\mathbf{x}\phi_L^2(\mathbf{x})} + \ldots + \frac{\int\limits_{B'(i)=n^3} \mathrm{d}^3\mathbf{x} \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x}-\mathbf{x}'|}}{\int\limits_{B'(i)=n^3} \mathrm{d}^3\mathbf{x}\phi_L^2(\mathbf{x})} \right\}$$

$$= k \sum_{B'(j(\neq i))=1}^{n^3} \int_{B'(j)} \mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x}') \left\{ \frac{\int\limits_{B'(i)=1} \mathrm{d}^3\mathbf{x} \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x}-\mathbf{x}'|}}{\frac{1}{k}} + \ldots + \frac{\int\limits_{B'(i)=n^3} \mathrm{d}^3\mathbf{x} \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x}-\mathbf{x}'|}}{\frac{1}{k}} \right\}$$

$$= k \sum_{B'(j(\neq i))=1}^{n^3} \int_{B'(j)} \mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x}') \sum_{B'(i)=1}^{n^3} k \int_{B'(i)} \mathrm{d}^3\mathbf{x} \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x}-\mathbf{x}'|}$$

$$= k^2 \sum_{B'(m)=1}^{n^3} \sum_{B'(q(\neq m))=1}^{n^3} \int_{B'(m)} \mathrm{d}^3\mathbf{x} \int_{B'(q)} \mathrm{d}^3\mathbf{x}'\ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}'). \tag{4.181}$$

Then we obtain the average of $A_3(k, \mathbf{R})$ as follows:

$$\langle A_3(k, \mathbf{R})\rangle = \frac{(2)^3}{2}\, e^2 k^2 \sum_{B'(m)=1}^{n^3} \sum_{B'(q(\neq m))=1}^{n^3} \int_{B'(m)} \mathrm{d}^3\mathbf{x} \int_{B'(q)} \mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}'). \tag{4.182}$$

Then, the average of $H_1(k, \mathbf{R})$ will be obtained below

$$\langle H_1(k, \mathbf{R})\rangle = \langle A_1(k, \mathbf{R})\rangle + A_2(k) + \langle A_3(k, \mathbf{R})\rangle$$

$$= -(2)^3\, k^2 e^2 \sum_{B'(m)=1}^{n^3} \sum_{B'(q)=1}^{n^3} \int_{B'(m)} \mathrm{d}^3\mathbf{x} \int_{B'(q)} \mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}')$$

$$+ (2)^3\, \frac{e^2}{2} k^2 \sum_{B'(m)=1}^{n^3} \sum_{B'(q)=1}^{n^3} \int_{B'(m)} \mathrm{d}^3\mathbf{x} \int_{B'(q)} \mathrm{d}^3\mathbf{x}'\phi_L^2\,(\mathbf{x})\, \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2\,(\mathbf{x}')$$

$$+\frac{(2)^3}{2}e^2k^2\sum_{B'(m)=1}^{n^3}\sum_{B'(q(\neq m))=1}^{n^3}\int_{B'(m)}\mathrm{d}^3\mathbf{x}\int_{B'(q)}\mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')$$

$$=-(2)^3\,k^2\frac{e^2}{2}\sum_{B'(m)=1}^{n^3}\sum_{B'(q)=1}^{n^3}\int_{B'(m)}\mathrm{d}^3\mathbf{x}\int_{B'(q)}\mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')$$

$$+(2)^3k^2\frac{e^2}{2}\sum_{B'(m)=1}^{n^3}\sum_{B'(q(\neq m))=1}^{n^3}\int_{B'(m)}\mathrm{d}^3\mathbf{x}\int_{B'(q)}\mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')$$

$$=-(2)^3\,\frac{e^2k^2}{2}\sum_{B'(m)=1}^{n^3}\sum_{B'(q)=1}^{n^3}\int_{B'(m)}\mathrm{d}^3\mathbf{x}\int_{B'(q)}\mathrm{d}^3\mathbf{x}'\phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')\delta_{mq}. \tag{4.183}$$

Eq. (4.183) may be rewritten as

$$\langle H_1(k,\mathbf{R})\rangle = -(2)^3\,\frac{e^2k^2}{2}\sum_{B'(m)=1}^{n^3}\int_{B'(m)}\mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\;\phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}'). \tag{4.184}$$

By the definition of an *average*, there must be at least one set of $\mathbf{R}$ such that

$$H_1(k,\mathbf{R}) \leqslant \langle H_1(k,\mathbf{R})\rangle\,. \tag{4.185}$$

Then, by using (4.163), we obtain

$$\langle H_1\rangle \leqslant -(2)^3\,\frac{e^2k^2}{2}\sum_{B'(m)=1}^{n^3}\int_{B'(m)}\mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\;\phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}'). \tag{4.186}$$

We may scale $\mathbf{x}$ to $\dfrac{\mathbf{x}}{L}\equiv\mathbf{u}$, then

$$\frac{1}{L}\int_{a'_{j-1}}^{a'_j}\mathrm{d}x_i\;\cos^2\left(\frac{\pi x_i}{2L}\right)=\int_{a'_{j-1}/L}^{a'_j/L}\mathrm{d}\left(\frac{x_i}{L}\right)\;\cos^2\left(\frac{\pi}{2}\left(\frac{x_i}{L}\right)\right) \tag{4.187}$$

then we obtain

$$\frac{1}{L}\int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i \ \cos^2\left(\frac{\pi x_i}{2L}\right) = \int_{a_{j-1}}^{a_j} \mathrm{d}u_i \ \cos^2\left(\frac{\pi u_i}{2}\right) \tag{4.188}$$

or

$$\int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i g^2(x_i) = \int_{a_{j-1}}^{a_j} \mathrm{d}u_i g_1^2(u_i) = \frac{1}{2n} \tag{4.189}$$

where

$$g_1(u_i) = \cos\left(\frac{\pi u_i}{2}\right). \tag{4.190}$$

For

$$0 = \frac{a'_0}{L} < \frac{a'_1}{L} < \frac{a'_2}{L} < \cdots < \frac{a'_n}{L} = 1$$

then

$$0 = a_0 < a_1 < a_2 < \cdots < a_n = 1, \tag{4.191}$$

$$\alpha_j = a_j - a_{j-1}, \qquad j = 1, \ldots, n, \tag{4.192}$$

$$\sum_{j=1}^{n} \alpha_j = 1. \tag{4.193}$$

Let

$$B(m) \equiv \text{ a box of sides } \alpha_{j_1} \times \alpha_{j_2} \times \alpha_{j_3}. \tag{4.194}$$

Therefore, we have the normalization condition such that

$$\int_{a_{j_1-1}}^{a_{j_1}} \mathrm{d}u_1 \ g_1^2(u_1) \int_{a_{j_2-1}}^{a_{j_2}} \mathrm{d}u_2 \ g_1^2(u_2) \int_{a_{j_3-1}}^{a_{j_3}} \mathrm{d}u_3 \ g_1^2(u_3)$$

$$= \int_{B(m)} \mathrm{d}^3\mathbf{u} \ \phi_1^2(\mathbf{u})$$

$$= \frac{1}{(2n)^3} = \frac{1}{k} \tag{4.195}$$

where

$$\phi_1(\mathbf{x}) = \prod_{i=1}^{3} \cos\left(\frac{\pi x_i}{2}\right), \qquad |x_i| \leqslant 1. \tag{4.196}$$

Then, we rewrite the integral on the right-hand side of (4.186) as below

$$\sum_{B'(m)=1}^{n^3} \int_{B'(m)} \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')$$

$$= \sum_{B(m)=1}^{n^3} \int_{B(m)} \mathrm{d}^3\mathbf{u}\mathrm{d}^3\mathbf{u}'\ \phi_1^2(\mathbf{u})\frac{1}{|L\mathbf{u}-L\mathbf{u}'|}\phi_1^2(\mathbf{u}')$$

$$= \frac{1}{L}\sum_{B(m)=1}^{n^3} \int_{B(m)} \mathrm{d}^3\mathbf{u}\mathrm{d}^3\mathbf{u}'\ \phi_1^2(\mathbf{u})\frac{1}{|\mathbf{u}-\mathbf{u}'|}\phi_1^2(\mathbf{u}') \tag{4.197}$$

where $0 \leqslant u_i \leqslant 1$. Substitute (4.197) in (4.186), we obtain

$$\langle H_1\rangle \leqslant -(2)^3\ \frac{e^2k^2}{2L}\sum_{B(m)=1}^{n^3} \int_{B(m)} \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\phi_1^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_1^2(\mathbf{x}') \tag{4.198}$$

where $0 \leqslant x_i \leqslant 1$.

Since $\mathbf{x}$ and $\mathbf{x}'$ lie within a box $B(j_1, j_2, j_3)$ of sides $\alpha_{j_1} \times \alpha_{j_2} \times \alpha_{j_3}$. Then, we may insert this box in a sphere of radius $\frac{1}{2}\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}$. And from the normalization condition (4.195), let $\phi_1^2(\mathbf{u})$ denotes the charge density in $B(m)$ of total charge $\frac{1}{k}$, i.e.,

$$\int_{B(m)} \mathrm{d}^3\mathbf{x}\ \phi_1^2(\mathbf{x}) = \frac{1}{k}. \tag{4.199}$$

Then, we obtain

$$\int_{B(m)} \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{x}'\ \phi_1^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_1^2(\mathbf{x}') \geqslant \frac{\left(\frac{1}{k}\right)^2}{\frac{1}{2}\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}}$$

$$= \frac{2}{k^2\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}}. \tag{4.200}$$

By substituting (4.203) in (4.198) and using

$$\sum_{B(m)=1}^{n^2} = \sum_{j_1=1}^{n}\sum_{j_2=1}^{n}\sum_{j_3=1}^{n} \tag{4.201}$$

then we have

$$\langle H_1 \rangle \leqslant -(2)^3\,\frac{e^2k^2}{2L}\sum_{j_1=1}^{n}\sum_{j_2=1}^{n}\sum_{j_3=1}^{n}\frac{2}{k^2\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}}$$

$$\leqslant -\frac{8e^2}{L}\sum_{j_1,j_2,j_3=1}^{n}\frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}}. \tag{4.202}$$

To obtain the bound of above summation, we consider

$$\sum_{j_1=1}^{n} 1 = n \tag{4.203}$$

then, for $f(\alpha_{j_1}) > 0$,

$$\sum_{j_1=1}^{n}\sqrt{f(\alpha_{j_1})}\frac{1}{f(\alpha_{j_1})} = n \tag{4.204}$$

where

$$f(\alpha_{j_1}) = \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}. \tag{4.205}$$

From Cauchy-Schwarz inequality,

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leqslant \sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2$$

we have

$$\left(\sum_{j_1=1}^{n}\sqrt{f(\alpha_{j_1})}\frac{1}{f(\alpha_{j_1})}\right)^2 \leqslant \sum_{j_1=1}^{n} f(\alpha_{j_1})\sum_{j_1=1}^{n}\frac{1}{f(\alpha_{j_1})}$$

or

$$\sum_{j_1=1}^{n} \frac{1}{f(\alpha_{j_1})} \geqslant \frac{n^2}{\sum\limits_{j_1=1}^{n} f(\alpha_{j_1})}. \tag{4.206}$$

Substitute $f(\alpha_{j_1})$ in above inequality, we obtain

$$\sum_{j_1=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}} \geqslant \frac{n^2}{\sum\limits_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}}. \tag{4.207}$$

Multiply above inequality by $\sum\limits_{j_2=1}^{n}$, we obtain

$$\begin{aligned} \sum_{j_2=1}^{n} \sum_{j_1=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}} &\geqslant \sum_{j_2=1}^{n} \frac{n^2}{\sum\limits_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}} \\ &= n^2 \sum_{j_2=1}^{n} \frac{1}{\sum\limits_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}}. \end{aligned} \tag{4.208}$$

Let

$$f(\alpha_{j_2}) = \frac{1}{\sum\limits_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \alpha_{j_3}^2}}. \tag{4.209}$$

From Cauchy-Schwarz inequality, we have

$$\sum_{j_2=1}^{n} \frac{1}{f(\alpha_{j_2})} \geqslant \frac{n^2}{\sum\limits_{j_2=1}^{n} f(\alpha_{j_2})}$$

then

$$\sum_{j_2=1}^{n} f(\alpha_{j_2}) \geqslant \frac{n^2}{\sum\limits_{j_2=1}^{n} \frac{1}{f(\alpha_{j_2})}}. \tag{4.210}$$

Replace $f(\alpha_{j_2})$ in above inequality, we obtain

$$\sum_{j_2=1}^{n}\frac{1}{\sum_{j_1=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2}}\geqslant\frac{n^2}{\sum_{j_2=1}^{n}\frac{1}{\frac{1}{\sum_{j_1=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2}}}}$$

$$=\frac{n^2}{\sum_{j_2=1}^{n}\sum_{j_1=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2}}. \tag{4.211}$$

Then, from (4.208), we have

$$\sum_{j_2=1}^{n}\sum_{j_1=1}^{n}\frac{1}{\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2}}\geqslant n^4\frac{1}{\sum_{j_2=1}^{n}\sum_{j_1=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2}}. \tag{4.212}$$

Multiply above inequality by $\sum_{j_3=1}^{n}$, we obtain

$$\sum_{j_3=1}^{n}\sum_{j_2=1}^{n}\sum_{j_1=1}^{n}\frac{1}{\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2}}\geqslant n^4\sum_{j_3=1}^{n}\frac{1}{\sum_{j_2=1}^{n}\sum_{j_1=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2}}. \tag{4.213}$$

The Cauchy-Schwarz inequality then yields

$$\sum_{j_1,j_2,j_3=1}^{n}\frac{1}{\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2}}\geqslant n^6\frac{1}{\sum_{j_1,j_2,j_3=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2}}. \tag{4.214}$$

Consider the right-hand side of (4.214)

$$\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2\leqslant(\alpha_{j_1}+\alpha_{j_2}+\alpha_{j_3})^2 \tag{4.215}$$

then, by using (4.193),

$$\begin{aligned}\sum_{j_1,j_2,j_3=1}^{n} \sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2} &\leqslant \sum_{j_1,j_2,j_3=1}^{n} (\alpha_{j_1}+\alpha_{j_2}+\alpha_{j_3}) \\ &= \sum_{j_1,j_2=1}^{n} (n\alpha_{j_1}+n\alpha_{j_2}+1) \\ &= \sum_{j_1=1}^{n}(n^2\alpha_{j_1}+n+n) \\ &= (n^2+n^2+n^2) \\ &= 3n^2. \end{aligned} \tag{4.216}$$

Substitute (4.216) in (4.214), we obtain

$$\begin{aligned}\sum_{j_1,j_2,j_3=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\alpha_{j_3}^2}} &\geqslant \frac{n^6}{3n^2} \\ &= \frac{n^4}{3}. \end{aligned} \tag{4.217}$$

By substituting (4.217) in (4.202), we obtain the upper bound of $\langle H_1 \rangle$

$$\begin{aligned}\langle H_1 \rangle &\leqslant -\frac{8e^2}{L}\frac{n^4}{3} \\ &= -\frac{e^2}{6L}k^{4/3} \end{aligned} \tag{4.218}$$

since $k=(2n)^3$.

Substitute (4.218) in (4.161), we obtain

$$\langle \Psi | H | \Psi \rangle \leqslant kT - \frac{e^2}{6L}k^{4/3} + (N-k)\left[T_0 + \frac{e^2(N+k-1)}{D} - \frac{e^2}{\sqrt{3}L_0}\right]. \tag{4.219}$$

Substitute $T$, $T_0$ and $D \geqslant \chi L_0$, where $\chi \geqslant 6$, hence

$$\langle\Psi|H|\Psi\rangle \leqslant \frac{3\pi^2\hbar^2}{8mL^2}k - \frac{e^2}{6L}k^{4/3} + (N-k)\left[\frac{3\pi^2\hbar^2}{8mL_0^2} + \frac{e^2(N+k-1)}{\chi L_0} - \frac{e^2}{\sqrt{3}L_0}\right]$$

$$\equiv B_1(L) + B_2(L_0) \tag{4.220}$$

where

$$B_1(L) = \frac{3\pi^2\hbar^2}{8mL^2}k - \frac{e^2}{6L}k^{4/3}, \tag{4.221}$$

$$B_2(L_0) = (N-k)\left[\frac{3\pi^2\hbar^2}{8mL_0^2} + \frac{e^2(N+k-1)}{\chi L_0} - \frac{e^2}{\sqrt{3}L_0}\right]. \tag{4.222}$$

Optimization of the right-hand side of equation (4.197) over $L$ and $L_0$ :

$$\frac{\partial}{\partial L}\Big(B_1(L) + B_2(L_0)\Big) = \frac{\mathrm{d}B_1(L)}{\mathrm{d}L}$$

$$= (-2)\frac{3\pi^2\hbar^2}{8mL^3}k - (-1)\frac{e^2}{6L^2}k^{4/3} \tag{4.223}$$

then, $L$ is obtained by

$$\frac{\mathrm{d}B_1(L)}{\mathrm{d}L} = 0,$$

$$-\frac{3\pi^2\hbar^2}{4mL^3}k + \frac{e^2}{6L^2}k^{4/3} = 0,$$

$$\frac{e^2k^{4/3}}{6L^2} = \frac{3\pi^2\hbar^2 k}{4mL^3}$$

that is

$$L = \left(\frac{3\pi^2\hbar^2 k}{4m}\right)\left(\frac{6}{e^2k^{4/3}}\right)$$

$$= \frac{9\pi^2\hbar^2}{2me^2}\frac{1}{k^{1/3}}. \tag{4.224}$$

Optimization of the right-hand side of equation (4.197) over $L_0$ is given by

$$\begin{aligned}
\frac{\partial}{\partial L_0}\Big(B_1(L)+B_2(L_0)\Big) &= \frac{\mathrm{d}B_2(L_0)}{\mathrm{d}L_0} \\
&= (N-k)\frac{\mathrm{d}}{\mathrm{d}L_0}\left[\frac{3\pi^2\hbar^2}{8mL_0^2} + \frac{e^2(N+k-1)}{\chi L_0} - \frac{e^2}{\sqrt{3}L_0}\right] \\
&= (N-k)\left[(-2)\frac{3\pi^2\hbar^2}{8mL_0^3} + (-1)\frac{e^2(N+k-1)}{\chi L_0^2} - (-1)\frac{e^2}{\sqrt{3}L_0^2}\right] \\
&= (N-k)\left[(-2)\frac{3\pi^2\hbar^2}{8mL_0^3} - \frac{e^2}{L_0^2}\left(\frac{(N+k-1)}{\chi} - \frac{1}{\sqrt{3}}\right)\right]
\end{aligned} \tag{4.225}$$

then, $L_0$ will be obtained from

$$\frac{\mathrm{d}B_2(L_0)}{\mathrm{d}L_0} = 0,$$

$$\left[-\frac{3\pi^2\hbar^2}{4mL_0^3} + \frac{e^2}{L_0^2}\left(\frac{1}{\sqrt{3}} - \frac{(N+k-1)}{\chi}\right)\right] = 0,$$

$$\frac{3\pi^2\hbar^2}{4mL_0^3} = \frac{e^2}{L_0^2}\left(\frac{1}{\sqrt{3}} - \frac{(N+k-1)}{\chi}\right).$$

Then,

$$L_0 = \frac{3\pi^2\hbar^2}{4me^2}\frac{1}{\left(\frac{1}{\sqrt{3}} - \frac{(N+k-1)}{\chi}\right)}$$

or

$$L_0 = \frac{3\sqrt{3}\pi^2\hbar^2}{2me^2}\frac{1}{\left(2 - \frac{2\sqrt{3}(N+k-1)}{\chi}\right)}. \tag{4.226}$$

Because $L_0 \geqslant L$, then

$$\frac{3\sqrt{3}\pi^2\hbar^2}{2me^2}\frac{1}{\left(2-\dfrac{2\sqrt{3}(N+k-1)}{\chi}\right)} \geqslant \frac{9\pi^2\hbar^2}{2me^2}\frac{1}{k^{1/3}}$$

leads to

$$2-\frac{2\sqrt{3}(N+k-1)}{\chi} \leqslant \frac{\sqrt{3}}{3}k^{1/3}. \tag{4.227}$$

Since $L_0 > 0$, then

$$2-\frac{2\sqrt{3}(N+k-1)}{\chi} > 0 \tag{4.228}$$

then

$$0 < 2-\frac{2\sqrt{3}(N+k-1)}{\chi} \leqslant \frac{\sqrt{3}}{3}k^{1/3} \tag{4.229}$$

and with $k^{1/3} \geqslant 2$, we may choose

$$\chi = 2\sqrt{3}(N+k-1) \tag{4.230}$$

which is obviously larger than 6, giving $L_0 \geqslant L$, where

$$L_0 = \frac{3\sqrt{3}\pi^2\hbar^2}{2me^2}\frac{1}{\left(2-\dfrac{2\sqrt{3}(N+k-1)}{2\sqrt{3}(N+k-1)}\right)}$$
$$= \frac{3\sqrt{3}\pi^2\hbar^2}{2me^2}. \tag{4.231}$$

Substitute (4.231) in (4.222), we obtain

$$B_2(L_0)\big|_{L_0=\frac{3\sqrt{3}\pi^2\hbar^2}{2me^2}} = (N-k)\left[\frac{3\pi^2\hbar^2}{8m}\left(\frac{4m^2e^4}{27\pi^4\hbar^4}\right)\right.$$
$$\left.+\frac{e^2(N+k-1)}{2\sqrt{3}(N+k-1)}\left(\frac{2me^2}{3\sqrt{3}\pi^2\hbar^2}\right)-\frac{e^2}{\sqrt{3}}\left(\frac{2me^2}{3\sqrt{3}\pi^2\hbar^2}\right)\right]$$

$$= (N-k)\left[\frac{me^4}{18\pi^2\hbar^2} + \frac{me^4}{9\pi^2\hbar^2} - \frac{2me^4}{9\pi^2\hbar^2}\right]$$

$$= -(N-k)\frac{me^4}{18\pi^2\hbar^2}. \tag{4.232}$$

Since $(N-k) \geqslant 0$, then

$$B_2(L_0) \leqslant 0. \tag{4.233}$$

Then, the addition of (4.233) and (4.221) leads to

$$\langle\Psi|H|\Psi\rangle \leqslant B_1(L) + B_2(L_0) \leqslant B_1(L)$$

$$= \frac{3\pi^2\hbar^2}{8mL^2}k - \frac{e^2}{6L}k^{4/3}. \tag{4.234}$$

Substitute $L = \left(\frac{9\pi^2\hbar^2}{2me^2}\right)\frac{1}{k^{1/3}}$ in above expression, we obtain

$$\langle\Psi|H|\Psi\rangle \leqslant \frac{3\pi^2\hbar^2 k}{8m}\left(\frac{4m^2e^4}{81\pi^4\hbar^4}\right)k^{2/3} - \frac{k^{4/3}e^2}{6}\left(\frac{2me^2k^{1/3}}{9\pi^2\hbar^2}\right)$$

$$= \left(\frac{me^4}{2\hbar^2}\right)\frac{k^{5/3}}{27\pi^2} - 2\left(\frac{me^4}{2\hbar^2}\right)\frac{k^{5/3}}{27\pi^2}$$

$$= -\left(\frac{me^4}{2\hbar^2}\right)\frac{k^{5/3}}{27\pi^2} \tag{4.235}$$

for *all* $N \geqslant 8$, where we have used the fact that $k = \frac{N}{(1+\varepsilon/n)^3}$. Then

$$k^{5/3} = \frac{N^{5/3}}{\left(1+\frac{\varepsilon}{n}\right)^5}. \tag{4.236}$$

Since $E_{N,N} < \langle\Psi|H|\Psi\rangle$, we substitute (4.236) in (4.235), then we obtain

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{5/3}}{27\pi^2}\frac{1}{\left(1+\frac{\varepsilon}{n}\right)^5}. \tag{4.237}$$

For the rather restrictive case with $\varepsilon = 0$, corresponding to $N = 8n^3$, $n = 1, 2, \ldots$, i.e., for $N = 8, 64, 216, \ldots$, we have

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{5/3}}{27\pi^2}. \tag{4.238}$$

And more interestingly for larger systems, e.g., with $n \geqslant 5000$, i.e., for $N \geqslant 10^{12}$, the term $(1 + \varepsilon/n)^5 \sim 1$. Therefore, the upper bound of such a system is the same as the one given in (4.238).

# CHAPTER V

# $N^2$ LAW FOR BOSONS IN $2D$

## 5.1 Introduction

There has been much interest in recent years in physics in $2D$ (e.g., Geyer, 1995; Bhaduri, Murthy and Srivastava, 1996; Semenoff and Wijewardhana, 1987; Forte, 1992) and the role of the Spin and Statistics Theorem which is tied up to the dimensionality of space (e.g., Forte, 1992). It has thus become important to investigate the nature of matter in $2D$ in the simplest case when the system is not being subjected to stringent constrained statistics. It is equally important to study the nature of such "bosonic matter" to see if the well known instability (implosive character) of such matter in $3D$ (Dyson and Lenard, 1967; Lenard and Dyson, 1968; Lieb, 1979; Manoukian and Muthaporn, 2003) will persist in $2D$ or it will turn it to a stable or even to an explosive phase. To answer such questions, we derive a rigorous upper bound for the ground-state energy $E_{N,N}$ of the system with $N$ negatively charged bosons and $N$ motionless, i.e., fixed $N$ positive charges, with Coulombic interactions. By doing so, in particular, we do not dwell on the fate and dynamics of the positive background which undoubtedly involves complicated dynamics. We obtain an $N^2$ behaviour which is to be compared to the $N^{5/3}$ one of Dyson (Dyson and Lenard, 1967; Lenard and Dyson, 1968; Lieb, 1979; Manoukian and Muthaporn, 2003) in $3D$, implying even a more violent collapse of such a system in $2D$ since the system of $(2N + 2N)$ particles will be favourable over two systems each with $(N+N)$ particles, brought into contact, and the energy release upon collapse will be proportional to $((2N)^2-2(N)^2)$ which will be overwhelmingly large for large $N$, e.g., $N \sim 10^{23}$. Thus the system becomes unstable and stable planar configurations, for example, do not even arise. The present chapter deals with a mathematically rigorous treatment of such a system by deriving an explicit upper bound for the exact ground-state energy $E_{N,N}$.

For $N \geqslant 4$ denoting the number of the negative (or positive) charges, $(N/4)^{1/2}$ being a real number may be written as

$$\left(\frac{N}{4}\right)^{1/2} = n + \varepsilon, \qquad 0 \leqslant \varepsilon < 1 \tag{5.1}$$

In this chapter we prove the following bound.

**Theorem 5.1.1**

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^2}{32\pi^2(1+\varepsilon/n)^4} \tag{5.2}$$

*for all* $N \geqslant 4$*. Here* $m$ *denotes the smallest mass of the negatively charged bosons.*

This is to be compared with the corresponding $N^{5/3}$ law derived in Chapter IV. The investigation carried out in this chapter then raises the serious question: Is instability a characteristic of the dimensionality of space? The answer to this question will be subject matter of our final chapter.

## 5.2 Derivation of Upper Bounds

The Hamiltonian under study is given by

$$H = \sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m} - \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{e^2}{|\mathbf{x}_i - \mathbf{R}_j|} + \sum_{i<j}^{N}\frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} + \sum_{i<j}^{N}\frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{5.3}$$

where the $\mathbf{x}_i$ and $\mathbf{R}_j$ refer, respectively, to the negative and positive charges, and $m$ is taken to be the smallest of the masses of the negative charges.

We introduce an $N$-particle trial function :

$$\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \frac{1}{\sqrt{N!k!}}\sum_{\pi}\phi\left(\mathbf{x}(\pi_1)\right)\ldots\phi\left(\mathbf{x}(\pi_k)\right)\psi_1\left(\mathbf{x}(\pi_{k+1})\right)\ldots\psi_{N-k}\left(\mathbf{x}(\pi_N)\right) \tag{5.4}$$

where $k = 4n^2$ (see (5.1)). The sum is over all permutations $\{\pi_1,\ldots,\pi_N\}$ of $\{1,\ldots,N\}$ such that

$$\int \mathrm{d}^2\mathbf{x}\ \psi_i^*(\mathbf{x})\psi_j(\mathbf{x}) = \delta_{ij}, \quad \int \mathrm{d}^2\mathbf{x}\ \phi^*(\mathbf{x})\psi_j(\mathbf{x}) = 0, \quad \int \mathrm{d}^2\mathbf{x}\ |\phi(\mathbf{x})|^2 = 1. \tag{5.5}$$

For the single-particle trial functions, we take

$$\phi(\mathbf{x}) = \prod_{i=1}^{2}\left(\frac{1}{\sqrt{L}}\cos\left(\frac{\pi x_i}{2L}\right)\right) \equiv \phi_L\left(\mathbf{x}\right), \qquad |x_i| \leqslant L \tag{5.6}$$

and is zero otherwise, and for $j = 1,\ldots,N-k$

$$\psi_j\left(\mathbf{x}\right) = \prod_{i=1}^{2}\left(\frac{1}{\sqrt{L_0}}\cos\left(\frac{\pi\left(x_i - L_{ji}\right)}{2L_0}\right)\right) \equiv \phi_{L_0}\left(\mathbf{x}-\mathbf{L}_j\right), \qquad |x_i - L_{ji}| \leqslant L_0 \tag{5.7}$$

and are zero otherwise, also.

$$\mathbf{L}_j = jD(1,1) \tag{5.8}$$

then

$$|\mathbf{L}_j| = j\sqrt{2}D \tag{5.9}$$

where $D$ is a positive constant. We can see from Fig. 5.1 that

$$|\mathbf{L}_1| = \sqrt{2}D > \sqrt{2}L + \sqrt{2}L_0,$$

$$|\mathbf{L}_2| = 2\sqrt{2}D > \sqrt{2}L + 2\sqrt{2}L_0 + \sqrt{2}L_0 = \sqrt{2}L + 3\sqrt{2}L_0,$$

$$|\mathbf{L}_3| = 3\sqrt{2}D > \sqrt{2}L + 5\sqrt{2}L_0,$$

$$\vdots$$

$$|\mathbf{L}_j| = j\sqrt{2}D > \sqrt{2}L + (2j-1)\sqrt{2}L_0 \tag{5.10}$$

then

$$jD > L + (2j-1)L_0 = (L - L_0) + 2jL_0. \tag{5.11}$$

Since $L_0 \geqslant L$, then

$$L - L_0 \leqslant 0. \tag{5.12}$$

Then (5.10) becomes

$$jD > 2jL_0$$

therefore

$$\frac{D}{2} > L_0. \tag{5.13}$$

Then, from (5.11), we have

$$L \leqslant L_0 < \frac{D}{2}. \tag{5.14}$$

Because $|x_i| \leqslant L$, then

$$-L \leqslant x_i \leqslant L. \tag{5.15}$$

Because $|x_i - L_{ji}| \leqslant L_0$, then

$$-L_0 \leqslant x_i - L_{ji} \leqslant L_0 \tag{5.16}$$

add (5.15) by $L_{ji}$, then we obtain

$$L_{ji} - L_0 \leqslant x_i \leqslant L_{ji} + L_0. \tag{5.17}$$

Because $\mathbf{L}_j = jD(1,1)$, then

$$L_{ji} = jD. \tag{5.18}$$

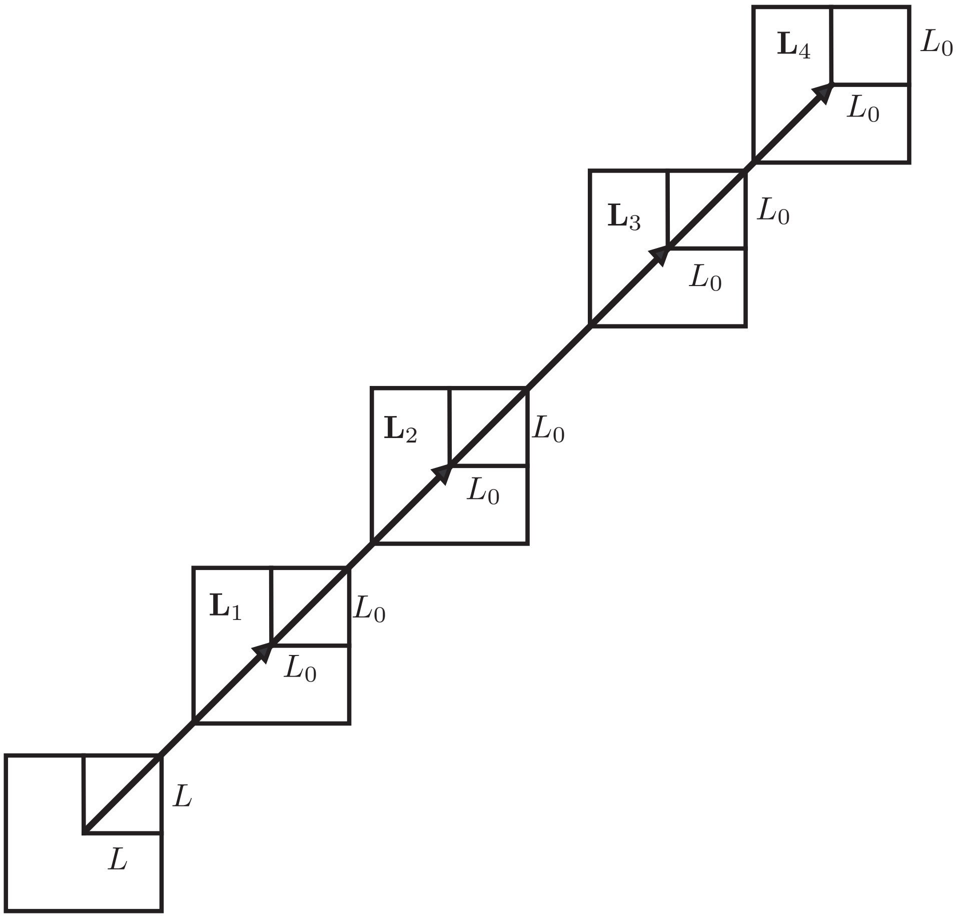


Figure 5.1: The figure displays vectors $\mathbf{L}_1, \ldots, \mathbf{L}_4$

Substitute (5.17) in (5.16), we obtain

$$jD - L_0 \leqslant x_i \leqslant jD + L_0. \tag{5.19}$$

From (5.13), we choose any $D$ that

$$D \geqslant \chi L_0 \tag{5.20}$$

where $\chi > 2$. Therefore, $D$ constrained such that $L \leqslant L_0 \leqslant \dfrac{D}{2}$, and will be optimally chosen later on below Lemma 5.2.1. The intervals $\{-L \leqslant x_i \leqslant L\}$, $\{jD - L_0 \leqslant x_i \leqslant jD + L_0\}$ for $j = 1, \dots, N-k$, $(i = 1, 2)$ are then all disjoint and the functions $\phi(\mathbf{x})$, $\psi_j(\mathbf{x})$ are non-overlapping and automatically satisfy (5.5). Physically, they correspond, respectively, to particles localized in boxes of sides $2L$ and $2L_0$ with the center of the first at the origin of the coordinate system, while the others, of sides $2L_0$, are translated by the vector $\mathbf{L}_j$ from the origin. Such localizations of the particles in these $(N - k + 1)$ boxes make the analysis manageable. The Coulomb interaction being of long range, there are non-trivial interactions between particles in different boxes as well. The key point is that we localize $k = 4n^2$ of the negative particles in the first box. Below, we will also set $k$ of the positive charges in the first box too.

Since $\Psi$ does not necessarily coincide with the ground-state wavefunction, we have for the ground-state energy the upper bound

$$E_{N,N} \leqslant \langle \Psi | H | \Psi \rangle \,. \tag{5.21}$$

The single-particle average kinetic energies are given by

$$T = \frac{\hbar^2}{2m} \int \mathrm{d}^2\mathbf{x} \;\left| \boldsymbol{\nabla} \phi(\mathbf{x}) \right|^2 \tag{5.22}$$

and

$$T_j = \frac{\hbar^2}{2m} \int \mathrm{d}^2\mathbf{x} \; |\boldsymbol{\nabla}\psi_j(\mathbf{x})|^2 \,. \tag{5.23}$$

From (5.6), with $\mathbf{x} = (x_1, x_2)$, we have

$$\phi(\mathbf{x}) = \frac{1}{L} \cos\left(\frac{\pi x_1}{2L}\right) \cos\left(\frac{\pi x_2}{2L}\right)$$

then

$$\begin{aligned} \boldsymbol{\nabla}\phi(\mathbf{x}) &= \frac{1}{L} \left\{ \hat{\mathbf{i}} \frac{\partial}{\partial x_1} \cos\left(\frac{\pi x_1}{2L}\right) \cos\left(\frac{\pi x_2}{2L}\right) \right. \\ &\qquad \left. + \hat{\mathbf{j}} \frac{\partial}{\partial x_2} \cos\left(\frac{\pi x_1}{2L}\right) \cos\left(\frac{\pi x_2}{2L}\right) \right\} \\ &= -\frac{\pi}{2L}\frac{1}{L} \left\{ \hat{\mathbf{i}} \sin\left(\frac{\pi x_1}{2L}\right) \cos\left(\frac{\pi x_2}{2L}\right) \right. \\ &\qquad \left. + \hat{\mathbf{j}} \cos\left(\frac{\pi x_1}{2L}\right) \sin\left(\frac{\pi x_2}{2L}\right) \right\} \end{aligned} \tag{5.24}$$

and

$$\begin{aligned} |\boldsymbol{\nabla}\phi(\mathbf{x})|^2 &= \frac{\pi^2}{4L^4} \left\{ \sin^2\left(\frac{\pi x_1}{2L}\right) \cos^2\left(\frac{\pi x_2}{2L}\right) \right. \\ &\qquad \left. + \cos^2\left(\frac{\pi x_1}{2L}\right) \sin^2\left(\frac{\pi x_2}{2L}\right) \right\}. \end{aligned} \tag{5.25}$$

Multiply (5.25) by $\int \mathrm{d}^2\, \mathbf{x}$, we obtain

$$\begin{aligned} \int \mathrm{d}^2\mathbf{x} \; |\boldsymbol{\nabla}\phi(\mathbf{x})|^2 &= \frac{\pi^2}{4L^4} \left\{ \int_{-L}^{L} \mathrm{d}x_1 \; \sin^2\left(\frac{\pi x_1}{2L}\right) \int_{-L}^{L} \mathrm{d}x_2 \; \cos^2\left(\frac{\pi x_2}{2L}\right) \right. \\ &\qquad \left. + \int_{-L}^{L} \mathrm{d}x_1 \; \cos^2\left(\frac{\pi x_1}{2L}\right) \int_{-L}^{L} \mathrm{d}x_2 \; \sin^2\left(\frac{\pi x_2}{2L}\right) \right\} \\ &= \frac{2\pi^2}{4L^4} \left\{ \int_{-L}^{L} \mathrm{d}x_1 \; \sin^2\left(\frac{\pi x_1}{2L}\right) \int_{-L}^{L} \mathrm{d}x_2 \; \cos^2\left(\frac{\pi x_2}{2L}\right) \right\} \end{aligned}$$

$$= \frac{2\pi^2}{4L^4} L^2$$

$$= \frac{\pi^2}{2L^2} \tag{5.26}$$

then

$$T = \frac{\pi^2 \hbar^2}{4mL^2}. \tag{5.27}$$

Consider

$$\begin{aligned}
\boldsymbol{\nabla}\psi_j(\mathbf{x}) = \frac{1}{L_0} \Bigg\{ &\hat{\mathbf{i}} \frac{\partial}{\partial x_1} \cos\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right) \cos\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right) \\
&+ \hat{\mathbf{j}} \frac{\partial}{\partial x_2} \cos\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right) \cos\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right) \Bigg\} \\
= -\frac{\pi}{2L_0}\frac{1}{L_0} \\
\times \Bigg\{ &\hat{\mathbf{i}} \sin\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right) \cos\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right) \\
&+ \hat{\mathbf{j}} \cos\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right) \sin\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right) \Bigg\}
\end{aligned} \tag{5.28}$$

then

$$\begin{aligned}
|\boldsymbol{\nabla}\psi_j(\mathbf{x})|^2 = \frac{\pi^2}{4L_0^4} \\
\times \Bigg\{ &\sin^2\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right) \cos^2\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right) \\
&+ \cos^2\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right) \sin^2\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right) \Bigg\}.
\end{aligned} \tag{5.29}$$

Let

$$a_i = Lji - L_0, \tag{5.30}$$

$$b_i = L_{ji} + L_0 \tag{5.31}$$

then

$$\begin{aligned}\int \mathrm{d}^2\mathbf{x}\ |\boldsymbol{\nabla}\psi_j(\mathbf{x})|^2 &= \frac{\pi^2}{4L_0^4} \\ &\times \left\{ \int_{a_1}^{b_1} \mathrm{d}x_1\ \sin^2\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right) \int_{a_2}^{b_2} \mathrm{d}x_2\ \cos^2\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right) \right. \\ &\left. + \int_{a_1}^{b_1} \mathrm{d}x_1\ \cos^2\left(\frac{\pi(x_1 - L_{j1})}{2L_0}\right) \int_{a_2}^{b_2} \mathrm{d}x_2\ \sin^2\left(\frac{\pi(x_2 - L_{j2})}{2L_0}\right) \right\}\end{aligned} \tag{5.32}$$

where

$$\int_{a_i}^{b_i} \mathrm{d}x_i\ \sin^2\left(\frac{\pi(x_i - L_{ji})}{2L_0}\right) = L_0, \tag{5.33}$$

$$\int_{a_i}^{b_i} \mathrm{d}x_i\ \cos^2\left(\frac{\pi(x_i - L_{ji})}{2L_0}\right) = L_0. \tag{5.34}$$

Substitute (5.33) and (5.34) in (5.32), then

$$\begin{aligned}\int \mathrm{d}^2\mathbf{x}\ |\boldsymbol{\nabla}\psi_j(\mathbf{x})|^2 &= \frac{\pi^2}{4L_0^5}\left\{L_0^2 + L_0^2\right\} \\ &= \frac{\pi^2}{2L_0^2}.\end{aligned} \tag{5.35}$$

Eq. (5.23) becomes

$$T_j = \frac{\pi^2\hbar^2}{4mL_0^2} \equiv T^0. \tag{5.36}$$

From Chapter IV, we have the total kinetic energy

$$\sum_{j=1}^{N} \frac{\hbar^2}{2m} \int \mathrm{d}^2\mathbf{x}_1 \ldots \mathrm{d}^2\mathbf{x}_N\ \left|\boldsymbol{\nabla}_j\Psi\left(\mathbf{x}_1, \ldots, \mathbf{x}_N\right)\right|^2 = \left[kT + (N-k)\,T^0\right] \tag{5.37}$$

and the expectation value on the right-hand side of (5.21) is given by

$$\langle\Psi|\, H\, |\Psi\rangle = \left[kT + (N-k)\, T^0\right] + \langle V_1\rangle + \langle V_2\rangle + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{5.38}$$

where

$$\langle V_1\rangle = -e^2 \sum_{j=1}^{N} \int \mathrm{d}^2\mathbf{x} \, \left[ \frac{k}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x}) + \left( \sum_{i=1}^{N-k} \frac{1}{|\mathbf{x}+\mathbf{L}_i-\mathbf{R}_j|} \right) \phi_{L_0}^2(\mathbf{x}) \right] \tag{5.39}$$

and

$$\begin{aligned} \langle V_2\rangle = {} & \frac{e^2}{2} k(k-1) \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}' \; \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}') \\ & + e^2 \sum_{j=1}^{N-k} \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}' \; \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_j|} \phi_{L_0}^2(\mathbf{x}') \\ & + e^2 \sum_{i<j}^{N-k} \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}' \; \phi_{L_0}^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|} \phi_{L_0}^2(\mathbf{x}'). \end{aligned} \tag{5.40}$$

We set $\mathbf{R}_{k+j} = \mathbf{L}_j$ and choose the vectors $\mathbf{R}_1, \ldots, \mathbf{R}_k$ to lie within the first box, with center at the origin, thus placing $k$ positive charges in this box. We then establish the following key inequality embodies in the following lemma.

**Lemma 5.2.1**

$$\langle\Psi|\, H\, |\Psi\rangle \leqslant kT + \langle H_1\rangle + (N-k) \left[ T^0 + \frac{e^2(N+k-1)}{D} - \frac{e^2}{\sqrt{2}L_0} \right] \tag{5.41}$$

*where*

$$\begin{aligned} \langle H_1\rangle = -ke^2 \sum_{j=1}^{k} \int \frac{\mathrm{d}^2\mathbf{x}}{|\mathbf{x}-\mathbf{R}_j|} \; \phi_L^2(\mathbf{x}) + \frac{e^2}{2} k(k-1) \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}' \; \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_{L_0}^2(\mathbf{x}') \\ + e^2 \sum_{i<j}^{k} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|}. \end{aligned} \tag{5.42}$$

To derive the above inequality, we note that $\langle V_1\rangle$, defined in (5.39), may be bounded as follows

$$\begin{aligned}\langle V_1\rangle &= -e^2k\sum_{j=1}^{N}\int d^2\mathbf{x}\,\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x})\\ &\quad -e^2\sum_{j=1}^{N}\int d^2\mathbf{x}\,\left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|}+\ldots+\frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\phi_{L_0}^2(\mathbf{x})\\ &= -e^2k\sum_{j=1}^{k}\int d^2\mathbf{x}\,\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x}) - e^2k\sum_{j=k+1}^{N}\int d^2\mathbf{x}\,\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x})\\ &\quad -e^2\sum_{j=1}^{k}\int d^2\mathbf{x}\,\left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|}+\ldots+\frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\phi_{L_0}^2(\mathbf{x})\\ &\quad -e^2\sum_{j=k+1}^{N}\int d^2\mathbf{x}\,\left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|}+\ldots+\frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\phi_{L_0}^2(\mathbf{x}).\end{aligned} \tag{5.43}$$

Since

$$e^2k\sum_{j=k+1}^{N}\int d^2\mathbf{x}\,\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x})\geqslant 0 \tag{5.44a}$$

and

$$e^2\sum_{j=1}^{k}\int d^2\mathbf{x}\,\left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|}+\ldots+\frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\phi_{L_0}^2(\mathbf{x})\geqslant 0 \tag{5.44b}$$

then, by using the sum of inequalities in (5.44), we obtain

$$\begin{aligned}\langle V_1\rangle &\leqslant -e^2k\sum_{j=1}^{k}\int d^2\mathbf{x}\,\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x})\\ &\quad -e^2\sum_{j=k+1}^{N}\int d^2\mathbf{x}\,\left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|}+\ldots+\frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\phi_{L_0}^2(\mathbf{x}).\end{aligned} \tag{5.45}$$

By setting $\mathbf{R}_{k+1} = \mathbf{L}_1, \ldots, \mathbf{R}_N = \mathbf{L}_{N-k}$, then we have

$$\sum_{j=k+1}^{N} \frac{1}{|\mathbf{x} + \mathbf{L}_i - \mathbf{R}_j|} \geqslant \frac{1}{|\mathbf{x}|}. \tag{5.46}$$

Above inequality leads to

$$\begin{aligned} \sum_{j=k+1}^{N} \left( \frac{1}{|\mathbf{x} + \mathbf{L}_1 - \mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x} + \mathbf{L}_{N-k} - \mathbf{R}_j|} \right) &\geqslant \sum_{j=k+1}^{N} \frac{1}{|\mathbf{x}|} \\ &\geqslant \frac{(N-k)}{|\mathbf{x}|}. \end{aligned} \tag{5.47}$$

Then,

$$\begin{aligned} -e^2 \sum_{j=k+1}^{N} \int \mathrm{d}^2\mathbf{x} \, &\left( \frac{1}{|\mathbf{x} + \mathbf{L}_1 - \mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x} + \mathbf{L}_{N-k} - \mathbf{R}_j|} \right) \phi^2_{L_0}(\mathbf{x}) \\ &\leqslant -e^2 \int \mathrm{d}^2\mathbf{x} \, \frac{(N-k)}{|\mathbf{x}|} \phi^2_{L_0}(\mathbf{x}) \\ &= -e^2 (N-k) \int \mathrm{d}^2\mathbf{x} \, \frac{1}{|\mathbf{x}|} \phi^2_{L_0}(\mathbf{x}). \end{aligned} \tag{5.48}$$

Substitute (5.48) in (5.45), we obtain the bound

$$\langle V_1 \rangle \leqslant -e^2 k \sum_{j=1}^{k} \int \mathrm{d}^2\mathbf{x} \, \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi^2_L(\mathbf{x}) - e^2 (N-k) \int \mathrm{d}^2\mathbf{x} \, \frac{1}{|\mathbf{x}|} \phi^2_{L_0}(\mathbf{x}) \tag{5.49}$$

where we have noted the overall negative sign of $\langle V_1 \rangle$, and we have conveniently chosen an upper bound with the summation going up to $k$ instead of up to $N$.

Consider the second integral in $\langle V_1 \rangle$, where $|x_i| \leqslant L_0$:

$$|\mathbf{x}|^2 = x_1^2 + x_2^2 \leqslant L_0^2 + L_0^2,$$

$$|\mathbf{x}|^2 \leqslant 2L_0^2$$

then

$$\frac{1}{|\mathbf{x}|} \geqslant \frac{1}{\sqrt{2}L_0}.$$

Multiply above inequality by $\int \mathrm{d}^2\,\mathbf{x}$, we obtain

$$\int \mathrm{d}^2\mathbf{x}\,\frac{\phi_{L_0}^2(\mathbf{x})}{|\mathbf{x}|} \geqslant \frac{1}{\sqrt{2}L_0}\int \mathrm{d}^2\mathbf{x}\,\phi_{L_0}^2(\mathbf{x})$$

$$= \frac{1}{\sqrt{2}L_0} \tag{5.50}$$

which leads to

$$-e^2(N-k)\int \mathrm{d}^2\mathbf{x}\,\frac{1}{|\mathbf{x}|}\phi_{L_0}^2(\mathbf{x}) \leqslant -\frac{e^2(N-k)}{\sqrt{2}L_0}. \tag{5.51}$$

Then, we obtain

$$\langle V_1\rangle \leqslant -e^2k\sum_{j=1}^{k}\int \mathrm{d}^2\mathbf{x}\,\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x}) - \frac{e^2(N-k)}{\sqrt{2}L_0}. \tag{5.52}$$

Now we use the following bounds,

$$j\sqrt{2}D \geqslant \sqrt{2}D$$

then

$$|\mathbf{L}_j| \geqslant \sqrt{2}D. \tag{5.53}$$

For $i \neq j$, we have

$$\mathbf{L}_i - \mathbf{L}_j = iD(1,1) - jD(1,1)$$

$$= (i-j)D(1,1)$$

then

$$|\mathbf{L}_i - \mathbf{L}_j| \geqslant \sqrt{2}D. \tag{5.54}$$

By considering $\mathbf{x} - \mathbf{x}' - \mathbf{L}_j = (\mathbf{x} - \mathbf{x}') - \mathbf{L}_j$, we have

$$|\mathbf{x} - \mathbf{x}' - \mathbf{L}_j|^2 = |\mathbf{x} - \mathbf{x}'|^2 + |\mathbf{L}_j|^2 - 2(\mathbf{x} - \mathbf{x}') \cdot \mathbf{L}_j$$

then

$$\begin{aligned} |\mathbf{x} - \mathbf{x}' - \mathbf{L}_j|^2 &\geqslant |\mathbf{x} - \mathbf{x}'|^2 + |\mathbf{L}_j|^2 - 2\,|\mathbf{x} - \mathbf{x}'|\,|\mathbf{L}_j| \\ &\geqslant |\mathbf{L}_j|^2 - 2\,|\mathbf{x} - \mathbf{x}'|\,|\mathbf{L}_j| \\ &= |\mathbf{L}_j|^2 \left(1 - 2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_j|}\right). \end{aligned} \tag{5.55}$$

Since $L \leqslant L_0$, then

$$|\mathbf{x} - \mathbf{x}'| \leqslant 2\sqrt{2}L_0,$$

the above inequality leads to

$$|\mathbf{x} - \mathbf{x}' - \mathbf{L}_j| \geqslant |\mathbf{L}_j| \left(1 - 2 \cdot \frac{2\sqrt{2}L_0}{|\mathbf{L}_j|}\right)^{1/2} \tag{5.56}$$

where $|\mathbf{L}_j| \geqslant \sqrt{2}D$, $L_0 \leqslant \dfrac{D}{\chi}$. We may choose $\chi \geqslant 8$, to obtain

$$\frac{L_0}{|\mathbf{L}_j|} \leqslant \frac{1}{8\sqrt{2}}.$$

This leads to

$$|\mathbf{L}_j| \left(1 - 2 \cdot \frac{2\sqrt{2}L_0}{|\mathbf{L}_j|}\right)^{1/2} \geqslant |\mathbf{L}_j| \frac{1}{\sqrt{2}} \geqslant \sqrt{2}D\frac{1}{\sqrt{2}}$$

$$= D. \tag{5.57}$$

Then, we obtain

$$|\mathbf{x} - \mathbf{x}' - \mathbf{L}_j| \geqslant D. \tag{5.58}$$

By considering $|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j|$, we have

$$|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j|^2 = |\mathbf{x} - \mathbf{x}'|^2 + |\mathbf{L}_i - \mathbf{L}_j|^2 - 2(\mathbf{x} - \mathbf{x}') \cdot (\mathbf{L}_i - \mathbf{L}_j)$$

then

$$\begin{aligned} |\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j|^2 &\geqslant |\mathbf{x} - \mathbf{x}'|^2 + |\mathbf{L}_i - \mathbf{L}_j|^2 - 2\,|\mathbf{x} - \mathbf{x}'|\,|\mathbf{L}_i - \mathbf{L}_j| \\ &\geqslant |\mathbf{L}_i - \mathbf{L}_j|^2 - 2\,|\mathbf{x} - \mathbf{x}'|\,|\mathbf{L}_i - \mathbf{L}_j| \\ &= |\mathbf{L}_i - \mathbf{L}_j|^2 \left(1 - 2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_i - \mathbf{L}_j|}\right) \end{aligned} \tag{5.59}$$

or

$$|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j| \geqslant |\mathbf{L}_i - \mathbf{L}_j| \left(1 - 2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_i - \mathbf{L}_j|}\right)^{1/2}. \tag{5.60}$$

Since

$$|\mathbf{x} - \mathbf{x}'| \leqslant 2\sqrt{2}L_0,$$

then

$$|\mathbf{L}_i - \mathbf{L}_j| \left(1 - 2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_i - \mathbf{L}_j|}\right)^{1/2} \geqslant |\mathbf{L}_i - \mathbf{L}_j| \left(1 - 2 \cdot \frac{2\sqrt{2}L_0}{|\mathbf{L}_i - \mathbf{L}_j|}\right)^{1/2}. \tag{5.61}$$

Since $|\mathbf{L}_i - \mathbf{L}_j| \geqslant \sqrt{2}D$ and $L_0 \leqslant \dfrac{D}{8}$, then

$$|\mathbf{L}_i - \mathbf{L}_j| \left(1 - 2 \cdot \frac{2\sqrt{2}L_0}{|\mathbf{L}_i - \mathbf{L}_j|}\right)^{1/2} \geqslant |\mathbf{L}_i - \mathbf{L}_j| \frac{1}{\sqrt{2}}$$

$$\geqslant \sqrt{2}D\frac{1}{\sqrt{2}}$$

$$= D. \tag{5.62}$$

Then, for $i \neq j$,

$$|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j| \geqslant D. \tag{5.63}$$

By using (5.58), we obtain

$$e^2 k \sum_{j=1}^{N-k} \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x} - \mathbf{x}' - \mathbf{L}_j|}\phi_{L_0}^2(\mathbf{x}') \leqslant e^2 k \sum_{j=1}^{N-k} \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \phi_L^2(\mathbf{x})\frac{1}{D}\phi_{L_0}^2(\mathbf{x}')$$

$$= \frac{e^2 k}{D} \sum_{j=1}^{N-k} \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \phi_L^2(\mathbf{x})\,\phi_{L_0}^2(\mathbf{x}')$$

$$= \frac{e^2 k}{D} \sum_{j=1}^{N-k} 1$$

$$= \frac{e^2 k}{D}(N-k) \tag{5.64}$$

and by using (5.63), we obtain

$$e^2 \sum_{i<j}^{N-k} \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \phi_{L_0}^2(\mathbf{x})\frac{1}{|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j|}\phi_{L_0}^2(\mathbf{x}')$$

$$\leqslant e^2 \sum_{i<j}^{N-k} \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \phi_{L_0}^2(\mathbf{x})\frac{1}{D}\phi_{L_0}^2(\mathbf{x}')$$

$$= \frac{e^2}{D} \sum_{i<j}^{N-k} \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \phi_{L_0}^2(\mathbf{x})\phi_{L_0}^2(\mathbf{x}')$$

$$= \frac{e^2}{D} \sum_{i<j}^{N-k} 1 \tag{5.65}$$

where

$$\frac{e^2}{D}\sum_{i<j}^{N-k} 1 = \frac{e^2(N-k)(N-k-1)}{2D}. \tag{5.66}$$

Then

$$e^2\sum_{i<j}^{N-k}\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\;\phi_{L_0}^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|}\phi_{L_0}^2(\mathbf{x}') \leqslant \frac{e^2(N-k)(N-k-1)}{2D}. \tag{5.67}$$

Substitute (5.52) and (5.67) in (5.40), we obtain

$$\begin{aligned}\langle V_2\rangle \leqslant e^2\frac{k(k-1)}{2}\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\;\phi_L^2(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')\\ +\frac{e^2k}{D}(N-k)+\frac{e^2(N-k)(N-k-1)}{2D}.\end{aligned} \tag{5.68}$$

Consider the right-hand side of above inequality, we have

$$\begin{aligned}\frac{e^2k}{D}(N-k)+\frac{e^2(N-k)(N-k-1)}{2D} &= \frac{e^2}{D}(N-k)\left(k+\frac{N-k-1}{2}\right)\\ &= \frac{e^2(N-k)(N+k-1)}{2D}.\end{aligned} \tag{5.69}$$

Then

$$\begin{aligned}\langle V_2\rangle \leqslant e^2\frac{k(k-1)}{2}\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\;\phi_L^2(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')\\ +\frac{e^2(N-k)(N+k-1)}{2D}.\end{aligned} \tag{5.70}$$

Also

$$\sum_{i<j}^{N}\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|} = \sum_{j=2}^{N}\sum_{i=1}^{j-1}\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|}$$

$$= \sum_{j=2}^{k} \sum_{i=1}^{j-1} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} + \sum_{j=k+1}^{N} \sum_{i=1}^{j-1} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|}. \tag{5.71}$$

We set $\mathbf{R}_j = \mathbf{L}_{j-k}$, for $j = k+1, \ldots, N$, then for $j \geqslant k+1$,

$$|\mathbf{R}_j| = |\mathbf{L}_{j-k}| \geqslant \sqrt{2}D. \tag{5.72}$$

And for $j \leqslant k$, we have

$$\begin{aligned} |\mathbf{R}_j| &\leqslant \sqrt{2}L \\ &\leqslant \sqrt{2}\frac{D}{8} < \frac{\sqrt{2}D}{4}. \end{aligned} \tag{5.73}$$

Consider $|\mathbf{R}_i - \mathbf{R}_j|^2$, we have

$$|\mathbf{R}_i - \mathbf{R}_j|^2 = |\mathbf{R}_i|^2 + |\mathbf{R}_j|^2 - 2\mathbf{R}_i \cdot \mathbf{R}_j$$

then

$$\begin{aligned} |\mathbf{R}_i - \mathbf{R}_j|^2 &\geqslant |\mathbf{R}_i|^2 + |\mathbf{R}_j|^2 - 2\,|\mathbf{R}_i|\,|\mathbf{R}_j| \\ &\geqslant |\mathbf{R}_j|^2 - 2\,|\mathbf{R}_i|\,|\mathbf{R}_j| \\ &= |\mathbf{R}_j|^2 \left(1 - 2\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|}\right) \end{aligned} \tag{5.74}$$

then, we obtain

$$|\mathbf{R}_i - \mathbf{R}_j| \geqslant |\mathbf{R}_j| \left(1 - 2\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|}\right)^{1/2}. \tag{5.75}$$

Consider the case of $i = 1, \ldots, k$, $j = k+1, \ldots, N$ with $i < j$, we obtain

$$\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|} \leqslant \frac{1}{4}.$$

The above inequality leads to

$$|\mathbf{R}_j|\left(1-2\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|}\right)^{1/2} \geqslant |\mathbf{R}_j|\left(\frac{1}{2}\right)^{1/2}$$

$$\geqslant \sqrt{2}D\frac{1}{\sqrt{2}}$$

$$= D \tag{5.76}$$

then

$$|\mathbf{R}_i-\mathbf{R}_j| \geqslant D, \quad i=1,\dots,k, \quad j=k+1,\dots,N. \tag{5.77}$$

Consider the case of $i=k+1,\dots,N-1$, $j=k+2,\dots,N$, with $i<j$, we obtain

$$|\mathbf{R}_i-\mathbf{R}_j| = |\mathbf{L}_{i-k}-\mathbf{L}_{j-k}|$$

$$\geqslant \sqrt{2}D$$

$$> D, \tag{5.78}$$

then from (5.77) and (5.78), we have

$$|\mathbf{R}_i-\mathbf{R}_j| \geqslant D \tag{5.79}$$

*for* $j=k+1,\dots,N$, and all $i$ such that $1\leqslant i<j$. Then

$$\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|} \leqslant \frac{1}{D}$$

which leads to

$$\sum_{j=k+1}^{N}\sum_{i=1}^{j-1}\frac{1}{|\mathbf{R}_i-\mathbf{R}_j|}\leqslant\frac{1}{D}\frac{(N-k)(N+k-1)}{2}. \tag{5.80}$$

Substitute (5.80) in (5.71), we obtain

$$\sum_{i<j}^{N}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}\leqslant\sum_{i<j}^{k}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}+\frac{e^2(N-k)(N+k-1)}{2D}. \tag{5.81}$$

Then, by using (5.70), (5.52) and (5.81), we obtain Lemma 5.2.1 as follow.

The expression for the expectation value of $H$ is given by

$$\begin{aligned}\langle\Psi|H|\Psi\rangle &= [kT+(N-k)T_0]+\langle V_1\rangle+\langle V_2\rangle+\sum_{i<j}^{N}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}\\ &\leqslant kT-ke^2\sum_{j=1}^{k}\int \mathrm{d}^2\mathbf{x}\frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x})\\ &\quad+\frac{k(k-1)e^2}{2}\int \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}'\phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')+\sum_{i<j}^{k}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}\\ &\quad+(N-k)T_0+\frac{e^2(N-k)(N+k-1)}{D}-\frac{e^2(N-k)}{\sqrt{2}L_0}\\ &= kT+\langle H_1\rangle+(N-k)\left[T_0+\frac{e^2(N+k-1)}{D}-\frac{e^2}{\sqrt{2}L_0}\right].\end{aligned} \tag{5.82}$$

By rewriting (5.41), that is

$$\langle\Psi|H|\Psi\rangle\leqslant kT+\langle H_1\rangle+(N-k)\left[T_0+\frac{e^2(N+k-1)}{D}-\frac{e^2}{\sqrt{2}L_0}\right]. \tag{5.83}$$

We finally use the following lemma, proved below, which gives an upper bound for $\langle H_1\rangle$ defined in (5.42). □

**Lemma 5.2.2**

$$\langle H_1 \rangle \leqslant -\frac{e^2 k^{3/2}}{8L}. \tag{5.84}$$

Since $k(k-1) < k^2$, then

$$\begin{aligned}\langle H_1 \rangle &< -ke^2 \sum_{j=1}^{k} \int \mathrm{d}^2\mathbf{x} \frac{1}{|\mathbf{x}-\mathbf{R}_j|} \phi_L^2(\mathbf{x}) \\ &\quad + \frac{e^2}{2} k^2 \int \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}' \phi_L^2\left(\mathbf{x}\right) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2\left(\mathbf{x}'\right) + \sum_{i<j}^{k} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \\ &\equiv H_1(k, \mathbf{R})\end{aligned} \tag{5.85}$$

where $\mathbf{R} = \{\mathbf{R}_1, \ldots, \mathbf{R}_k\}$ and

$$\begin{aligned}H_1(k, \mathbf{R}) = &-ke^2 \sum_{j=1}^{k} \int \mathrm{d}^2\mathbf{x} \frac{1}{|\mathbf{x}-\mathbf{R}_j|} \phi_L^2(\mathbf{x}) \\ &+ \frac{e^2}{2} k^2 \int \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}' \phi_L^2\left(\mathbf{x}\right) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2\left(\mathbf{x}'\right) \\ &+ \sum_{i<j}^{k} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|}.\end{aligned} \tag{5.86}$$

We define

$$A_1(k, \mathbf{R}) = -ke^2 \sum_{j=1}^{k} \int \mathrm{d}^2\mathbf{x} \frac{1}{|\mathbf{x}-\mathbf{R}_j|} \phi_L^2(\mathbf{x}), \tag{5.87a}$$

$$A_2(k) = \frac{e^2}{2} k^2 \int \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}' \phi_L^2\left(\mathbf{x}\right) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2\left(\mathbf{x}'\right), \tag{5.87b}$$

$$A_3(k, \mathbf{R}) = \sum_{i<j}^{k} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{5.87c}$$

then

$$H_1(k,\mathbf{R}) = A_1(k,\mathbf{R}) + A_2(k) + A_3(k,\mathbf{R}). \tag{5.88}$$

Therefore, to derive the upper bound of $\langle H_1\rangle$, we partition the interval $[0, L]$ in to $n$ subintervals: $0 = a'_0 < a'_1 < a'_2 < \ldots < a'_n = L$ and we choose $a'_j, a'_{j-1}$ such that

$$\frac{1}{L}\int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i \, \cos^2\left(\frac{\pi x_i}{2L}\right) \equiv \int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i \, g^2(x_i) = \frac{1}{2n} \tag{5.89}$$

where

$$g(x_i) = \frac{1}{\sqrt{L}} \cos\left(\frac{\pi x_i}{2L}\right) \tag{5.90}$$

for $j = 1, \ldots, n$. By doing so, we divide the rectangle of side $2L, 2L$ into $(2n)^2 = 4n^2 = k$ smaller rectangles which labeled $B'(m)$.

Let

$$0 = a'_0 < a'_1 < a'_2 < \cdots < a'_n = L, \tag{5.91}$$

$$\alpha'_j = a'_j - a'_{j-1}, \qquad j = 1, \ldots, n \tag{5.92}$$

where

$$\sum_{j=1}^{n} \alpha'_j = L. \tag{5.93}$$

Let $m = (j_1, j_2)$, then

$$B'(m) \text{ is equivalent to rectangle of sides } \alpha'_{j_1} \times \alpha'_{j_2} \tag{5.94}$$

where we have the normalization condition such that

$$\left(\frac{1}{L}\right)^2 \int_{a'_{j_1-1}}^{a'_{j_1}} \mathrm{d}x_1 \, \cos^2\left(\frac{\pi x_1}{2L}\right) \int_{a'_{j_2-1}}^{a'_{j_2}} \mathrm{d}x_2 \, \cos^2\left(\frac{\pi x_2}{2L}\right)$$

$$= \int_{a'_{j_1-1}}^{a'_{j_1}} \mathrm{d}x_1\, g^2(x_1) \int_{a'_{j_2-1}}^{a'_{j_2}} \mathrm{d}x_2\, g^2(x_2)$$

$$= \int_{B'(m)} \mathrm{d}^2\mathbf{x}\, \phi_L^2(\mathbf{x})$$

$$= \frac{1}{(2n)^2} = \frac{1}{k}. \tag{5.95}$$

Therefore

$$\int \mathrm{d}^2\mathbf{x}\, \phi_L^2(\mathbf{x}) = (2)^2 \sum_{B'(m)=1}^{k/(2)^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x}\, \phi_L^2(\mathbf{x})$$

$$= (2)^2 \sum_{B'(m)=1}^{k/(2)^2} \left(\frac{1}{k}\right)$$

$$= (2)^2 \frac{k}{(2)^2}\frac{1}{k}$$

$$= 1. \tag{5.96}$$

Now we place $\mathbf{R}_1$ in rectangle $B'(m) = 1$, $\mathbf{R}_2$ in rectangle $B'(m) = 2, \ldots, \mathbf{R}_k$ in rectangle $B'(m) = k$, and then we average $H_1(k, \mathbf{R})$ over the positions, $\mathbf{R}_1, \ldots, \mathbf{R}_k$, of the positive particles within the rectangles with a relative weight $\phi_L^2(\mathbf{R}_1), \ldots, \phi_L^2(\mathbf{R}_k)$ in rectangle $B'(m) = 1, \ldots, B'(m) = k$, respectively.

## The Average of $A_1(k, \mathbf{R})$

The term $A_1(k, \mathbf{R})$ may be rewritten as sums of integrals over such rectangles as follows:

$$A_1(k, \mathbf{R}) = -(2)^2 k e^2 \sum_{B'(m)=1}^{k/2^2} \sum_{j=1}^{k/2^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x}\, \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x})$$

$$= -(2)^2 k e^2 \sum_{B'(m)=1}^{n^2} \sum_{j=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x}\ \frac{1}{|\mathbf{x}-\mathbf{R}_j|} \phi_L^2(\mathbf{x})$$

$$= -(2)^2 k e^2 \sum_{B'(m)=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x}\ \phi_L^2(\mathbf{x}) \sum_{j=1}^{n^2} \frac{1}{|\mathbf{x}-\mathbf{R}_j|}. \tag{5.97}$$

Then $\langle A_1(k,\mathbf{R})\rangle$ will be derived below. Since

$$\sum_{j=1}^{n^2} \frac{1}{|\mathbf{x}-\mathbf{R}_j|} = \frac{1}{|\mathbf{x}-\mathbf{R}_1|} + \ldots + \frac{1}{|\mathbf{x}-\mathbf{R}_{n^2}|}$$

then we have

$$\left(\sum_{j=1}^{n^2} \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\right)\Bigg|_{\text{average}} = \frac{\displaystyle\int_{B'(j)=1} \mathrm{d}^2\mathbf{x}'\ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}}{\displaystyle\int_{B'(j)=1} \mathrm{d}^2\mathbf{x}'\ \phi_L^2(\mathbf{x}')} + \ldots + \frac{\displaystyle\int_{B'(j)=n^2} \mathrm{d}^2\mathbf{x}'\ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}}{\displaystyle\int_{B'(j)=n^2} \mathrm{d}^2\mathbf{x}'\ \phi_L^2(\mathbf{x}')}$$

$$= \frac{\displaystyle\int_{B'(j)=1} \mathrm{d}^2\mathbf{x}'\ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}}{\displaystyle\frac{1}{k}} + \ldots + \frac{\displaystyle\int_{B'(j)=n^2} \mathrm{d}^2\mathbf{x}'\ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}}{\displaystyle\frac{1}{k}}$$

$$= k \int_{B'(j)=1} \mathrm{d}^2\mathbf{x}'\ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} + \ldots + k \int_{B'(j)=n^2} \mathrm{d}^2\mathbf{x}'\ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

$$= k \sum_{B'(q)=1}^{n^2} \int_{B'(q)} \mathrm{d}^2\mathbf{x}'\ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \tag{5.98}$$

then

$$\langle A_1(k,\mathbf{R})\rangle = -(2)^2 k e^2 \sum_{B'(m)=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x}\ \phi_L^2(\mathbf{x}) k \sum_{B'(q)=1}^{n^2} \int_{B'(q)} \mathrm{d}^2\mathbf{x}'\ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}$$

$$= -(2)^2 k^2 e^2 \sum_{B'(m)=1}^{n^2} \sum_{B'(q)=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x} \int_{B'(q)} \mathrm{d}^2\mathbf{x}' \; \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}'). \tag{5.99}$$

## The Average of $A_2(k)$

The term $A_2(k)$ may be rewritten as sums of integrals over such rectangles directly as follows:

$$A_2(k) = \frac{e^2}{2} k^2 \int \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}' \; \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}')$$

$$= \frac{(2)^2 e^2}{2} k^2 \sum_{B'(m)=1}^{n^2} \sum_{B'(q)=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x} \int_{B'(q)} \mathrm{d}^2\mathbf{x}' \; \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}'). \tag{5.100}$$

## The Average of $A_3(k, \mathbf{R})$

Since

$$A_3(k, \mathbf{R}) = \frac{1}{2} \sum_{i \neq j}^{k} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} = \frac{(2)^2}{2} \sum_{i \neq j}^{n^2} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{5.101}$$

then we have

$$\left( \sum_{i \neq j}^{n^2} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} \right) \Bigg|_{\text{average over } \mathbf{R}_j}$$

$$= \sum_{i=1}^{n^2} \sum_{j(\neq i)=1}^{n^2} \left( \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} \right) \Bigg|_{\text{average over } \mathbf{R}_j}$$

$$= \sum_{i(\neq j)=1}^{n^2} \left\{ \frac{\displaystyle\int\limits_{B'(j)=1} \mathrm{d}^2\mathbf{x}' \; \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|}}{\displaystyle\int\limits_{B'(j)=1} \mathrm{d}^2\mathbf{x}' \; \phi_L^2(\mathbf{x}')} + \ldots + \frac{\displaystyle\int\limits_{B'(j)=n^2} \mathrm{d}^2\mathbf{x}' \; \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|}}{\displaystyle\int\limits_{B'(j)=n^2} \mathrm{d}^2\mathbf{x}' \; \phi_L^2(\mathbf{x}')} \right\}$$

$$= \sum_{i(\neq j)=1}^{n^2} \left\{ \frac{\displaystyle\int\limits_{B'(j)=1} \mathrm{d}^2\mathbf{x}' \; \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|}}{\dfrac{1}{k}} + \ldots + \frac{\displaystyle\int\limits_{B'(j)=n^2} \mathrm{d}^2\mathbf{x}' \; \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|}}{\dfrac{1}{k}} \right\}$$

$$= \sum_{i(\neq j)=1}^{n^2} \left\{ k \int\limits_{B'(j)=1} \mathrm{d}^2\mathbf{x}' \; \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|} + \ldots + k \int\limits_{B'(j)=n^2} \mathrm{d}^2\mathbf{x}' \; \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|} \right\}$$

$$= k \sum_{i(\neq j)=1}^{n^2} \sum_{B'(j)=1}^{n^2} \int_{B'(j)} \mathrm{d}^2\mathbf{x}' \; \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|}. \tag{5.102}$$

The average of above equation over $\mathbf{R}_i$ is given by

$$\left( \sum_{i\neq j}^{n^2} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} \right)\Bigg|_{\text{average}}$$

$$= k \sum_{B'(j(\neq i))=1}^{n^2} \int_{B'(j)} \mathrm{d}^2\mathbf{x}' \; \phi_L^2(\mathbf{x}') \left\{ \frac{\displaystyle\int\limits_{B'(i)=1} \mathrm{d}^2\mathbf{x} \; \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}}{\displaystyle\int\limits_{B'(i)=1} \mathrm{d}^2\mathbf{x} \; \phi_L^2(\mathbf{x})} + \ldots + \frac{\displaystyle\int\limits_{B'(i)=n^2} \mathrm{d}^2\mathbf{x} \; \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}}{\displaystyle\int\limits_{B'(i)=n^2} \mathrm{d}^2\mathbf{x} \; \phi_L^2(\mathbf{x})} \right\}$$

$$= k \sum_{B'(j(\neq i))=1}^{n^2} \int_{B'(j)} \mathrm{d}^2\mathbf{x}' \; \phi_L^2(\mathbf{x}') \left\{ \frac{\displaystyle\int\limits_{B'(i)=1} \mathrm{d}^2\mathbf{x} \; \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}}{\dfrac{1}{k}} + \ldots + \frac{\displaystyle\int\limits_{B'(i)=n^2} \mathrm{d}^2\mathbf{x} \; \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}}{\dfrac{1}{k}} \right\}$$

$$= k \sum_{B'(j(\neq i))=1}^{n^2} \int_{B'(j)} \mathrm{d}^2\mathbf{x}' \; \phi_L^2(\mathbf{x}') \sum_{B'(i)=1}^{n^2} k \int_{B'(i)} \mathrm{d}^2\mathbf{x} \; \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}$$

$$= k^2 \sum_{B'(m)=1}^{n^2} \sum_{B'(q(\neq m))=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x} \int_{B'(q)} \mathrm{d}^2\mathbf{x}' \ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}'). \tag{5.103}$$

Then we obtain the average of $A_3(k, \mathbf{R})$ as follows:

$$\langle A_3(k, \mathbf{R}) \rangle = \frac{(2)^2}{2} e^2 k^2 \sum_{B'(m)=1}^{n^2} \sum_{B'(q(\neq m))=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x} \int_{B'(q)} \mathrm{d}^2\mathbf{x}' \ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}'). \tag{5.104}$$

The average of $H_1(k, \mathbf{R})$ is given by

$$\begin{aligned}
\langle H_1(k, \mathbf{R}) \rangle &= \langle A_1(k, \mathbf{R}) \rangle + A_2(k) + \langle A_3(k, \mathbf{R}) \rangle \\
&= -(2)^2 k^2 e^2 \sum_{B'(m)=1}^{n^2} \sum_{B'(q)=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x} \int_{B'(q)} \mathrm{d}^2\mathbf{x}' \ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}') \\
&\quad + \frac{(2)^2 e^2}{2} k^2 \sum_{B'(m)=1}^{n^2} \sum_{B'(q)=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x} \int_{B'(q)} \mathrm{d}^2\mathbf{x}' \ \phi_L^2 (\mathbf{x}) \ \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2 (\mathbf{x}') \\
&\quad + \frac{(2)^2}{2} e^2 k^2 \sum_{B'(m)=1}^{n^2} \sum_{B'(q(\neq m))=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x} \int_{B'(q)} \mathrm{d}^2\mathbf{x}' \ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}') \\
&= -(2)^2 \ k^2 \frac{e^2}{2} \sum_{B'(m)=1}^{n^2} \sum_{B'(q)=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x} \int_{B'(q)} \mathrm{d}^2\mathbf{x}' \ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}') \\
&\quad + (2)^2 \ k^2 \frac{e^2}{2} \sum_{B'(m)=1}^{n^2} \sum_{B'(q(\neq m))=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x} \int_{B'(q)} \mathrm{d}^2\mathbf{x}' \ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}') \\
&= -(2)^2 \ \frac{e^2 k^2}{2} \sum_{B'(m)=1}^{n^2} \sum_{B'(q)=1}^{n^2} \int_{B'(m)} \mathrm{d}^2\mathbf{x} \int_{B'(q)} \mathrm{d}^2\mathbf{x}' \ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}') \delta_{mq}.
\end{aligned} \tag{5.105}$$

Eq. (5.105) may be rewritten as

$$\langle H_1(k,\mathbf{R})\rangle = -(2)^2\,\frac{e^2k^2}{2}\sum_{B'(m)=1}^{n^2}\int_{B'(m)} \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}'\;\phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}'). \tag{5.106}$$

By the definition of an *average*, there must be at least one set of $\mathbf{R}$ such that

$$H_1(k,\mathbf{R}) \leqslant \langle H_1(k,\mathbf{R})\rangle\,. \tag{5.107}$$

Then, we obtain

$$\langle H_1\rangle \leqslant -(2)^2\,\frac{e^2k^2}{2}\sum_{B'(m)=1}^{n^2}\int_{B'(m)} \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}'\;\phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}'). \tag{5.108}$$

We may scale $\mathbf{x}$ to $\dfrac{\mathbf{x}}{L} \equiv \mathbf{u}$ , then

$$\frac{1}{L}\int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i\;\cos^2\left(\frac{\pi x_i}{2L}\right) = \int_{a'_{j-1}/L}^{a'_j/L} \mathrm{d}\left(\frac{x_i}{L}\right)\;\cos^2\left[\frac{\pi}{2}\left(\frac{x_i}{L}\right)\right] \tag{5.109}$$

then we obtain

$$\frac{1}{L}\int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i\;\cos^2\left(\frac{\pi x_i}{2L}\right) = \int_{a_{j-1}}^{a_j} \mathrm{d}u_i\;\cos^2\left(\frac{\pi u_i}{2}\right) = \frac{1}{2n} \tag{5.110}$$

or

$$\int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i\;g^2(x_i) = \int_{a_{j-1}}^{a_j} \mathrm{d}u_i\;g_1^2(u_i) = \frac{1}{2n} \tag{5.111}$$

where

$$g_1(u_i) = \cos\left(\frac{\pi u_i}{2}\right). \tag{5.112}$$

For

$$0 = \frac{a'_0}{L} < \frac{a'_1}{L} < \frac{a'_2}{L} < \cdots < \frac{a'_n}{L} = 1$$

then

$$0 = a_0 < a_1 < a_2 < \cdots < a_n = 1, \tag{5.113}$$

$$\alpha_j = a_j - a_{j-1}, \qquad j = 1, \ldots, n, \tag{5.114}$$

where

$$\sum_{j=1}^{n} \alpha_j = 1. \tag{5.115}$$

Let

$$B(m) \equiv \text{ a rectangle of sides } \alpha_{j_1} \times \alpha_{j_2}. \tag{5.116}$$

Therefore, we have the normalization condition such that

$$\begin{aligned}\int_{a_{j_1-1}}^{a_{j_1}} \mathrm{d}u_1 \, g_1^2(u_1) \int_{a_{j_2-1}}^{a_{j_2}} \mathrm{d}u_2 \, g_1^2(u_2) &= \int\limits_{B(m)} \mathrm{d}^2\mathbf{u} \, \phi_1^2(\mathbf{u}) \\ &= \frac{1}{(2n)^2} = \frac{1}{k}\end{aligned} \tag{5.117}$$

where

$$\phi_1(\mathbf{x}) = \prod_{i=1}^{2} \cos\left(\frac{\pi x_i}{2}\right), \qquad |x_i| \leqslant 1. \tag{5.118}$$

Then, we rewrite the integral on the right-hand side of (5.108) as below

$$\begin{aligned}&\sum_{B'(m)=1}^{n^2} \int\limits_{B'(m)} \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}' \, \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}') \\ &\quad = \sum_{B(m)=1}^{n^2} \int\limits_{B(m)} \mathrm{d}^2\mathbf{u}\mathrm{d}^2\mathbf{u}' \, \phi_1^2(\mathbf{u}) \frac{1}{|L\mathbf{u}-L\mathbf{u}'|} \phi_1^2(\mathbf{u}') \\ &\quad = \frac{1}{L} \sum_{B(m)=1}^{n^2} \int\limits_{B(m)} \mathrm{d}^2\mathbf{u}\mathrm{d}^2\mathbf{u}' \, \phi_1^2(\mathbf{u}) \frac{1}{|\mathbf{u}-\mathbf{u}'|} \phi_1^2(\mathbf{u}')\end{aligned} \tag{5.119}$$

where $0 \leqslant u_i \leqslant 1$. Substitute (5.119) in (5.108), we obtain

$$\langle H_1 \rangle \leqslant -(2)^2 \, \frac{e^2 k^2}{2L} \sum_{B(m)=1}^{n^2} \int_{B(m)} \mathrm{d}^2\mathbf{x} \, \mathrm{d}^2\mathbf{x}' \; \phi_1^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_1^2(\mathbf{x}') \tag{5.120}$$

where $0 \leqslant x_i \leqslant 1$.

Since $\mathbf{x}$ and $\mathbf{x}'$ lie in rectangle $B(m)$ of the length $\alpha_{j_1} \times \alpha_{j_2}$. Then the maximum magnitude of $|\mathbf{x}-\mathbf{x}'|$ is the diagonal line in $B(m)$ of length $\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}$,

$$|\mathbf{x}-\mathbf{x}'| \leqslant \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2} \tag{5.121}$$

or

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} \geqslant \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}}. \tag{5.122}$$

Let $m = (j_1, j_2)$, then

$$\sum_{B(m)=1}^{n^2} = \sum_{j_1=1}^{n} \sum_{j_2=1}^{n}. \tag{5.123}$$

By using (5.122), we have

$$\begin{aligned}
\langle H_1 \rangle &\leqslant -(2)^2 \, \frac{e^2 k^2}{2L} \sum_{B(m)=1}^{n^2} \int_{B(m)} \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}' \; \phi_1^2(\mathbf{x}) \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \phi_1^2(\mathbf{x}') \\
&= -(2)^2 \, \frac{e^2 k^2}{2L} \sum_{j_1=1}^{n} \sum_{j_2=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \int_{B(j_1,j_2)} \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}' \; \phi_1^2(\mathbf{x}) \phi_1^2(\mathbf{x}') \\
&= -(2)^2 \, \frac{e^2 k^2}{2L} \sum_{j_1=1}^{n} \sum_{j_2=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \int_{B(j_1,j_2)} \mathrm{d}^2\mathbf{x} \; \phi_1^2(\mathbf{x}) \int_{B(j_1,j_2)} \mathrm{d}^2\mathbf{x}' \; \phi_1^2(\mathbf{x}') \\
&= -(2)^2 \, \frac{e^2 k^2}{2L} \sum_{j_1=1}^{n} \sum_{j_2=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \left(\frac{1}{k}\right) \left(\frac{1}{k}\right)
\end{aligned}$$

$$= -(2)^2 \, \frac{e^2}{2L} \sum_{j_1=1}^{n} \sum_{j_2=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}}. \tag{5.124}$$

We define $f(\alpha_{j_1})$ as

$$f(\alpha_{j_1}) = \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}. \tag{5.125}$$

Since $\sum_{j_1=1}^{n} 1 = n$, then

$$\sum_{j_1=1}^{n} \left( \sqrt{f(\alpha_{j_1})} \frac{1}{f(\alpha_{j_1})} \right) = n. \tag{5.126}$$

From Cauchy-Schwarz inequality,

$$\left( \sum_{i=1}^{n} a_i b_i \right)^2 \leqslant \sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2$$

we have

$$\left( \sum_{j_1=1}^{n} \sqrt{f(\alpha_{j_1})} \frac{1}{f(\alpha_{j_1})} \right)^2 \leqslant \sum_{j_1=1}^{n} f(\alpha_{j_1}) \sum_{j_1=1}^{n} \frac{1}{f(\alpha_{j_1})}$$

or

$$\sum_{j_1=1}^{n} \frac{1}{f(\alpha_{j_1})} \geqslant \frac{n^2}{\sum_{j_1=1}^{n} f(\alpha_{j_1})}. \tag{5.127}$$

Substitute $f(\alpha_{j_1})$ in above inequality, we obtain

$$\sum_{j_1=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \geqslant \frac{n^2}{\sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}}. \tag{5.128}$$

Multiply above inequality by $\sum_{j_2=1}^{n}$, we obtain

$$\sum_{j_2=1}^{n} \sum_{j_1=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \geqslant \sum_{j_2=1}^{n} \frac{n^2}{\sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}}$$

$$= n^2 \sum_{j_2=1}^{n} \frac{1}{\sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}}. \tag{5.129}$$

Let

$$f(\alpha_{j_2}) = \frac{1}{\sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}}. \tag{5.130}$$

From Cauchy-Schwarz inequality, we have

$$\sum_{j_2=1}^{n} \frac{1}{f(\alpha_{j_2})} \geqslant \frac{n^2}{\sum_{j_2=1}^{n} f(\alpha_{j_2})}$$

then

$$\sum_{j_2=1}^{n} f(\alpha_{j_2}) \geqslant \frac{n^2}{\sum_{j_2=1}^{n} \frac{1}{f(\alpha_{j_2})}}. \tag{5.131}$$

Substitute $f(\alpha_{j_2})$ in above inequality, we obtain

$$\sum_{j_2=1}^{n} \frac{1}{\sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \geqslant \frac{n^2}{\sum_{j_2=1}^{n} \frac{1}{\frac{1}{\sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}}}}$$

$$= \frac{n^2}{\sum_{j_2=1}^{n} \sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}}. \tag{5.132}$$

Substitute (5.132) in (5.129), we obtain

$$\sum_{j_2=1}^{n} \sum_{j_1=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \geqslant \frac{n^4}{\sum_{j_2=1}^{n} \sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \tag{5.133}$$

where $\sum_{j_1=1}^{n} \alpha_{j_1} = 1$, $\sum_{j_2=1}^{n} \alpha_{j_2} = 1$. We have

$$(\alpha_{j_1} + \alpha_{j_2})^2 = \alpha_{j_1}^2 + \alpha_{j_2}^2 + 2\alpha_{j_1}\alpha_{j_2} \geqslant \alpha_{j_1}^2 + \alpha_{j_2}^2$$

then

$$\alpha_{j_1} + \alpha_{j_2} \geqslant \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}.$$

Multiply above inequality by $\sum_{j_1=1}^{n}$, we obtain

$$\sum_{j_1=1}^{n} (\alpha_{j_1} + \alpha_{j_2}) \geqslant \sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}$$

or

$$\left( \sum_{j_1=1}^{n} \alpha_{j_1} + \sum_{j_1=1}^{n} \alpha_{j_2} \right) \geqslant \sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}$$

then

$$(1 + n\alpha_{j_2}) \geqslant \sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}. \tag{5.134}$$

Multiply above inequality by $\sum_{j_2=1}^{n}$, we obtain

$$\sum_{j_2=1}^{n} (1 + n\alpha_{j_2}) \geqslant \sum_{j_2=1}^{n} \sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2},$$

$$\left( \sum_{j_2=1}^{n} 1 + n \sum_{j_2=1}^{n} \alpha_{j_2} \right) \geqslant \sum_{j_2=1}^{n} \sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2},$$

$$(n + n) \geqslant \sum_{j_2=1}^{n} \sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}.$$

We obtain the bound

$$\sum_{j_2=1}^{n} \sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2} \leqslant 2n \tag{5.135}$$

or

$$\frac{1}{\sum_{j_1,j_2=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \geqslant \frac{1}{2n}.$$

Then, we obtain

$$\frac{n^4}{\sum_{j_1,j_2=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \geqslant \frac{n^4}{2n}. \tag{5.136}$$

Substitute above inequality in (5.129), we obtain

$$\sum_{j_2=1}^{n} \sum_{j_1=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2}} \geqslant \frac{n^4}{2n} = \frac{n^3}{2}. \tag{5.137}$$

This above inequality leads to

$$\langle H_1 \rangle \leqslant -(2)^2 \, \frac{e^2}{2L} \frac{n^3}{2} = -\frac{e^2 n^3}{L}. \tag{5.138}$$

For $k = (2n)^2$, we obtain

$$n^3 = \frac{k^{3/2}}{2^3} = \frac{k^{2/3}}{8}. \tag{5.139}$$

Then, Lemma 5.2.2 follows

$$\langle H_1 \rangle \leqslant -\frac{e^2 k^{3/2}}{8L}. \tag{5.140}$$

□

This inequality then leads to

$$\langle \Psi | H | \Psi \rangle \leqslant kT - \frac{e^2 k^{3/2}}{8L} + (N-k) \left[ T_0 + \frac{e^2(N+k-1)}{D} - \frac{e^2}{\sqrt{2} L_0} \right]. \tag{5.141}$$

Substitute $T$, $T_0$ and $D \geqslant \chi L_0$, where $\chi \geqslant 8$

$$\langle \Psi | H | \Psi \rangle \leqslant \frac{\pi^2 \hbar^2}{4mL^2} k - \frac{e^2 k^{3/2}}{8L} + (N-k) \left[ \frac{\pi^2 \hbar^2}{4mL_0^2} + \frac{e^2(N+k-1)}{\chi L_0} - \frac{e^2}{\sqrt{2} L_0} \right]$$

$$\equiv B_1(L) + B_2(L_0) \tag{5.142}$$

where

$$B_1(L) = \frac{\pi^2\hbar^2}{4mL^2}k - \frac{e^2k^{3/2}}{8L}, \tag{5.143}$$

$$B_2(L_0) = (N-k)\left[\frac{\pi^2\hbar^2}{4mL_0^2} + \frac{e^2(N+k-1)}{\chi L_0} - \frac{e^2}{\sqrt{2}L_0}\right]. \tag{5.144}$$

Optimization of the right-hand side of equation (5.142) over $L$ and $L_0$ :

$$\begin{aligned}\frac{\partial}{\partial L}\Big(B_1(L) + B_2(L_0)\Big) &= \frac{\mathrm{d}B_1(L)}{\mathrm{d}L} \\ &= (-2)\frac{\pi^2\hbar^2}{4mL^3}k - (-1)\frac{k^{3/2}e^2}{8L^2} \\ &= -\frac{\pi^2\hbar^2 k}{2mL^3} + \frac{k^{3/2}e^2}{8L^2}\end{aligned} \tag{5.145}$$

then $L$ will be obtained below

$$\frac{\mathrm{d}B_1(L)}{\mathrm{d}L} = 0,$$

$$-\frac{\pi^2\hbar^2 k}{2mL^3} + \frac{k^{3/2}e^2}{8L^2} = 0$$

then

$$\begin{aligned}L &= \left(\frac{\pi^2\hbar^2 k}{2m}\right)\left(\frac{8}{e^2k^{3/2}}\right) \\ &= \frac{4\pi^2\hbar^2}{me^2k^{1/2}}.\end{aligned} \tag{5.146}$$

Optimization of the right-hand side of equation (5.142) over $L_0$ is given by

$$
\begin{aligned}
\frac{\partial}{\partial L_0}\Big(B_1(L)+B_2(L_0)\Big) &= \frac{\mathrm{d}B_2(L_0)}{\mathrm{d}L_0} \\
&= (N-k)\frac{\mathrm{d}}{\mathrm{d}L_0}\left[\frac{\pi^2\hbar^2}{4mL_0^2}+\frac{e^2(N+k-1)}{\chi L_0}-\frac{e^2}{\sqrt{2}L_0}\right] \\
&= (N-k)\left[-\frac{\pi^2\hbar^2}{2mL_0^3}-\frac{e^2(N+k-1)}{\chi L_0^2}+\frac{e^2}{\sqrt{2}L_0^2}\right] \\
&= (N-k)\left[-\frac{\pi^2\hbar^2}{2mL_0^3}+\frac{e^2}{L_0^2}\left(\frac{1}{\sqrt{2}}-\frac{(N+k-1)}{\chi}\right)\right]
\end{aligned}
\tag{5.147}
$$

then $L_0$ will be obtained below

$$
\begin{aligned}
\frac{\mathrm{d}B_2(L_0)}{\mathrm{d}L_0} &= 0, \\
-\frac{\pi^2\hbar^2}{2mL_0^3}+\frac{e^2}{L_0^2}\left(\frac{1}{\sqrt{2}}-\frac{(N+k-1)}{\chi}\right) &= 0, \\
\frac{e^2}{L_0^2}\left(\frac{1}{\sqrt{2}}-\frac{(N+k-1)}{\chi}\right) &= \frac{\pi^2\hbar^2}{2mL_0^3}
\end{aligned}
$$

then

$$
\begin{aligned}
L_0 &= \frac{\pi^2\hbar^2}{2m}\frac{1}{e^2\left(\dfrac{1}{\sqrt{2}}-\dfrac{(N+k-1)}{\chi}\right)} \\
&= \frac{2\sqrt{2}\pi^2\hbar^2}{me^2 4}\frac{1}{\left(1-\dfrac{\sqrt{2}(N+k-1)}{\chi}\right)}.
\end{aligned}
\tag{5.148}
$$

Because $L_0 \geqslant L$ then

$$\frac{2\sqrt{2}\pi^2\hbar^2}{me^2 4}\frac{1}{\left(1-\dfrac{\sqrt{2}(N+k-1)}{\chi}\right)} \geqslant \frac{4\pi^2\hbar^2}{me^2 k^{1/2}},$$

$$4\left(1-\frac{\sqrt{2}(N+k-1)}{\chi}\right) \leqslant \frac{\sqrt{2}k^{1/2}}{2}. \tag{5.149}$$

For $L_0 > 0$, then

$$\frac{2\sqrt{2}\pi^2\hbar^2}{me^2 4}\frac{1}{\left(1-\dfrac{\sqrt{2}(N+k-1)}{\chi}\right)} > 0, \qquad \text{then}$$

$$1-\frac{\sqrt{2}(N+k-1)}{\chi} > 0. \tag{5.150}$$

Then we obtain

$$0 < 4\left(1-\frac{\sqrt{2}(N+k-1)}{\chi}\right) \leqslant \frac{\sqrt{2}k^{1/2}}{2}. \tag{5.151}$$

We choose $\chi = \dfrac{4\sqrt{2}}{3}(N+k-1) \geqslant 8$, we obtain $L_0$

$$\begin{aligned} L_0 &= \frac{2\sqrt{2}\pi^2\hbar^2}{me^2 4}\frac{1}{\left(1-\dfrac{\sqrt{2}(N+k-1)}{\dfrac{4\sqrt{2}}{3}(N+k-1)}\right)} \\ &= \frac{2\sqrt{2}\pi^2\hbar^2}{me^2 4}\frac{1}{\left(1-\dfrac{3}{4}\right)} \\ &= \frac{2\sqrt{2}\pi^2\hbar^2}{me^2} \end{aligned} \tag{5.152}$$

and

$$
\begin{aligned}
&B_2(L_0)\big|_{L_0=\frac{2\sqrt{2}\pi^2\hbar^2}{me^2}} \\
&= (N-k)\left[\frac{\pi^2\hbar^2}{4m}\left(\frac{m^2e^4}{8\pi^4\hbar^4}\right)+\frac{3e^2(N+k-1)}{4\sqrt{2}(N+k-1)}\left(\frac{me^2}{2\sqrt{2}\pi^2\hbar^2}\right)\right. \\
&\qquad\qquad \left.-\frac{e^2}{\sqrt{2}}\left(\frac{me^2}{2\sqrt{2}\pi^2\hbar^2}\right)\right] \\
&= (N-k)\left[\frac{me^4}{32\pi^2\hbar^2}+\frac{3me^4}{16\pi^2\hbar^2}-\frac{me^4}{4\pi^2\hbar^2}\right] \\
&= (N-k)\frac{me^4}{2\hbar^2}\frac{1}{16\pi^2}\left[1+6-8\right] \\
&= -(N-k)\frac{me^4}{2\hbar^2}\frac{1}{16\pi^2}.
\end{aligned} \tag{5.153}
$$

Since $(N-k)\geqslant 0$, then

$$
B_2(L_0)\leqslant 0. \tag{5.154}
$$

Add above inequality by $B_1(L)$, then

$$
\begin{aligned}
B_1(L)+B_2(L_0) &\leqslant B_1(L) \\
&= \frac{\pi^2\hbar^2}{4mL^2}k-\frac{e^2k^{3/2}}{8L}.
\end{aligned} \tag{5.155}
$$

Substitute $L=\dfrac{4\pi^2\hbar^2}{me^2k^{1/2}}$ in above inequality, then

$$
\begin{aligned}
B_1(L) &\leqslant \frac{\pi^2\hbar^2k}{4m}\left(\frac{m^2e^4k}{16\pi^4\hbar^4}\right)-\frac{e^2k^{3/2}}{8}\left(\frac{me^2k^{1/2}}{4\pi^2\hbar^2}\right) \\
&= \frac{me^4}{2\pi^2\hbar^2}\left(\frac{k^2}{32}\right)-\frac{me^4}{2\pi^2\hbar^2}\left(\frac{k^2}{16}\right)
\end{aligned}
$$

$$= \frac{me^4}{2\hbar^2}\left(\frac{k^2}{32\pi^2}\right)(1-2)$$

$$= -\left(\frac{me^4}{2\hbar^2}\right)\frac{k^2}{32\pi^2} \tag{5.156}$$

which leads to

$$\langle\Psi|H|\Psi\rangle \leqslant -\left(\frac{me^4}{2\hbar^2}\right)\frac{k^2}{32\pi^2}. \tag{5.157}$$

Since we have

$$k^2 = \frac{N^2}{\left(1+\dfrac{\varepsilon}{n}\right)^4} \tag{5.158}$$

then, for $E_{N,N} < \langle\Psi|H|\Psi\rangle$, we obtain the upper bound

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^2}{32\pi^2\left(1+\dfrac{\varepsilon}{n}\right)^4} \tag{5.159}$$

for *all* $N \geqslant 4$, where we have used the fact that $k = N(1+\varepsilon/n)^{-2} = 4n^2$. Since $(1+\varepsilon/n) < 2$, we also have the conservative bound

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^2}{512\pi^2}$$

for all $N \geqslant 4$.

For large bosonic systems, e.g., for $n \geqslant 50$, i.e., for $N \geqslant 10^4$,

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^2}{36\pi^2}.$$

# CHAPTER VI

# INSTABILITY OF "BOSONIC MATTER" IN ALL DIMENSIONS

## 6.1 Introduction

In this final chapter, we will answer the question raised at the end of the introduction to the last chapter: Is instability of "bosonic matter" a characteristic of the dimensionality of space? We will prove that instability is not a characteristic of the dimensionality of space and that such systems are unstable in all dimensions. We have been seriously concerned with this question since the beginning of this project and have succeeded in answering the above question. We were able to derive an explicit upper bound for the exact $E_{N,N}$ in all dimensions $\nu$

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{(2+\nu)/\nu}}{16\pi^2\nu^3(2)^\nu} \tag{6.1}$$

for all $N \geqslant (2)^\nu$, where $m$ is the smallest of the masses of the $N$ negatively charged bosons. Thus we conclude, in particular, that the instability of such matter is not a characteristic of the dimensionality of space. For example, no stable planar configurations may be formed corresponding to $\nu = 2$. There has been much interest in recent years in the physics of arbitrary dimensions (Geyer, 1995; Bhaduri, Murthy and Srivastava, 1996; Semenoff and Wijewardhana, 1987; Forte, 1992) and the role of the Spin and Statistics Theorem in such dimensions. It is well known that the latter is tied up (Geyer, 1995) to the dimensionality of space and we learn that such a system not being subjected to stringent constrained statistics is necessarily unstable in all dimensions. It is also an important theoretical question to investigate if the change of the dimensionality of space will change such matter from, e.g., an "implosive" to a "stable" or to an "explosive" phase. The present work shows that this does not happen. (Some of present field theories speculate that at early stages of the universe the dimensionality of space was not necessarily 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 of the universe.) The potentials considered are the $1/r$ type, and we do not dwell on the fate and the dynamics of the positive charges which, undoubtedly, involve complicated interactions, and instability is established down to and above the nuclear level. Also since both signs of the charges are involved in this work, the analysis becomes more involved than one dealing with one sign of the charges only (Hall, 2000). Needless to say, if for some $\nu$, $E_{N,N}$ goes to minus infinity, then (6.1) is automatically satisfied.

## 6.2 Derivation of Upper Bounds

The Hamiltonian under study is given by

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} - \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{R}_j|} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{6.2}$$

the $\mathbf{x}_i$, $\mathbf{R}_j$ refer to the negative and positive charges, respectively. Quite generally, we may write for any $N \geqslant (2)^\nu$,

$$\left(\frac{N}{2^\nu}\right)^{1/\nu} = n + \varepsilon \tag{6.3}$$

then

$$N = 2^\nu (n + \varepsilon)^\nu$$

$$= (2n)^\nu \left(1 + \frac{\varepsilon}{n}\right)^\nu < (2n)^\nu (2)^\nu, \qquad (2n)^\nu \equiv k. \tag{6.4}$$

where $0 \leqslant \varepsilon < 1$, $n = 1, 2, \ldots$. We introduce an $N$-particle trial function

$$\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \frac{1}{\sqrt{N!k!}} \sum_\pi \phi\left(\mathbf{x}(\pi_1)\right) \ldots \phi\left(\mathbf{x}(\pi_k)\right) \psi_1\left(\mathbf{x}(\pi_{k+1})\right) \ldots \psi_{N-k}\left(\mathbf{x}(\pi_N)\right) \tag{6.5}$$

with the sum over all permutations $\{\pi_1, \ldots, \pi_N\}$ of $\{1, \ldots, N\}$, such that $\phi(\mathbf{x})$, $\psi_j(\mathbf{x})$ are pairwise orthonormal,

$$\int \mathrm{d}^\nu\mathbf{x}\ \psi_i^*(\mathbf{x})\psi_j(\mathbf{x}) = \delta_{ij}, \quad \int \mathrm{d}^\nu\mathbf{x}\ \phi^*(\mathbf{x})\psi_j(\mathbf{x}) = 0, \quad \int \mathrm{d}^\nu\mathbf{x}\ |\phi(\mathbf{x})|^2 = 1. \tag{6.6}$$

For the single-particle trial functions, we take

$$\phi(\mathbf{x}) = \prod_{i=1}^{\nu} \left(\frac{1}{\sqrt{L}} \cos\left(\frac{\pi x_i}{2L}\right)\right) \equiv \phi_L\left(\mathbf{x}\right), \qquad |x_i| \leqslant L \tag{6.7}$$

and is zero otherwise, and for $j = 1, \ldots, N - k$

$$\psi_j\left(\mathbf{x}\right) = \prod_{i=1}^{\nu} \left(\frac{1}{\sqrt{L_0}} \cos\left(\frac{\pi\left(x_i - L_{ji}\right)}{2L_0}\right)\right) \equiv \phi_{L_0}\left(\mathbf{x} - \mathbf{L}_j\right), \qquad |x_i - L_{ji}| \leqslant L_0 \tag{6.8}$$

and are zero otherwise. Let

$$\mathbf{L}_j = jD_0(1, 1, \ldots, 1) \tag{6.9}$$

then

$$|\mathbf{L}_j| = jD_0\sqrt{1^2 + 1^2 + \ldots + 1^2} = j\sqrt{\nu}D_0. \tag{6.10}$$

We have

$$|\mathbf{L}_1| = \sqrt{\nu}D_0 > \sqrt{\nu}L + \sqrt{\nu}L_0,$$

$$
\begin{aligned}
|\mathbf{L}_2| &= 2\sqrt{\nu}D_0 > \sqrt{\nu}L + 2\sqrt{\nu}L_0 + \sqrt{\nu}L_0 = \sqrt{\nu}L + 3\sqrt{\nu}L_0,\\
|\mathbf{L}_3| &= 3\sqrt{\nu}D_0 > \sqrt{\nu}L + 5\sqrt{\nu}L_0,\\
&\vdots\\
|\mathbf{L}_j| &= j\sqrt{\nu}D_0 > \sqrt{\nu}L + (2j-1)\sqrt{\nu}L_0.
\end{aligned} \tag{6.11}
$$

Then,

$$jD_0 > L + (2j-1)L_0 = (L - L_0) + 2jL_0.$$

Since $L_0 \geqslant L$, then

$$L - L_0 \leqslant 0.$$

We obtain

$$jD_0 > 2jL_0,$$

$$\frac{D_0}{2} > L_0.$$

We have

$$L \leqslant L_0 < \frac{D_0}{2}. \tag{6.12}$$

Because $|x_i| \leqslant L$, then

$$-L \leqslant x_i \leqslant L. \tag{6.13}$$

Because $|x_i - L_{ji}| \leqslant L_0$, then

$$-L_0 \leqslant x_i - L_{ji} \leqslant L_0,$$

$$L_{ji} - L_0 \leqslant x_i \leqslant L_{ji} + L_0. \tag{6.14}$$

Because $\mathbf{L}_j = jD_0(1, 1, \ldots, 1)$, then

$$L_{ji} = jD_0. \tag{6.15}$$

Then substitute (6.15) to (6.14), we obtain

$$jD_0 - L_0 \leqslant x_i \leqslant jD_0 + L_0. \tag{6.16}$$

From $\dfrac{D_0}{2} > L_0 \geqslant L$, we can choose any $D_0$ that

$$D_0 \geqslant \chi L_0 \tag{6.17}$$

where $\chi > 2$.

Let

$$T = \frac{\hbar^2}{2m} \int \mathrm{d}^\nu \mathbf{x}\ \left|\boldsymbol{\nabla}\phi(\mathbf{x})\right|^2, \tag{6.18}$$

and

$$T_j = \frac{\hbar^2}{2m} \int \mathrm{d}^\nu \mathbf{x}\ \left|\boldsymbol{\nabla}\psi_j(\mathbf{x})\right|^2. \tag{6.19}$$

The elementary computation gives

$$\int \mathrm{d}^\nu \mathbf{x}\ \left|\boldsymbol{\nabla}\phi(\mathbf{x})\right|^2 = \frac{\nu\pi^2}{4L^2}. \tag{6.20}$$

Substitute (6.20) to (6.18), we obtain

$$T = \frac{\nu\pi^2\hbar^2}{8mL^2}. \tag{6.21}$$

Also, we have

$$\begin{aligned}\int \mathrm{d}^\nu \mathbf{x}\ \left|\boldsymbol{\nabla}\psi_j(\mathbf{x})\right|^2 &= \nu \left(\frac{\pi}{2L_0}\right)^2 \left(\frac{1}{L_0}\right)^\nu (L_0)^\nu \\ &= \frac{\nu\pi^2}{4\,(L_0)^2}.\end{aligned} \tag{6.22}$$

Substitute (6.22) in (6.19) we obtain

$$T_j = \frac{\hbar^2}{2m}\frac{\nu\pi^2}{4\left(L_0\right)^2}$$

$$= \frac{\nu\pi^2\hbar^2}{8m\left(L_0\right)^2} \equiv T^0 \tag{6.23}$$

and we use the results from Chapter V, to obtain

$$\frac{\hbar^2}{2m}\sum_{i=1}^{N}\int \mathrm{d}^\nu \mathbf{x}(\pi_1)\ldots \mathrm{d}^\nu \mathbf{x}(\pi_N)\ \left|\boldsymbol{\nabla}_i \Psi\right|^2$$

$$= \frac{N!}{\sqrt{N!k!}}\frac{k!}{\sqrt{N!k!}}\sum_{i=1}^{N}\left\{\sum_{\ell=1}^{k} T\delta_{i\ell} + \sum_{\ell=k+1}^{N} T_0\delta_{i\ell}\right\}$$

$$= kT + (N-k)T_0, \tag{6.24}$$

$$-\left\langle \Psi \left| \sum_{j=1}^{N}\sum_{i=1}^{N}\frac{e^2}{|\mathbf{x}_i - \mathbf{R}_j|}\right| \Psi \right\rangle = -e^2 k \sum_{j=1}^{N}\int \mathrm{d}^\nu \mathbf{x}\ \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x})$$

$$- e^2 \sum_{j=1}^{N}\sum_{i=1}^{N-k}\int \mathrm{d}^\nu \mathbf{x}\ \frac{1}{|\mathbf{x}+\mathbf{L}_i-\mathbf{R}_j|}\phi_{L_0}^2(\mathbf{x})$$

$$\equiv \left\langle V_1 \right\rangle, \tag{6.25}$$

$$\left\langle \Psi \left| \sum_{i<j}^{N}\frac{e^2}{|\mathbf{x}_i-\mathbf{x}_j|}\right| \Psi \right\rangle = e^2 \sum_{j=2}^{N}\sum_{i=1}^{j-1}\left\langle \Psi \left| \frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}\right| \Psi \right\rangle$$

$$= e^2\frac{k(k-1)}{2}\int \mathrm{d}^\nu \mathbf{x}\, \mathrm{d}^\nu \mathbf{x}'\ \phi_L^2\left(\mathbf{x}\right)\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2\left(\mathbf{x}'\right)$$

$$+\, e^2 k \sum_{j=1}^{N-k} \int \mathrm{d}^\nu \mathbf{x}\, \mathrm{d}^\nu \mathbf{x}'\ \phi_L^2\,(\mathbf{x})\, \frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_j|} \phi_{L_0}^2(\mathbf{x}')$$

$$+\, e^2 \sum_{i<j}^{N-k} \int \mathrm{d}^\nu \mathbf{x}\, \mathrm{d}^\nu \mathbf{x}'\ \phi_{L_0}^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|} \phi_{L_0}^2(\mathbf{x}')$$

$$\equiv \langle V_2 \rangle\,, \tag{6.26}$$

and

$$\left\langle \Psi \left| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|} \right| \Psi \right\rangle = \left\langle \Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) \left| \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|} \right| \Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) \right\rangle$$

$$= \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|} \left\langle \Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) \,|\, \Psi(\mathbf{x}_1,\ldots,\mathbf{x}_N) \right\rangle$$

$$= \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}. \tag{6.27}$$

From (6.24), (6.25), (6.26) and (6.27) we obtain the expectation value of the Hamiltonian

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

$$+ \sum_{i<j}^{N} \left\langle \Psi \left| \frac{e^2}{|\mathbf{x}_i-\mathbf{x}_j|} \right| \Psi \right\rangle + \sum_{i<j}^{N} \left\langle \Psi \left| \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|} \right| \Psi \right\rangle$$

$$= [kT + (N-k)T_0] + \langle V_1 \rangle + \langle V_2 \rangle + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}. \tag{6.28}$$

The upper bound of $\langle V_1 \rangle$ will be derived below. Then, from (6.25), we obtain

$$\begin{aligned}
\langle V_1\rangle &= -e^2 k \sum_{j=1}^{N} \int \mathrm{d}^\nu \mathbf{x}\, \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x}) \\
&\quad - e^2 \sum_{j=1}^{N} \int \mathrm{d}^\nu \mathbf{x}\, \left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\phi_{L_0}^2(\mathbf{x}) \\
&= -e^2 k \sum_{j=1}^{k} \int \mathrm{d}^\nu \mathbf{x}\, \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x}) - e^2 k \sum_{j=k+1}^{N} \int \mathrm{d}^\nu \mathbf{x}\, \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x}) \\
&\quad - e^2 \sum_{j=1}^{k} \int \mathrm{d}^\nu \mathbf{x}\, \left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\phi_{L_0}^2(\mathbf{x}) \\
&\quad - e^2 \sum_{j=k+1}^{N} \int \mathrm{d}^\nu \mathbf{x}\, \left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\phi_{L_0}^2(\mathbf{x}).
\end{aligned} \tag{6.29}$$

Since

$$e^2 k \sum_{j=k+1}^{N} \int \mathrm{d}^\nu \mathbf{x}\, \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x}) \geqslant 0 \tag{6.30a}$$

and

$$e^2 \sum_{j=1}^{k} \int \mathrm{d}^\nu \mathbf{x}\, \left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\phi_{L_0}^2(\mathbf{x}) \geqslant 0 \tag{6.30b}$$

then, by using (6.30), Eq. (6.29) becomes

$$\begin{aligned}
\langle V_1\rangle &\leqslant -e^2 k \sum_{j=1}^{k} \int \mathrm{d}^\nu \mathbf{x}\, \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x}) \\
&\quad - e^2 \sum_{j=k+1}^{N} \int \mathrm{d}^\nu \mathbf{x}\, \left(\frac{1}{|\mathbf{x}+\mathbf{L}_1-\mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x}+\mathbf{L}_{N-k}-\mathbf{R}_j|}\right)\phi_{L_0}^2(\mathbf{x}).
\end{aligned} \tag{6.31}$$

For $i = 1, \ldots, N-k$, we set $\mathbf{R}_{k+1} = \mathbf{L}_1$, $\mathbf{R}_{k+2} = \mathbf{L}_2, \ldots, \mathbf{R}_{k+j} = \mathbf{L}_j$. We obtain the bound

$$\sum_{j=k+1}^{N} \frac{1}{|\mathbf{x} + \mathbf{L}_i - \mathbf{R}_j|} \geqslant \frac{1}{|\mathbf{x}|}. \tag{6.32}$$

Eq. (6.32) leads to

$$\sum_{j=k+1}^{N} \left( \frac{1}{|\mathbf{x} + \mathbf{L}_1 - \mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x} + \mathbf{L}_{N-k} - \mathbf{R}_j|} \right) \geqslant \sum_{j=k+1}^{N} \frac{1}{|\mathbf{x}|}$$

$$= \frac{(N-k)}{|\mathbf{x}|}. \tag{6.33}$$

Substitute (6.33) in the second term of (6.31), we obtain

$$-e^2 \sum_{j=k+1}^{N} \int \mathrm{d}^\nu \mathbf{x} \left( \frac{1}{|\mathbf{x} + \mathbf{L}_1 - \mathbf{R}_j|} + \ldots + \frac{1}{|\mathbf{x} + \mathbf{L}_{N-k} - \mathbf{R}_j|} \right) \phi_{L_0}^2(\mathbf{x})$$

$$\leqslant -e^2 \int \mathrm{d}^\nu \mathbf{x} \, \frac{(N-k)}{|\mathbf{x}|} \phi_{L_0}^2(\mathbf{x})$$

$$= -e^2 (N-k) \int \mathrm{d}^\nu \mathbf{x} \, \frac{1}{|\mathbf{x}|} \phi_{L_0}^2(\mathbf{x}). \tag{6.34}$$

Then, substitute (6.34) in (6.31), we obtain

$$\langle V_1 \rangle \leqslant -e^2 k \sum_{j=1}^{k} \int \mathrm{d}^\nu \mathbf{x} \, \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x}) - e^2 (N-k) \int \mathrm{d}^\nu \mathbf{x} \, \frac{1}{|\mathbf{x}|} \phi_{L_0}^2(\mathbf{x}). \tag{6.35}$$

Consider the second integral in $\langle V_1 \rangle$, where $|x_i| \leqslant L_0$:

$$|\mathbf{x}|^2 = x_1^2 + \ldots + x_\nu^2 \leqslant L_0^2 + \ldots + L_0^2$$

then

$$|\mathbf{x}| \leqslant \sqrt{\nu} L_0 \tag{6.36}$$

or

$$\frac{1}{|\mathbf{x}|} \geqslant \frac{1}{\sqrt{\nu}L_0}.$$

Multiply above inequality by $\int \mathrm{d}^\nu \mathbf{x}\, \phi_{L_0}^2(\mathbf{x})$, we obtain

$$\int \mathrm{d}^\nu \mathbf{x}\, \frac{\phi_{L_0}^2(\mathbf{x})}{|\mathbf{x}|} \geqslant \frac{1}{\sqrt{\nu}L_0} \int \mathrm{d}^\nu \mathbf{x}\, \phi_{L_0}^2(\mathbf{x})$$

$$= \frac{1}{\sqrt{\nu}L_0}. \tag{6.37}$$

Multiply above inequality by $-e^2(N-k)$, we obtain

$$-e^2(N-k) \int \mathrm{d}^\nu \mathbf{x}\, \frac{1}{|\mathbf{x}|} \phi_{L_0}^2(\mathbf{x}) \leqslant -\frac{e^2(N-k)}{\sqrt{\nu}L_0}. \tag{6.38}$$

Substitute (6.38) in (6.35), we obtain

$$\langle V_1 \rangle \leqslant -e^2 k \sum_{j=1}^{k} \int \mathrm{d}^\nu \mathbf{x}\, \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x}) - \frac{e^2(N-k)}{\sqrt{\nu}L_0}. \tag{6.39}$$

The upper bound of $\langle V_2 \rangle$ will be derived below. For $j \geqslant 1$, $|\mathbf{L}_j| = j\sqrt{\nu}D_0$, we have

$$|\mathbf{L}_j| \geqslant \sqrt{\nu}D_0 \tag{6.40}$$

and for $i \neq j$, we have

$$\mathbf{L}_i - \mathbf{L}_j = iD_0(1,1,\ldots,1) - jD_0(1,1,\ldots,1)$$

$$= (i-j)D_0(1,1,\ldots,1),$$

$$|\mathbf{L}_i - \mathbf{L}_j| = \sqrt{(i-j)^2}\sqrt{\nu}D_0$$

$$\geqslant \sqrt{\nu}D_0. \tag{6.41}$$

Consider $\mathbf{x}-\mathbf{x}'-\mathbf{L}_j=(\mathbf{x}-\mathbf{x}')-\mathbf{L}_j$, we obtain

$$|\mathbf{x}-\mathbf{x}'-\mathbf{L}_j|^2=|\mathbf{x}-\mathbf{x}'|^2+|\mathbf{L}_j|^2-2(\mathbf{x}-\mathbf{x}')\cdot\mathbf{L}_j$$

then

$$\begin{aligned}|\mathbf{x}-\mathbf{x}'-\mathbf{L}_j|^2 &\geqslant |\mathbf{x}-\mathbf{x}'|^2+|\mathbf{L}_j|^2-2\,|\mathbf{x}-\mathbf{x}'|\,|\mathbf{L}_j| \\ &\geqslant |\mathbf{L}_j|^2-2\,|\mathbf{x}-\mathbf{x}'|\,|\mathbf{L}_j| \\ &= |\mathbf{L}_j|^2\left(1-2\frac{|\mathbf{x}-\mathbf{x}'|}{|\mathbf{L}_j|}\right). \end{aligned} \tag{6.42}$$

We consider $|\mathbf{x}-\mathbf{x}'|$ in (6.42), for $L\leqslant L_0$, we have

$$|\mathbf{x}-\mathbf{x}'|\leqslant 2\sqrt{\nu}L_0.$$

Substitute above inequality in (6.42), we obtain

$$2\frac{|\mathbf{x}-\mathbf{x}'|}{|\mathbf{L}_j|}\leqslant 2\cdot\frac{2\sqrt{\nu}L_0}{|\mathbf{L}_j|}.$$

The above inequality leads to

$$|\mathbf{L}_j|^2\left(1-2\frac{|\mathbf{x}-\mathbf{x}'|}{|\mathbf{L}_j|}\right)\geqslant |\mathbf{L}_j|^2\left(1-2\cdot\frac{2\sqrt{\nu}L_0}{|\mathbf{L}_j|}\right). \tag{6.43}$$

Then, from (6.42) and (6.43), we obtain

$$|\mathbf{x}-\mathbf{x}'-\mathbf{L}_j|\geqslant |\mathbf{L}_j|\left(1-2\cdot\frac{2\sqrt{\nu}L_0}{|\mathbf{L}_j|}\right)^{1/2}. \tag{6.44}$$

From (6.40), we have $|\mathbf{L}_j|\geqslant\sqrt{\nu}D_0$ and from (6.17), we have $L_0\leqslant\dfrac{D_0}{\chi}$ where

$\chi > 2$, these equations leads to

$$\frac{L_0}{|\mathbf{L}_j|} \leqslant \frac{1}{\chi\sqrt{\nu}}$$

which gives

$$\begin{aligned} |\mathbf{L}_j| \left(1 - 2 \cdot \frac{2\sqrt{\nu}L_0}{|\mathbf{L}_j|}\right)^{1/2} &\geqslant |\mathbf{L}_j| \left(1 - \frac{4}{\chi}\right)^{1/2} \\ &\geqslant \sqrt{\nu} D_0 \left(1 - \frac{4}{\chi}\right)^{1/2} \\ &\geqslant D_0. \end{aligned} \tag{6.45}$$

Compare (6.45) with (6.44), we obtain

$$|\mathbf{x} - \mathbf{x}' - \mathbf{L}_j| \geqslant D_0. \tag{6.46}$$

Consider $|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j|$, we have

$$|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j|^2 = |\mathbf{x} - \mathbf{x}'|^2 + |\mathbf{L}_i - \mathbf{L}_j|^2 - 2(\mathbf{x} - \mathbf{x}') \cdot (\mathbf{L}_i - \mathbf{L}_j)$$

then

$$|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j|^2 \geqslant |\mathbf{x} - \mathbf{x}'|^2 + |\mathbf{L}_i - \mathbf{L}_j|^2 - 2\,|\mathbf{x} - \mathbf{x}'|\,|\mathbf{L}_i - \mathbf{L}_j|\,.$$

This leads to

$$|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j| \geqslant |\mathbf{L}_i - \mathbf{L}_j| \left(1 - 2\frac{|\mathbf{x} - \mathbf{x}'|}{|\mathbf{L}_i - \mathbf{L}_j|}\right)^{1/2} \tag{6.47}$$

where

$$|\mathbf{x} - \mathbf{x}'| \leqslant 2\sqrt{\nu}L_0.$$

Then,

$$2\frac{|\mathbf{x}-\mathbf{x}'|}{|\mathbf{L}_i-\mathbf{L}_j|} \leqslant 2\cdot\frac{2\sqrt{\nu}L_0}{|\mathbf{L}_i-\mathbf{L}_j|}$$

which gives

$$|\mathbf{L}_i-\mathbf{L}_j|\left(1-2\frac{|\mathbf{x}-\mathbf{x}'|}{|\mathbf{L}_i-\mathbf{L}_j|}\right)^{1/2} \geqslant |\mathbf{L}_i-\mathbf{L}_j|\left(1-2\cdot\frac{2\sqrt{\nu}L_0}{|\mathbf{L}_i-\mathbf{L}_j|}\right)^{1/2}. \tag{6.48}$$

From (6.41), we have $|\mathbf{L}_i-\mathbf{L}_j| \geqslant \sqrt{\nu}D_0$, and for $L_0 \leqslant \dfrac{D_0}{\chi}$, then

$$\frac{L_0}{|\mathbf{L}_i-\mathbf{L}_j|} \leqslant \frac{1}{\chi\sqrt{\nu}}.$$

This inequality leads to

$$\begin{aligned}|\mathbf{L}_i-\mathbf{L}_j|\left(1-2\cdot\frac{2\sqrt{\nu}L_0}{|\mathbf{L}_i-\mathbf{L}_j|}\right)^{1/2} &\geqslant |\mathbf{L}_i-\mathbf{L}_j|\left(1-\frac{4}{\chi}\right)^{1/2}\\ &\geqslant \sqrt{\nu}D_0\left(1-\frac{4}{\chi}\right)^{1/2}\\ &\geqslant D_0.\end{aligned} \tag{6.49}$$

Compare (6.49) with (6.48), we obtain

$$|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j| \geqslant D_0. \tag{6.50}$$

From (6.46), we have $|\mathbf{x}-\mathbf{x}'-\mathbf{L}_j| \geqslant D_0$, then

$$\frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_j|} \leqslant \frac{1}{D_0}.$$

Multiply above inequality by $\phi_L^2(\mathbf{x})\,\phi_{L_0}^2(\mathbf{x}')$, we obtain

$$\phi_L^2(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_j|}\phi_{L_0}^2(\mathbf{x}') \leqslant \phi_L^2(\mathbf{x})\,\frac{1}{D_0}\phi_{L_0}^2(\mathbf{x}').$$

Multiply above inequality by $e^2k\sum_{j=1}^{N-k}\int \mathrm{d}^\nu\mathbf{x}\,\mathrm{d}^\nu\mathbf{x}'$ we obtain

$$\begin{aligned}
e^2k\sum_{j=1}^{N-k}\int \mathrm{d}^\nu\mathbf{x}\,\mathrm{d}^\nu\mathbf{x}'\;\phi_L^2\left(\mathbf{x}\right)\frac{1}{|\mathbf{x}-\mathbf{x}'-\mathbf{L}_j|}\phi_{L_0}^2(\mathbf{x}')
&\leqslant e^2k\sum_{j=1}^{N-k}\int \mathrm{d}^\nu\mathbf{x}\,\mathrm{d}^\nu\mathbf{x}'\;\phi_L^2\left(\mathbf{x}\right)\frac{1}{D_0}\phi_{L_0}^2(\mathbf{x}')\\
&= \frac{e^2k}{D_0}\sum_{j=1}^{N-k}\int \mathrm{d}^\nu\mathbf{x}\,\mathrm{d}^\nu\mathbf{x}'\;\phi_L^2\left(\mathbf{x}\right)\phi_{L_0}^2(\mathbf{x}')\\
&= \frac{e^2k}{D_0}\sum_{j=1}^{N-k}1\\
&= \frac{e^2k}{D_0}(N-k). \qquad (6.51)
\end{aligned}$$

From (6.50), we have $|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|\geqslant D_0$, then

$$\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|}\leqslant\frac{1}{D_0}.$$

Multiply above inequality by $\phi_L^2\left(\mathbf{x}\right)\phi_{L_0}^2(\mathbf{x}')$, we obtain

$$\phi_{L_0}^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|}\phi_{L_0}^2(\mathbf{x}')\leqslant\phi_{L_0}^2(\mathbf{x})\frac{1}{D_0}\phi_{L_0}^2(\mathbf{x}').$$

Multiply above inequality by $e^2k\sum_{i<j}^{N-k}\int \mathrm{d}^\nu\mathbf{x}\mathrm{d}^\nu\mathbf{x}'$, we obtain

$$\begin{aligned}
e^2\sum_{i<j}^{N-k}\int \mathrm{d}^\nu\mathbf{x}\,\mathrm{d}^\nu\mathbf{x}'\;\phi_{L_0}^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'+\mathbf{L}_i-\mathbf{L}_j|}\phi_{L_0}^2(\mathbf{x}')
&\leqslant e^2\sum_{i<j}^{N-k}\int \mathrm{d}^\nu\mathbf{x}\,\mathrm{d}^\nu\mathbf{x}'\;\phi_{L_0}^2(\mathbf{x})\frac{1}{D_0}\phi_{L_0}^2(\mathbf{x}')
\end{aligned}$$

$$= \frac{e^2}{D_0} \sum_{i<j}^{N-k} \int \mathrm{d}^\nu \mathbf{x}\, \mathrm{d}^\nu \mathbf{x}'\ \phi_{L_0}^2(\mathbf{x}) \phi_{L_0}^2(\mathbf{x}')$$

$$= \frac{e^2}{D_0} \sum_{i<j}^{N-k} 1 \tag{6.52}$$

where

$$\frac{e^2}{D_0} \sum_{i<j}^{N-k} 1 = \frac{e^2(N-k)(N-k-1)}{2D_0}. \tag{6.53}$$

Then, (6.52) becomes

$$e^2 \sum_{i<j}^{N-k} \int \mathrm{d}^\nu \mathbf{x}\, \mathrm{d}^\nu \mathbf{x}'\ \phi_{L_0}^2(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}' + \mathbf{L}_i - \mathbf{L}_j|} \phi_{L_0}^2(\mathbf{x}') \leqslant \frac{e^2(N-k)(N-k-1)}{2D_0}. \tag{6.54}$$

From (6.51), (6.54) and (6.129), we obtain the upper bound of $\langle V_2 \rangle$

$$\langle V_2 \rangle \leqslant e^2 \frac{k(k-1)}{2} \int \mathrm{d}^\nu \mathbf{x}\, \mathrm{d}^\nu \mathbf{x}'\ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \phi_L^2(\mathbf{x}')$$

$$+ \frac{e^2 k}{D_0}(N-k) + \frac{e^2(N-k)(N-k-1)}{2D_0} \tag{6.55}$$

where the sum of the latter two terms on the right-hand side of (6.55) is given by

$$\frac{e^2 k}{D_0}(N-k) + \frac{e^2(N-k)(N-k-1)}{2D_0} = \frac{e^2}{D_0}(N-k)\left(k + \frac{N-k-1}{2}\right)$$

$$= \frac{e^2(N-k)(N+k-1)}{2D_0}. \tag{6.56}$$

Substitute (6.56) in (6.55), we obtain

$$\langle V_2 \rangle \leqslant e^2 \frac{k(k-1)}{2} \int \mathrm{d}^\nu \mathbf{x} \mathrm{d}^\nu \mathbf{x}' \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \phi_L^2(\mathbf{x}')$$

$$+ \frac{e^2(N-k)(N+k-1)}{2D_0}. \tag{6.57}$$

Consider the interaction term of positive charged particles,

$$\sum_{i<j}^{N} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} = \sum_{j=2}^{N}\sum_{i=1}^{j-1} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|}$$

$$= \sum_{j=2}^{k}\sum_{i=1}^{j-1} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} + \sum_{j=k+1}^{N}\sum_{i=1}^{j-1} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|}. \tag{6.58}$$

We set $\mathbf{R}_j = \mathbf{L}_{j-k}$, for $j = k+1, \ldots, N$, then for $j \geqslant k+1$,

$$|\mathbf{R}_j| = |\mathbf{L}_{j-k}| \geqslant \sqrt{\nu} D_0. \tag{6.59}$$

For $j \leqslant k$, and from (6.17) we obtain

$$|\mathbf{R}_j| \leqslant \sqrt{\nu} L$$

$$\leqslant \sqrt{\nu} \frac{D_0}{\chi}. \tag{6.60}$$

Since $|\mathbf{R}_i - \mathbf{R}_j|^2 = |\mathbf{R}_i|^2 + |\mathbf{R}_j|^2 - 2\mathbf{R}_i \cdot \mathbf{R}_j$, then

$$|\mathbf{R}_i - \mathbf{R}_j|^2 \geqslant |\mathbf{R}_i|^2 + |\mathbf{R}_j|^2 - 2\,|\mathbf{R}_i|\,|\mathbf{R}_j|$$

$$\geqslant |\mathbf{R}_j|^2 - 2\,|\mathbf{R}_i|\,|\mathbf{R}_j|$$

$$= |\mathbf{R}_j|^2 \left(1 - 2\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|}\right) \tag{6.61}$$

or

$$|\mathbf{R}_i - \mathbf{R}_j| \geqslant |\mathbf{R}_j| \left(1 - 2\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|}\right)^{1/2}. \tag{6.62}$$

**1. Consider the case of** $i = 1, \ldots, k,\ j = k+1, \ldots, N,\ i < j$.

We have

$$\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|} \leqslant \frac{\sqrt{\nu}L}{\sqrt{\nu}D_0} \leqslant \frac{D_0}{\chi}\frac{1}{D_0}.$$

The above inequality leads to

$$\begin{aligned} |\mathbf{R}_j|\left(1 - 2\frac{|\mathbf{R}_i|}{|\mathbf{R}_j|}\right)^{1/2} &\geqslant |\mathbf{R}_j|\left(1 - \frac{2}{\chi}\right)^{1/2} \\ &\geqslant \sqrt{\nu}D_0\left(1 - \frac{2}{\chi}\right)^{1/2} \\ &\geqslant D_0. \end{aligned} \tag{6.63}$$

Then compare (6.63) with (6.62), we obtain

$$|\mathbf{R}_i - \mathbf{R}_j| \geqslant D_0. \tag{6.64}$$

**2. Consider the case** $i = k+1, \ldots, N-1,\ j = k+2, \ldots, N,\ i < j$.

We have

$$\begin{aligned} |\mathbf{R}_i - \mathbf{R}_j| &= |\mathbf{L}_{i-k} - \mathbf{L}_{j-k}| \\ &\geqslant \sqrt{\nu}D_0 \\ &\geqslant D_0. \end{aligned} \tag{6.65}$$

Therefore, from (6.64) and (6.65), we obtain

$$|\mathbf{R}_i - \mathbf{R}_j| \geqslant D_0 \tag{6.66}$$

then

$$\frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} \leqslant \frac{1}{D_0}.$$

This inequality gives

$$\sum_{j=k+1}^{N} \sum_{i=1}^{j-1} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} \leqslant \sum_{j=k+1}^{N} \sum_{i=1}^{j-1} \frac{1}{D_0}$$

$$= \frac{1}{D_0} \sum_{j=k+1}^{N} \sum_{i=1}^{j-1} 1$$

$$= \frac{1}{D_0} \frac{(N-k)(N+k-1)}{2}. \tag{6.67}$$

Substitute (6.67) in (6.58), we obtain

$$\sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \leqslant \sum_{i<j}^{k} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} + \frac{e^2(N-k)(N+k-1)}{2D_0}. \tag{6.68}$$

Then, substitute (6.39), (6.57) and (6.68) in (6.28), we obtain the upper bound

$$\langle \Psi | H | \Psi \rangle \leqslant kT - ke^2 \sum_{j=1}^{k} \int \mathrm{d}^\nu \mathbf{x} \, \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x})$$

$$+ \frac{k(k-1)e^2}{2} \int \mathrm{d}^\nu \mathbf{x} \, \mathrm{d}^\nu \mathbf{x}' \, \phi_L^2\,(\mathbf{x}) \, \frac{1}{|\mathbf{x} - \mathbf{x}'|} \phi_L^2\,(\mathbf{x}') + \sum_{i<j}^{k} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|}$$

$$+ (N-k)T_0 + \frac{e^2(N-k)(N+k-1)}{D_0} - \frac{e^2(N-k)}{\sqrt{\nu} L_0} \tag{6.69}$$

therefore

$$\langle \Psi | H | \Psi \rangle \leqslant kT + \langle H_1 \rangle + (N-k) \left[ T_0 + \frac{e^2(N+k-1)}{D_0} - \frac{e^2}{\sqrt{2} L_0} \right] \tag{6.70}$$

where

$$\langle H_1\rangle = -ke^2\sum_{j=1}^{k}\int \mathrm{d}^\nu\mathbf{x}\ \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x})$$

$$+\frac{k(k-1)e^2}{2}\int \mathrm{d}^\nu\mathbf{x}\,\mathrm{d}^\nu\mathbf{x}'\ \phi_L^2\left(\mathbf{x}\right)\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2\left(\mathbf{x}'\right)+\sum_{i<j}^{k}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}. \quad (6.71)$$

Since $k(k-1) < k^2$, then

$$\langle H_1\rangle < -ke^2\sum_{j=1}^{k}\int \mathrm{d}^\nu\mathbf{x}\ \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x})$$

$$+\frac{e^2}{2}k^2\int \mathrm{d}^\nu\mathbf{x}\,\mathrm{d}^\nu\mathbf{x}'\ \phi_L^2\left(\mathbf{x}\right)\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2\left(\mathbf{x}'\right)+\sum_{i<j}^{k}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}$$

$$\equiv H_1(k,\mathbf{R}) \quad (6.72)$$

where $\mathbf{R} = \{\mathbf{R}_1,\ldots,\mathbf{R}_k\}$ and

$$H_1(k,\mathbf{R}) = A_1(k,\mathbf{R}) + A_2(k) + A_3(k,\mathbf{R}). \quad (6.73)$$

We define

$$A_1(k,\mathbf{R}) = -ke^2\sum_{j=1}^{k}\int \mathrm{d}^\nu\mathbf{x}\ \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\phi_L^2(\mathbf{x}), \quad (6.74a)$$

$$A_2(k) = \frac{e^2}{2}k^2\int \mathrm{d}^\nu\mathbf{x}\,\mathrm{d}^\nu\mathbf{x}'\ \phi_L^2\left(\mathbf{x}\right)\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2\left(\mathbf{x}'\right), \quad (6.74b)$$

$$A_3(k,\mathbf{R}) = \sum_{i<j}^{k}\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}. \quad (6.74c)$$

Therefore, to derive the upper bound of $\langle H_1\rangle$, we partition the interval $[0, L]$ in to $n$ subintervals: $0 = a'_0 < a'_1 < a'_2 < \ldots < a'_n = L$ and we choose $a'_j$, $a'_{j-1}$ such that

$$\frac{1}{L}\int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i \ \cos^2\left(\frac{\pi x_i}{2L}\right) \equiv \int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i \ g^2(x_i) = \frac{1}{2n} \tag{6.75}$$

where

$$g(x_i) = \frac{1}{\sqrt{L}} \cos\left(\frac{\pi x_i}{2L}\right) \tag{6.76}$$

for $j = 1, \ldots, n$. By doing so, we divide the box of sides $2L, 2L, \ldots, 2L$ into $(2n)^\nu = k$ smaller boxes which labeled $B'(m)$, where $m = (j_1, j_2, \ldots, j_\nu)$.

Let

$$0 = a'_0 < a'_1 < a'_2 < \cdots < a'_n = L, \tag{6.77}$$

$$\alpha'_j = a'_j - a'_{j-1}, \qquad j = 1, \ldots, n, \tag{6.78}$$

where

$$\sum_{j=1}^{n} \alpha'_j = L. \tag{6.79}$$

Then

$$B'(m) \text{ is equivalent to boxes of sides } \alpha'_{j_1} \times \alpha'_{j_2} \times \ldots \times \alpha'_{j_\nu} \tag{6.80}$$

where we have the normalization condition such that

$$\begin{aligned}
&\frac{1}{L}\int_{a'_{j_1-1}}^{a'_{j_1}} \mathrm{d}x_1 \ \cos^2\left(\frac{\pi x_1}{2L}\right) \ldots \frac{1}{L}\int_{a'_{j_\nu-1}}^{a'_{j_\nu}} \mathrm{d}x_\nu \ \cos^2\left(\frac{\pi x_\nu}{2L}\right) \\
&\qquad\qquad \equiv \int_{a'_{j_1-1}}^{a'_{j_1}} \mathrm{d}x_1 \ g^2\left(x_1\right) \ldots \int_{a'_{j_\nu-1}}^{a'_{j_\nu}} \mathrm{d}x_\nu \ g^2\left(x_\nu\right) \\
&\qquad\qquad = \int\limits_{B'(m)} \mathrm{d}^\nu \mathbf{x} \ \phi_L^2(\mathbf{x}) \\
&\qquad\qquad = \frac{1}{(2n)^\nu} = \frac{1}{k}.
\end{aligned} \tag{6.81}$$

Therefore,

$$\int \mathrm{d}^{\nu}\mathbf{x}\ \phi_L^2(\mathbf{x}) = (2)^{\nu} \sum_{B'(m)=1}^{k/(2)^{\nu}} \int_{B'(m)} \mathrm{d}^{\nu}\mathbf{x}\ \phi_L^2(\mathbf{x})$$

$$= (2)^{\nu} \sum_{B'(m)=1}^{k/(2)^{\nu}} \left(\frac{1}{k}\right)$$

$$= (2)^{\nu} \frac{k}{(2)^{\nu}} \frac{1}{k}$$

$$= 1. \tag{6.82}$$

Now we place $\mathbf{R}_1$ in box $B'(m) = 1$, $\mathbf{R}_2$ in box $B'(m) = 2, \ldots, \mathbf{R}_k$ in box $B'(m) = k$, and then we average $H_1(k, \mathbf{R})$ over the positions, $\mathbf{R}_1, \ldots, \mathbf{R}_k$, of the positive particles within the box with a relative weight $\phi_L^2(\mathbf{R}_1), \ldots, \phi_L^2(\mathbf{R}_k)$ in rectangle $B'(m) = 1, \ldots, B'(m) = k$, respectively.

## The Average of $A_1(k, \mathbf{R})$

The term $A_1(k, \mathbf{R})$, for $k = (2n)^{\nu}$, may be rewritten as sums of integrals over such boxes as follows:

$$A_1(k, \mathbf{R}) = -(2)^{\nu} k e^2 \sum_{B'(m)=1}^{k/2^{\nu}} \sum_{j=1}^{k/2^{\nu}} \int_{B'(m)} \mathrm{d}^{\nu}\mathbf{x} \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x})$$

$$= -(2)^{\nu} k e^2 \sum_{B'(m)=1}^{n^{\nu}} \sum_{j=1}^{n^{\nu}} \int_{B'(m)} \mathrm{d}^{\nu}\mathbf{x}\ \frac{1}{|\mathbf{x} - \mathbf{R}_j|} \phi_L^2(\mathbf{x})$$

$$= -(2)^{\nu} k e^2 \sum_{B'(m)=1}^{n^{\nu}} \int_{B'(m)} \mathrm{d}^{\nu}\mathbf{x}\ \phi_L^2(\mathbf{x}) \sum_{j=1}^{n^{\nu}} \frac{1}{|\mathbf{x} - \mathbf{R}_j|}. \tag{6.83}$$

Then $\langle A_1(k, \mathbf{R}) \rangle$ will be derived below and it is obtained by the average of

$\sum_{j=1}^{n^\nu} \frac{1}{|\mathbf{x}-\mathbf{R}_j|}$. Since

$$\sum_{j=1}^{n^\nu} \frac{1}{|\mathbf{x}-\mathbf{R}_j|} = \frac{1}{|\mathbf{x}-\mathbf{R}_1|} + \ldots + \frac{1}{|\mathbf{x}-\mathbf{R}_{n^\nu}|}$$

then we have

$$\begin{aligned}
\left(\sum_{j=1}^{n^\nu} \frac{1}{|\mathbf{x}-\mathbf{R}_j|}\right)\Bigg|_{\text{average}} &= \frac{\displaystyle\int\limits_{B'(j)=1} \mathrm{d}^\nu\mathbf{x}' \ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}}{\displaystyle\int\limits_{B'(j)=1} \mathrm{d}^\nu\mathbf{x}' \ \phi_L^2(\mathbf{x}')} + \ldots + \frac{\displaystyle\int\limits_{B'(j)=n^\nu} \mathrm{d}^\nu\mathbf{x}' \ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}}{\displaystyle\int\limits_{B'(j)=n^\nu} \mathrm{d}^\nu\mathbf{x}' \ \phi_L^2(\mathbf{x}')} \\
&= \frac{\displaystyle\int\limits_{B'(j)=1} \mathrm{d}^\nu\mathbf{x}' \ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}}{\frac{1}{k}} + \ldots + \frac{\displaystyle\int\limits_{B'(j)=n^\nu} \mathrm{d}^\nu\mathbf{x}' \ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}}{\frac{1}{k}} \\
&= k \int\limits_{B'(j)=1} \mathrm{d}^\nu\mathbf{x}' \ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} + \ldots + k \int\limits_{B'(j)=n^\nu} \mathrm{d}^\nu\mathbf{x}' \ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \\
&= k \sum_{B'(q)=1}^{n^\nu} \int\limits_{B'(q)} \mathrm{d}^\nu\mathbf{x}' \ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}.
\end{aligned} \tag{6.84}$$

Then, we obtain

$$\begin{aligned}
\langle A_1(k,\mathbf{R})\rangle &= -(2)^\nu k e^2 \sum_{B'(m)=1}^{n^\nu} \int\limits_{B'(m)} \mathrm{d}^\nu\mathbf{x} \ \phi_L^2(\mathbf{x}) k \sum_{B'(q)=1}^{n^\nu} \int\limits_{B'(q)} \mathrm{d}^\nu\mathbf{x}' \ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \\
&= -(2)^\nu k^2 e^2 \sum_{B'(m)=1}^{n^\nu} \sum_{B'(q)=1}^{n^\nu} \int\limits_{B'(m)} \mathrm{d}^\nu\mathbf{x} \int\limits_{B'(q)} \mathrm{d}^\nu\mathbf{x}' \ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}').
\end{aligned} \tag{6.85}$$

## The Average of $A_2(k)$

The term $A_2(k)$ may be rewritten as sums of integrals over such boxes directly as follows:

$$\begin{aligned} A_2(k) &= \frac{e^2}{2} k^2 \int \mathrm{d}^\nu \mathbf{x}\, \mathrm{d}^\nu \mathbf{x}'\ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}') \\ &= \frac{(2)^\nu e^2}{2} k^2 \sum_{B'(m)=1}^{n^\nu} \sum_{B'(q)=1}^{n^\nu} \int_{B'(m)} \mathrm{d}^\nu \mathbf{x} \int_{B'(q)} \mathrm{d}^\nu \mathbf{x}'\ \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \phi_L^2(\mathbf{x}')\,. \end{aligned} \tag{6.86}$$

## The Average of $A_3(k, \mathbf{R})$

Since

$$A_3(k,\mathbf{R}) = \frac{1}{2} \sum_{i \neq j}^{k} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} = \frac{(2)^\nu}{2} \sum_{i \neq j}^{n^\nu} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{6.87}$$

then, the average of $A_3(k, \mathbf{R})$ over $\mathbf{R}_j$ is given by

$$\begin{aligned} &\left( \sum_{i\neq j}^{n^\nu} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} \right) \Bigg|_{\text{average over } \mathbf{R}_j} \\ &= \sum_{i=1}^{n^\nu} \sum_{j(\neq i)=1}^{n^\nu} \left( \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} \right) \Bigg|_{\text{average over } \mathbf{R}_j} \\ &= \sum_{i(\neq j)=1}^{n^\nu} \left\{ \frac{\displaystyle\int_{B'(j)=1} \mathrm{d}^\nu \mathbf{x}'\ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|}}{\displaystyle\int_{B'(j)=1} \mathrm{d}^\nu \mathbf{x}'\ \phi_L^2(\mathbf{x}')} + \ldots + \frac{\displaystyle\int_{B'(j)=n^\nu} \mathrm{d}^\nu \mathbf{x}'\ \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|}}{\displaystyle\int_{B'(j)=n^\nu} \mathrm{d}^\nu \mathbf{x}'\ \phi_L^2(\mathbf{x}')} \right\} \end{aligned}$$

$$= \sum_{i(\neq j)=1}^{n^\nu} \left\{ \frac{\displaystyle\int_{B'(j)=1} \mathrm{d}^\nu \mathbf{x}' \, \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|}}{\dfrac{1}{k}} + \ldots + \frac{\displaystyle\int_{B'(j)=n^\nu} \mathrm{d}^\nu \mathbf{x}' \, \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|}}{\dfrac{1}{k}} \right\}$$

$$= \sum_{i(\neq j)=1}^{n^\nu} \left\{ k \int_{B'(j)=1} \mathrm{d}^\nu \mathbf{x}' \, \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|} + \ldots + k \int_{B'(j)=n^\nu} \mathrm{d}^\nu \mathbf{x}' \, \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|} \right\}$$

$$= k \sum_{i(\neq j)=1}^{n^\nu} \sum_{B'(j)=1}^{n^\nu} \int_{B'(j)} \mathrm{d}^\nu \mathbf{x}' \, \frac{\phi_L^2(\mathbf{x}')}{|\mathbf{R}_i - \mathbf{x}'|}. \tag{6.88}$$

Now, we average above inequality over $\mathbf{R}_i$

$$\left( \sum_{i \neq j}^{n^\nu} \frac{1}{|\mathbf{R}_i - \mathbf{R}_j|} \right) \Bigg|_{\text{average}}$$

$$= k \sum_{B'(j(\neq i))=1}^{n^\nu} \int_{B'(j)} \mathrm{d}^\nu \mathbf{x}' \, \phi_L^2(\mathbf{x}') \left\{ \frac{\displaystyle\int_{B'(i)=1} \mathrm{d}^\nu \mathbf{x} \, \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}}{\displaystyle\int_{B'(i)=1} \mathrm{d}^\nu \mathbf{x} \, \phi_L^2(\mathbf{x})} + \ldots + \frac{\displaystyle\int_{B'(i)=n^\nu} \mathrm{d}^\nu \mathbf{x} \, \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}}{\displaystyle\int_{B'(i)=n^\nu} \mathrm{d}^\nu \mathbf{x} \, \phi_L^2(\mathbf{x})} \right\}$$

$$= k \sum_{B'(j(\neq i))=1}^{n^\nu} \int_{B'(j)} \mathrm{d}^\nu \mathbf{x}' \, \phi_L^2(\mathbf{x}') \left\{ \frac{\displaystyle\int_{B'(i)=1} \mathrm{d}^\nu \mathbf{x} \, \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}}{\dfrac{1}{k}} + \ldots + \frac{\displaystyle\int_{B'(i)=n^\nu} \mathrm{d}^\nu \mathbf{x} \, \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}}{\dfrac{1}{k}} \right\}$$

$$= k \sum_{B'(j(\neq i))=1}^{n^\nu} \int_{B'(j)} \mathrm{d}^\nu \mathbf{x}' \, \phi_L^2(\mathbf{x}') \sum_{B'(i)=1}^{n^\nu} k \int_{B'(i)} \mathrm{d}^\nu \mathbf{x} \, \frac{\phi_L^2(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}$$

$$= k^2 \sum_{B'(m)=1}^{n^\nu} \sum_{B'(q(\neq m))=1}^{n^\nu} \int_{B'(m)} \mathrm{d}^\nu \mathbf{x} \int_{B'(q)} \mathrm{d}^\nu \mathbf{x}' \, \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \phi_L^2(\mathbf{x}'). \tag{6.89}$$

Then, we obtain

$$\langle A_3(k,\mathbf{R})\rangle = \frac{(2)^\nu e^2k^2}{2} \sum_{B'(m)=1}^{n^\nu} \sum_{B'(q(\neq m))=1}^{n^\nu} \int_{B'(m)} \mathrm{d}^\nu\mathbf{x} \int_{B'(q)} \mathrm{d}^\nu\mathbf{x}' \; \phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}'). \tag{6.90}$$

From (6.73), we have the average of $H_1(k,\mathbf{R})$ as below

$$\begin{aligned}
\langle H_1(k,\mathbf{R})\rangle &= \langle A_1(k,\mathbf{R})\rangle + A_2(k) + \langle A_3(k,\mathbf{R})\rangle \\
&= -(2)^\nu k^2e^2 \sum_{B'(m)=1}^{n^\nu} \sum_{B'(q)=1}^{n^\nu} \int_{B'(m)} \mathrm{d}^\nu\mathbf{x} \int_{B'(q)} \mathrm{d}^\nu\mathbf{x}' \; \phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}') \\
&\quad + \frac{(2)^\nu e^2k^2}{2} \sum_{B'(m)=1}^{n^\nu} \sum_{B'(q)=1}^{n^\nu} \int_{B'(m)} \mathrm{d}^\nu\mathbf{x} \int_{B'(q)} \mathrm{d}^\nu\mathbf{x}' \; \phi_L^2\,(\mathbf{x})\,\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2\,(\mathbf{x}') \\
&\quad + \frac{(2)^\nu e^2k^2}{2} \sum_{B'(m)=1}^{n^\nu} \sum_{B'(q(\neq m))=1}^{n^\nu} \int_{B'(m)} \mathrm{d}^\nu\mathbf{x} \int_{B'(q)} \mathrm{d}^\nu\mathbf{x}' \; \phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}') \\
&= -\frac{(2)^\nu e^2k^2}{2} \sum_{B'(m)=1}^{n^\nu} \sum_{B'(q)=1}^{n^\nu} \int_{B'(m)} \mathrm{d}^\nu\mathbf{x} \int_{B'(q)} \mathrm{d}^\nu\mathbf{x}' \; \phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}') \\
&\quad + \frac{(2)^\nu e^2k^2}{2} \sum_{B'(m)=1}^{n^\nu} \sum_{B'(q(\neq m))=1}^{n^\nu} \int_{B'(m)} \mathrm{d}^\nu\mathbf{x} \int_{B'(q)} \mathrm{d}^\nu\mathbf{x}' \; \phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}') \\
&= -\frac{(2)^\nu e^2k^2}{2} \sum_{B'(m)=1}^{n^\nu} \sum_{B'(q)=1}^{n^\nu} \int_{B'(m)} \mathrm{d}^\nu\mathbf{x} \int_{B'(q)} \mathrm{d}^\nu\mathbf{x}' \; \phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}')\delta_{mq}.
\end{aligned} \tag{6.91}$$

Eq. (6.91) may be rewritten as

$$\langle H_1(k,\mathbf{R})\rangle = -(2)^\nu \,\frac{e^2k^2}{2} \sum_{B'(m)=1}^{n^\nu} \int_{B'(m)} \mathrm{d}^\nu\mathbf{x}\,\mathrm{d}^\nu\mathbf{x}' \; \phi_L^2(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\phi_L^2(\mathbf{x}'). \tag{6.92}$$

By the definition of an *average*, there must be at least one set of $\mathbf{R}$ such that

$$H_1(k, \mathbf{R}) \leqslant \langle H_1(k, \mathbf{R}) \rangle \, . \tag{6.93}$$

Then, (6.73) becomes

$$\langle H_1 \rangle \leqslant -\frac{(2)^\nu e^2 k^2}{2} \sum_{B'(m)=1}^{n^\nu} \int_{B'(m)} \mathrm{d}^\nu \mathbf{x} \, \mathrm{d}^\nu \mathbf{x}' \; \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \phi_L^2(\mathbf{x}'). \tag{6.94}$$

We scale $\mathbf{x}$ to $\dfrac{\mathbf{x}}{L} \equiv \mathbf{u}$ , then

$$\frac{1}{L} \int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i \; \cos^2\left(\frac{\pi x_i}{2L}\right) = \int_{a'_{j-1}/L}^{a'_j/L} \mathrm{d}\left(\frac{x_i}{L}\right) \; \cos^2\left(\frac{\pi}{2}\left(\frac{x_i}{L}\right)\right) \tag{6.95}$$

or

$$\frac{1}{L} \int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i \; \cos^2\left(\frac{\pi x_i}{2L}\right) = \int_{a_{j-1}}^{a_j} \mathrm{d}u_i \; \cos^2\left(\frac{\pi u_i}{2}\right) = \frac{1}{2n} \tag{6.96}$$

or

$$\int_{a'_{j-1}}^{a'_j} \mathrm{d}x_i \; g^2(x_i) = \int_{a_{j-1}}^{a_j} \mathrm{d}u_i \; g_1^2(u_i) = \frac{1}{2n} \tag{6.97}$$

where

$$g_1(u_i) = \cos\left(\frac{\pi u_i}{2}\right) \tag{6.98}$$

and

$$0 = \frac{a'_0}{L} < \frac{a'_1}{L} < \frac{a'_2}{L} < \cdots < \frac{a'_n}{L} = 1.$$

Then

$$0 = a_0 < a_1 < a_2 < \cdots < a_n = 1, \tag{6.99}$$

$$\alpha_j = a_j - a_{j-1}, \qquad j = 1, \ldots, n, \tag{6.100}$$

where

$$\sum_{j=1}^{n} \alpha_j = 1. \tag{6.101}$$

Let

$$B(m) \equiv \text{ a box of sides } \alpha_{j_1} \times \alpha_{j_2} \times \ldots \times \alpha_{j_\nu}. \tag{6.102}$$

Therefore, we have the normalization condition such that

$$\int_{a_{j_1-1}}^{a_{j_1}} \mathrm{d}u_1 \, g_1^2(u_1) \ldots \int_{a_{j_\nu-1}}^{a_{j_\nu}} \mathrm{d}u_\nu \, g_1^2(u_\nu) = \int\limits_{B(m)} \mathrm{d}^\nu \mathbf{u} \, \phi_1^2(\mathbf{u})$$

$$= \frac{1}{(2n)^\nu} = \frac{1}{k} \tag{6.103}$$

where

$$\phi_1(\mathbf{x}) = \prod_{i=1}^{\nu} \cos\left(\frac{\pi x_i}{2}\right), \qquad |x_i| \leqslant 1. \tag{6.104}$$

Then, we rewrite the integral on the right-hand side of (6.94) as below

$$\sum_{B'(m)=1}^{n^\nu} \int\limits_{B'(m)} \mathrm{d}^\nu \mathbf{x} \, \mathrm{d}^\nu \mathbf{x}' \, \phi_L^2(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \phi_L^2(\mathbf{x}')$$

$$= \sum_{B(m)=1}^{n^\nu} \int\limits_{B(m)} \mathrm{d}^\nu \mathbf{u} \, \mathrm{d}^\nu \mathbf{u}' \, \phi_1^2(\mathbf{u}) \frac{1}{|L\mathbf{u} - L\mathbf{u}'|} \phi_1^2(\mathbf{u}')$$

$$= \frac{1}{L} \sum_{B(m)=1}^{n^\nu} \int\limits_{B(m)} \mathrm{d}^\nu \mathbf{u} \, \mathrm{d}^\nu \mathbf{u}' \, \phi_1^2(\mathbf{u}) \frac{1}{|\mathbf{u} - \mathbf{u}'|} \phi_1^2(\mathbf{u}') \tag{6.105}$$

where $0 \leqslant u_i \leqslant 1$. Substitute (6.105) in (6.94), we obtain

$$\langle H_1 \rangle \leqslant -\frac{(2)^\nu e^2 k^2}{2L} \sum_{B(m)=1}^{n^\nu} \int\limits_{B(m)} \mathrm{d}^\nu \mathbf{x} \, \mathrm{d}^\nu \mathbf{x}' \, \phi_1^2(\mathbf{x}) \frac{1}{|\mathbf{x} - \mathbf{x}'|} \phi_1^2(\mathbf{x}') \tag{6.106}$$

where $0 \leqslant x_i \leqslant 1$.

Since $\mathbf{x}$ and $\mathbf{x}'$ lie in box $B(m)$ of the length $\alpha_{j_1} \times \alpha_{j_2} \times \ldots \times \alpha_{j_\nu}$. Then the maximum magnitude of $|\mathbf{x} - \mathbf{x}'|$ is the diagonal line in $B(m)$ of length $\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}$. That is,

$$|\mathbf{x} - \mathbf{x}'| \leqslant \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2} \tag{6.107}$$

or

$$\frac{1}{|\mathbf{x} - \mathbf{x}'|} \geqslant \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}}. \tag{6.108}$$

For $m = (j_1, j_2, \ldots, j_\nu)$, we have

$$\sum_{B(m)=1}^{n^\nu} = \sum_{j_1=1}^{n} \sum_{j_2=1}^{n} \cdots \sum_{j_\nu=1}^{n}. \tag{6.109}$$

Substitute (6.108) and (6.109) in (6.106), we obtain

$$\langle H_1 \rangle \leqslant -\frac{(2)^\nu e^2 k^2}{2L} \sum_{B(m)=1}^{n^\nu} \int_{B(m)} \mathrm{d}^\nu \mathbf{x}\, \mathrm{d}^\nu \mathbf{x}' \; \phi_1^2(\mathbf{x}) \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}} \phi_1^2(\mathbf{x}')$$

$$= -\frac{(2)^\nu e^2 k^2}{2L} \sum_{j_1=1}^{n} \sum_{j_2=1}^{n} \cdots \sum_{j_\nu=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}}$$

$$\times \int_{B(j_1, j_2, \ldots, j_\nu)} \mathrm{d}^\nu \mathbf{x}\, \mathrm{d}^\nu \mathbf{x}' \; \phi_1^2(\mathbf{x}) \phi_1^2(\mathbf{x}')$$

$$= -\frac{(2)^\nu e^2 k^2}{2L} \sum_{j_1=1}^{n} \sum_{j_2=1}^{n} \cdots \sum_{j_\nu=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}}$$

$$\times \int_{B(j_1, j_2, \ldots, j_\nu)} \mathrm{d}^\nu \mathbf{x} \; \phi_1^2(\mathbf{x}) \int_{B(j_1, j_2, \ldots, j_\nu)} \mathrm{d}^\nu \mathbf{x}' \; \phi_1^2(\mathbf{x}').$$

From (6.103), we obtain above inequality as below

$$\langle H_1 \rangle \leqslant -\frac{(2)^\nu e^2 k^2}{2L} \sum_{j_1=1}^{n} \sum_{j_2=1}^{n} \cdots \sum_{j_\nu=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}} \left(\frac{1}{k}\right)\left(\frac{1}{k}\right)$$

$$= -\frac{(2)^\nu e^2}{2L} \sum_{j_1=1}^{n} \sum_{j_2=1}^{n} \cdots \sum_{j_\nu=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}}. \qquad (6.110)$$

Now, we define $f(\alpha_{j_1})$ as

$$f(\alpha_{j_1}) = \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}. \qquad (6.111)$$

Since

$$\sum_{j_1=1}^{n} 1 = n$$

then

$$\sum_{j_1=1}^{n} \left( \sqrt{f(\alpha_{j_1})} \frac{1}{f(\alpha_{j_1})} \right) = n. \qquad (6.112)$$

By using the Cauchy-Schwarz inequality,

$$\left( \sum_{i=1}^{n} a_i b_i \right)^2 \leqslant \sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2$$

then, we have

$$\left( \sum_{j_1=1}^{n} \sqrt{f(\alpha_{j_1})} \frac{1}{f(\alpha_{j_1})} \right)^2 \leqslant \sum_{j_1=1}^{n} f(\alpha_{j_1}) \sum_{j_1=1}^{n} \frac{1}{f(\alpha_{j_1})},$$

$$\sum_{j_1=1}^{n} \frac{1}{f(\alpha_{j_1})} \geqslant \frac{n^2}{\sum_{j_1=1}^{n} f(\alpha_{j_1})} \qquad (6.113)$$

or

$$\sum_{j_1=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}} \geqslant \frac{n^2}{\sum\limits_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}}. \qquad (6.114)$$

Multiply above inequality by $\sum\limits_{j_2=1}^{n}$ ,we obtain

$$\sum_{j_2=1}^{n}\sum_{j_1=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}} \geqslant \sum_{j_2=1}^{n} \frac{n^2}{\sum\limits_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}}$$

$$= n^2 \sum_{j_2=1}^{n} \frac{1}{\sum\limits_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}}. \qquad (6.115)$$

Let

$$f(\alpha_{j_2}) = \frac{1}{\sum\limits_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}}. \qquad (6.116)$$

From Cauchy-Schwarz inequality

$$\sum_{j_2=1}^{n} \frac{1}{f(\alpha_{j_2})} \geqslant \frac{n^2}{\sum\limits_{j_2=1}^{n} f(\alpha_{j_2})}$$

or

$$\sum_{j_2=1}^{n} f(\alpha_{j_2}) \geqslant \frac{n^2}{\sum\limits_{j_2=1}^{n} \frac{1}{f(\alpha_{j_2})}}. \qquad (6.117)$$

Substitution of $f(\alpha_{j_2})$ gives

$$\sum_{j_2=1}^{n} \frac{1}{\sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}} \geqslant \frac{n^2}{\sum_{j_2=1}^{n} \frac{1}{\frac{1}{\sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}}}}$$

$$= \frac{n^2}{\sum_{j_2=1}^{n}\sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}}. \qquad (6.118)$$

Substitute (6.118) in (6.115), we obtain

$$\sum_{j_2=1}^{n}\sum_{j_1=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}} \geqslant \frac{n^4}{\sum_{j_2=1}^{n}\sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}} \qquad (6.119)$$

which leads to

$$\sum_{j_1=1}^{n} \cdots \sum_{j_\nu=1}^{n} \frac{1}{\sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}} \geqslant \frac{n^{2\nu}}{\sum_{j_1=1}^{n} \cdots \sum_{j_\nu=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}} \qquad (6.120)$$

where $\sum_{j_1=1}^{n} \alpha_{j_1} = 1, \sum_{j_2=1}^{n} \alpha_{j_2} = 1, \ldots, \sum_{j_\nu=1}^{n} \alpha_{j_\nu} = 1$. We have

$$(\alpha_{j_1} + \alpha_{j_2} + \ldots + \alpha_{j_\nu})^2 \geqslant \alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2$$

or

$$\alpha_{j_1} + \alpha_{j_2} + \ldots + \alpha_{j_\nu} \geqslant \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2}$$

then

$$\sum_{j_1=1}^{n} (\alpha_{j_1} + \alpha_{j_2} + \ldots + \alpha_{j_\nu}) \geqslant \sum_{j_1=1}^{n} \sqrt{\alpha_{j_1}^2 + \alpha_{j_2}^2 + \ldots + \alpha_{j_\nu}^2},$$

$$\left(\sum_{j_1=1}^{n}\alpha_{j_1}+\sum_{j_1=1}^{n}\alpha_{j_2}+\ldots+\sum_{j_\nu=1}^{n}\alpha_{j_\nu}\right)\geqslant\sum_{j_1=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\ldots+\alpha_{j_\nu}^2}.$$

Then, we obtain

$$(1+n\alpha_{j_2}+\ldots+n\alpha_{j_\nu})\geqslant\sum_{j_1=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\ldots+\alpha_{j_\nu}^2}. \tag{6.121}$$

Multiply above inequality by $\sum_{j_2=1}^{n}$, we obtain

$$\sum_{j_2=1}^{n}(1+n\alpha_{j_2}+\ldots+n\alpha_{j_\nu})\geqslant\sum_{j_2=1}^{n}\sum_{j_1=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\ldots+\alpha_{j_\nu}^2},$$

$$\left(\sum_{j_2=1}^{n}1+n\sum_{j_2=1}^{n}\alpha_{j_2}+\ldots+n\sum_{j_2=1}^{n}\alpha_{j_\nu}\right)\geqslant\sum_{j_2=1}^{n}\sum_{j_1=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\ldots+\alpha_{j_\nu}^2},$$

$$\left(n+n+\ldots+n^2\alpha_{j_\nu}\right)\geqslant\sum_{j_2=1}^{n}\sum_{j_1=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\ldots+\alpha_{j_\nu}^2}$$

which leads to

$$\sum_{j_1=1}^{n}\cdots\sum_{j_\nu=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\ldots+\alpha_{j_\nu}^2}\leqslant n^{\nu-1}+n^{\nu-1}+\ldots+n^{\nu-1}$$

$$=\nu n^{\nu-1} \tag{6.122}$$

or

$$\frac{1}{\sum_{j_1=1}^{n}\cdots\sum_{j_\nu=1}^{n}\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\ldots+\alpha_{j_\nu}^2}}\geqslant\frac{1}{\nu n^{\nu-1}},$$

$$\sum_{j_1=1}^{n}\cdots\sum_{j_\nu=1}^{n}\frac{1}{\sqrt{\alpha_{j_1}^2+\alpha_{j_2}^2+\ldots+\alpha_{j_\nu}^2}}\geqslant\frac{n^{2\nu}}{\nu n^{\nu-1}}$$

$$= \frac{n^{\nu+1}}{\nu}. \tag{6.123}$$

Substitute (6.123) in (6.110), we obtain

$$\langle H_1 \rangle \leqslant -(2)^{\nu} \frac{e^2}{2L} \frac{n^{\nu+1}}{\nu} = -\frac{2^{\nu-1} e^2 \, n^{\nu+1}}{\nu L}. \tag{6.124}$$

Since $k = (2n)^{\nu}$, then

$$\frac{k^{1/\nu}}{2} = n \tag{6.125}$$

then

$$\langle H_1 \rangle \leqslant -\frac{2^{\nu-1} e^2 \left( \frac{k^{1/\nu}}{2} \right)^{\nu+1}}{\nu L} = -\frac{e^2 k^{(\nu+1)/\nu}}{4\nu L}. \tag{6.126}$$

Substitute (6.126) in (6.70) we obtain

$$\langle \Psi | H | \Psi \rangle \leqslant kT - \frac{e^2 k^{(\nu+1)/\nu}}{4\nu L} + (N-k) \left[ T_0 + \frac{e^2 (N+k-1)}{D_0} - \frac{e^2}{\sqrt{\nu} L_0} \right]. \tag{6.127}$$

Substitute $T$, $T_0$ and $D_0 \geqslant \chi L_0$, then

$$\langle \Psi | H | \Psi \rangle \leqslant \frac{\nu \pi^2 \hbar^2}{8mL^2} k - \frac{e^2 k^{(\nu+1)/\nu}}{4\nu L} + (N-k) \left[ \frac{\nu \pi^2 \hbar^2}{8m(L_0)^2} + \frac{e^2 (N+k-1)}{\chi L_0} - \frac{e^2}{\sqrt{\nu} L_0} \right]$$

$$\equiv B_1(L) + B_2(L_0) \tag{6.128}$$

where

$$B_1(L) = \frac{\nu \pi^2 \hbar^2}{8mL^2} k - \frac{e^2 k^{(\nu+1)/\nu}}{4\nu L}, \tag{6.129}$$

$$B_2(L_0) = (N-k) \left[ \frac{\nu \pi^2 \hbar^2}{8m(L_0)^2} + \frac{e^2 (N+k-1)}{\chi L_0} - \frac{e^2}{\sqrt{\nu} L_0} \right]. \tag{6.130}$$

Optimization of the right-hand side of equation (6.148) over $L$ and $L_0$ :

$$\frac{\partial}{\partial L}(B_1(L)+B_2(L_0)) = \frac{\mathrm{d}B_1(L)}{\mathrm{d}L}$$

$$= (-2)\frac{\nu\pi^2\hbar^2}{8mL^3}k + \frac{k^{(\nu+1)/\nu}e^2}{4\nu L^2}. \tag{6.131}$$

Then, $L$ will be obtained from

$$\frac{\mathrm{d}B_1(L)}{\mathrm{d}L} = 0,$$

$$(-2)\frac{\nu\pi^2\hbar^2}{8mL^3}k + \frac{k^{(\nu+1)/\nu}e^2}{4\nu L^2} = 0 \tag{6.132}$$

then

$$L = \frac{\nu^2\pi^2\hbar^2}{me^2k^{1/\nu}}. \tag{6.133}$$

We can find $L_0$ from,

$$\frac{\partial}{\partial L_0}(B_1(L)+B_2(L_0)) = \frac{\mathrm{d}B_2(L_0)}{\mathrm{d}L_0}$$

$$= (N-k)\frac{\mathrm{d}}{\mathrm{d}L_0}\left[\frac{\nu\pi^2\hbar^2}{8m(L_0)^2} + \frac{e^2(N+k-1)}{\chi L_0} - \frac{e^2}{\sqrt{\nu}L_0}\right]$$

$$= (N-k)\left[-2\frac{\nu\pi^2\hbar^2}{8m(L_0)^3} - \frac{e^2(N+k-1)}{\chi(L_0)^2} + \frac{e^2}{\sqrt{\nu}(L_0)^2}\right]$$

$$= (N-k)\left[-\frac{\nu\pi^2\hbar^2}{4m(L_0)^3} + \frac{e^2}{(L_0)^2}\left(\frac{1}{\sqrt{\nu}} - \frac{(N+k-1)}{\chi}\right)\right] \tag{6.134}$$

and

$$\frac{\mathrm{d}B_2(L_0)}{\mathrm{d}L_0} = 0$$

then

$$-\frac{\nu\pi^2\hbar^2}{4m(L_0)^3}+\frac{e^2}{(L_0)^2}\left(\frac{1}{\sqrt{\nu}}-\frac{(N+k-1)}{\chi}\right)=0,$$

$$\frac{e^2}{(L_0)^2}\left(\frac{1}{\sqrt{\nu}}-\frac{(N+k-1)}{\chi}\right)=\frac{\nu\pi^2\hbar^2}{4m(L_0)^3}$$

then

$$L_0=\frac{\nu^2\pi^2\hbar^2}{me^2}\frac{1}{\left(4\sqrt{\nu}-\dfrac{4\nu(N+k-1)}{\chi}\right)}. \tag{6.135}$$

Because $L_0 \geqslant L$, then

$$\frac{\nu^2\pi^2\hbar^2}{me^2}\frac{1}{\left(4\sqrt{\nu}-\dfrac{4\nu(N+k-1)}{\chi}\right)}\geqslant\frac{\nu^2\pi^2\hbar^2}{me^2k^{1/\nu}},$$

$$4\sqrt{\nu}-\frac{4\nu(N+k-1)}{\chi}\leqslant k^{1/\nu}. \tag{6.136}$$

Since $L_0 > 0$, then

$$4\sqrt{\nu}-\frac{4\nu(N+k-1)}{\chi}>0. \tag{6.137}$$

Then, we have the bound

$$0<4\sqrt{\nu}-\frac{4\nu(N+k-1)}{\chi}\leqslant k^{1/\nu}. \tag{6.138}$$

We may choose $\chi=\dfrac{4\sqrt{\nu}}{3}(N+k-1)>2$, then $L_0$ is given by

$$L_0=\frac{\nu^2\pi^2\hbar^2}{me^2}\frac{1}{\left(4\sqrt{\nu}-\dfrac{4\nu(N+k-1)}{\dfrac{4\sqrt{\nu}}{3}(N+k-1)}\right)}$$

$$=\frac{\nu^2\pi^2\hbar^2}{me^2}\frac{1}{(4\sqrt{\nu}-3\sqrt{\nu})}$$

$$= \frac{\nu^{3/2}\pi^2\hbar^2}{me^2}. \tag{6.139}$$

From (6.130), we obtain

$$\begin{aligned}
B_2(L_0)\big|_{L_0=\frac{\nu^{3/2}\pi^2\hbar^2}{me^2}} &= (N-k)\left[\frac{\nu\pi^2\hbar^2}{8m}\left(\frac{m^2e^4}{\pi^4\hbar^4\nu^3}\right)\right. \\
&\quad \left. + \frac{3e^2(N+k-1)me^2}{4\nu^2(N+k-1)\pi^2\hbar^2} - \frac{me^4}{\nu^2\pi^2\hbar^2}\right] \\
&= (N-k)\left[\frac{me^4}{8\pi^2\hbar^2\nu^2} + \frac{3me^4}{4\pi^2\hbar^2\nu^2} - \frac{me^4}{\pi^2\hbar^2\nu^2}\right] \\
&= (N-k)\frac{me^4}{\pi^2\hbar^2\nu^2}\left[\frac{1}{8} + \frac{3}{4} - 1\right] \\
&= -(N-k)\frac{me^4}{8\pi^2\hbar^2\nu^2}. \qquad (6.140)
\end{aligned}$$

Since $(N-k) \geqslant 0$ then

$$B_2(L_0) \leqslant 0. \tag{6.141}$$

Add (6.141) by $B_1$ from (6.129), we obtain

$$\begin{aligned}
B_1(L) + B_2(L_0) &\leqslant B_1(L) \\
&= \frac{\nu\pi^2\hbar^2}{8mL^2}k - \frac{e^2k^{(\nu+1)/\nu}}{4\nu L}. \qquad (6.142)
\end{aligned}$$

Replace $L = \dfrac{\nu^2\pi^2\hbar^2}{me^2k^{1/\nu}}$, then (6.129) becomes

$$\begin{aligned}
B_1(L) &\leqslant \frac{\nu\pi^2\hbar^2}{8m}\left(\frac{m^2e^4k^{2/\nu}}{\nu^4\pi^4\hbar^4}\right)k - \frac{e^2k^{(\nu+1)/\nu}}{4\nu}\left(\frac{me^2k^{1/\nu}}{\nu^2\pi^2\hbar^2}\right) \\
&= \frac{me^4}{\pi^2\hbar^2}\frac{k^{\left(\frac{2}{\nu}+1\right)}}{8\nu^3} - \frac{me^4}{\pi^2\hbar^2}\frac{k^{\left(\frac{\nu+1}{\nu}+\frac{1}{\nu}\right)}}{4\nu^3}
\end{aligned}$$

$$= \frac{me^4}{\pi^2\hbar^2}\frac{k^{\left(\frac{2}{\nu}+1\right)}}{\nu^3}\left(\frac{1}{8}-\frac{1}{4}\right)$$

$$= -\frac{me^4}{\pi^2\hbar^2}\frac{k^{\left(\frac{2}{\nu}+1\right)}}{8\nu^3}$$

$$= -\left(\frac{me^4}{2\hbar^2}\right)\frac{k^{\left(\frac{2}{\nu}+1\right)}}{4\pi^2\nu^3}. \tag{6.143}$$

From (6.142), (6.128) and (6.143), we obtain the bound

$$\langle\Psi|H|\Psi\rangle \leqslant -\left(\frac{me^4}{2\hbar^2}\right)\frac{k^{\left(\frac{2}{\nu}+1\right)}}{4\pi^2\nu^3}. \tag{6.144}$$

Since $N = k\left(1+\frac{\varepsilon}{n}\right)^{\nu}$, then

$$k^{\left(\frac{2}{\nu}+1\right)} = \frac{N^{(2+\nu)/\nu}}{\left(1+\frac{\varepsilon}{n}\right)^{2+\nu}}. \tag{6.145}$$

Since $E_{N,N} \leqslant \langle\Psi|H|\Psi\rangle$, and by substituting (6.145) in (6.144), then

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{(2+\nu)/\nu}}{4\pi^2\nu^3}\frac{1}{\left(1+\frac{\varepsilon}{n}\right)^{2+\nu}}. \tag{6.146}$$

Since $0 \leqslant \varepsilon < 1$ and $n \geqslant 1$, therefore

$$\left(1+\frac{\varepsilon}{n}\right)^{2+\nu} \leqslant 2^{2+\nu}$$

or

$$\frac{1}{\left(1+\frac{\varepsilon}{n}\right)^{2+\nu}} \geqslant \frac{1}{4(2)^{\nu}}. \tag{6.147}$$

Upon substituting (6.147) in (6.146), we obtain the following upper bound for the ground-state energy

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{(2+\nu)/\nu}}{16\pi^2\nu^3(2)^\nu}. \tag{6.148}$$

# CHAPTER VII

# CONCLUSION AND DISCUSSION

In this work, we have provided a detailed rigorous quantitative analysis of the collapse of "bosonic matter" in the bulk with Coulomb interactions. To do this, we have derived several upper bounds for the exact ground-state energy of such matter as functions of the number of the charged particles involved which may be as large as $10^{23}$ or even more, and we have also considered numbers as low as 8. As every step in the derivations was justified and the results were stated in the form of Propositions, the complexity encountered in the analysis were of the following nature: (i) Estimates were needed that control the negative part of the interaction of the Hamiltonians in question over their positive repulsive parts and the positive kinetic energies part. (ii) Both signs of the couplings were needed which complicated the investigation to a large extent. (iii) Special choices of trial functions were needed to be considered in an optimal way. (iv) Detailed estimates were needed for counting the states available for the trial wavefunctions corresponding to large numbers of particles as large as $10^{23}$ and even more. (v) Several new Theorems had to be introduced and proved, one of which we have found is an unsolved problem in mathematics which we had to modify in order to obtain the upper bound of the ground-state energy of central importance in Chapter IV and is quoted below in (7.1). As mentioned above, several upper bounds of the exact ground-state energy were derived in this thesis. We have been able to obtain a new bound corresponding to the Hamiltonian in (1.1) which improved the classic bound of Dyson by a factor of 31. This result was also extended for the first time in $2D$. An upper bound of central importance in the entire project was obtained in Chapter IV for the corresponding Hamiltonian in

(1.2) with fixed positive charges, given by

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{5/3}}{27\pi^2} \tag{7.1}$$

for $N \geqslant 10^{12}$, in $3D$, where $m$ is the smallest of the masses of the negative charged particles involved in the system. Other bounds were also obtained in analogy to (7.1) valid for $N$ as low as 8. To obtain (7.1), we had to group our particles, which may be as large as $10^{23}$ or even more, in a very special way to obtain our bound. One of the interesting results embodied in (7.1) is that the more matter is added to the system, the more negative the ground-state energy becomes and this occurs in a non-linear way and a more violent collapse is encountered. This is unlike the situations with standard fermionic matter were the ground-state energy becomes more negative only linearly and guarantees its stability. We have proved for the first time that instability of "bosonic matter" is not a characteristic of the dimensionality of space and is not a mere property of the dimension of space chosen by nature. Our interest in this latter investigation came about our curiosity in finding out whether the instability of such matter in $3D$ would change in other dimensions from an "implosive" to a "stable" or even to an "explosive" phase. Our rigorous investigation shows that this does not happen. As is well known, there has been much interest in recent years in physics in arbitrary dimensions such as in $2D$ superconductivity and eleven dimensions of supersymmetric string field theories. It has thus become important for us to investigate the nature of such matter in arbitrary dimensions in the simplest case when the system is not being subjected to stringent constrained statistics. In Chapter VI, we have derived the following remarkable inequality in a unified manner valid in all dimensions $\nu$:

$$E_{N,N} < -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{(2+\nu)/\nu}}{16\pi^2\nu^3(2)^\nu} \tag{7.2}$$

and for all $N \geqslant (2)^{\nu}$, where $m$, as before, is the smallest of the masses of the negatively charged particles, corresponding to the Hamiltonian in (1.2). As in all of our derivations, the bounds obtained are for the exact ground-state energy $E_{N,N}$ and the result embodied in (7.2), as a proven Theorem, we hope will be valuable in the future of the quantum physics of bulk matter. In particular we note, that the collapse of "bosonic matter" is more violent in $2D$ than $3D$ and becomes less violent with increasing $\nu$ for large $N$. It states, for example, that not even two-dimensional stable planar configurations may arise. Our precise estimate in (7.1) together with the lower bound obtained by our group (Manoukian and Sirininlakul, 2005) as a byproduct of its investigation on fermionic matter (see Appendix C) allows us to estimate the range of the energy released upon the collapse of two objects of relatively small $N$ and is found to be of several orders of magnitude higher than that of the Hiroshima and Nagasaki bombs in conformity with Dyson's famous statement quoted in the introduction to this project and such matter is surely unpleasant stuff to have around the house. The energy release estimated is even higher than that of the Tsunami disaster off the west coast of northern Sumatra on December 26, 2004. As is often stated, the Spin and Statistics connection is indeed a very clever design of nature and without it the whole of the universe would collapse.

# REFERENCES

# REFERENCES


Balàzs, N. L. (1967). Formation of stable molecules within the statistical theory of atoms. **Physical Review** 156 (1): 42–47.

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.

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.]

Eidelman, S. et al. (Particle Data Group). (2004). Review of Particle Physics. **Physics Letters B** 592 (1–4): 1–1109.

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. **Review 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.

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.

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. **Review 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. (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. **Inventiones 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. 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.

Manoukain, E. B. and Sirininlakul, S. (2005). 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.

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.

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.

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**. 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.

Wightman, A. S. (1956). Quantum field theory in terms of vacuum expectation values. **Physical Review** 101 (2): 860–866.

Wikipedia, the Free Encyclopedia (2005). **Megaton** [On-line]. Available: `http://en.wikipedia.org/wiki/Megaton`

Yosida, K. (1980). **Functional analysis** (6th ed.). Berlin: Springer-Verlag.

# APPENDICES

# APPENDIX A

# NUMBER OF DISTINCT STATES IN $3D$

Table A.1: Number of distinct states for $6 \leqslant n^2 \leqslant 51$

| $n_1$ | $n_2$ | $n_3$ | $n$ | $n^2$ | $k$ |
|---|---|---|---|---|---|
| 1 | 1 | 2 | 2.449490 | 6 | 3 |
| 1 | 2 | 2 | 3.000000 | 9 | 6 |
| 1 | 1 | 3 | 3.316625 | 11 | 9 |
| 2 | 2 | 2 | 3.464102 | 12 | 10 |
| 1 | 2 | 3 | 3.741657 | 14 | 16 |
| 2 | 2 | 3 | 4.123106 | 17 | 19 |
| 1 | 1 | 4 | 4.242641 | 18 | 22 |
| 1 | 3 | 3 | 4.358899 | 19 | 25 |
| 1 | 2 | 4 | 4.582576 | 21 | 31 |
| 2 | 3 | 3 | 4.690416 | 22 | 34 |
| 2 | 2 | 4 | 4.898979 | 24 | 37 |
| 1 | 3 | 4 | 5.099020 | 26 | 43 |
| 3 | 3 | 3 | 5.196152 | 27 | 47 |
| 2 | 3 | 4 | 5.385165 | 29 | 53 |

| $n_1$ | $n_2$ | $n_3$ | $n$ | $n^2$ | $k$ |
|---|---|---|---|---|---|
| 1 | 2 | 5 | 5.477226 | 30 | 59 |
| 1 | 4 | 4 | 5.744563 | 33 | 65 |
| 3 | 3 | 4 | 5.830952 | 34 | 68 |
| 1 | 3 | 5 | 5.916080 | 35 | 74 |
| 2 | 4 | 4 | 6.000000 | 36 | 77 |
| 2 | 3 | 5 | 6.164414 | 38 | 86 |
| 3 | 4 | 4 | 6.403124 | 41 | 95 |
| 1 | 4 | 5 | 6.480741 | 42 | 101 |
| 3 | 3 | 5 | 6.557439 | 43 | 104 |
| 2 | 2 | 6 | 6.633250 | 44 | 107 |
| 2 | 4 | 5 | 6.708204 | 45 | 113 |
| 1 | 3 | 6 | 6.782330 | 46 | 119 |
| 4 | 4 | 4 | 6.928203 | 48 | 120 |
| 1 | 1 | 7 | 7.141428 | 51 | 138 |

Table A.2: Number of distinct states for $53 \leqslant n^2 \leqslant 101$

| $n_1$ | $n_2$ | $n_3$ | $n$ | $n^2$ | $k$ |
|---|---|---|---|---|---|
| 1 | 4 | 6 | 7.280110 | 53 | 144 |
| 3 | 3 | 6 | 7.348469 | 54 | 156 |
| 2 | 4 | 6 | 7.483315 | 56 | 162 |
| 4 | 4 | 5 | 7.549834 | 57 | 168 |
| 3 | 5 | 5 | 7.681146 | 59 | 177 |
| 3 | 4 | 6 | 7.810250 | 61 | 183 |
| 2 | 3 | 7 | 7.874008 | 62 | 195 |
| 2 | 5 | 6 | 8.062258 | 65 | 201 |
| 4 | 5 | 5 | 8.124038 | 66 | 213 |
| 3 | 3 | 7 | 8.185353 | 67 | 216 |
| 4 | 4 | 6 | 8.246211 | 68 | 219 |
| 2 | 4 | 7 | 8.306624 | 69 | 231 |
| 3 | 5 | 6 | 8.366600 | 70 | 237 |
| 2 | 2 | 8 | 8.485281 | 72 | 240 |
| 1 | 6 | 6 | 8.544004 | 73 | 243 |
| 3 | 4 | 7 | 8.602325 | 74 | 255 |
| 5 | 5 | 5 | 8.660254 | 75 | 262 |
| 2 | 6 | 6 | 8.717798 | 76 | 265 |

| $n_1$ | $n_2$ | $n_3$ | $n$ | $n^2$ | $k$ |
|---|---|---|---|---|---|
| 4 | 5 | 6 | 8.774964 | 77 | 277 |
| 2 | 5 | 7 | 8.831761 | 78 | 283 |
| 4 | 4 | 7 | 9.000000 | 81 | 295 |
| 3 | 3 | 8 | 9.055385 | 82 | 298 |
| 3 | 5 | 7 | 9.110434 | 83 | 307 |
| 2 | 4 | 8 | 9.165151 | 84 | 313 |
| 5 | 5 | 6 | 9.273618 | 86 | 328 |
| 4 | 6 | 6 | 9.380832 | 88 | 331 |
| 3 | 4 | 8 | 9.433981 | 89 | 346 |
| 4 | 5 | 7 | 9.486833 | 90 | 358 |
| 1 | 3 | 9 | 9.539392 | 91 | 364 |
| 2 | 5 | 8 | 9.643651 | 93 | 370 |
| 3 | 6 | 7 | 9.695360 | 94 | 382 |
| 4 | 4 | 8 | 9.797959 | 96 | 385 |
| 5 | 6 | 6 | 9.848858 | 97 | 388 |
| 3 | 5 | 8 | 9.899495 | 98 | 400 |
| 5 | 5 | 7 | 9.949874 | 99 | 409 |
| 4 | 6 | 7 | 10.049876 | 101 | 427 |

Table A.3: Number of distinct states for $9933 \leqslant n^2 \leqslant 9974$

| $n_1$ | $n_2$ | $n_3$ | $n$ | $n^2$ | $k$ |
|---|---|---|---|---|---|
| 12 | 68 | 72 | 99.759711 | 9952 | 508133 |
| 2 | 43 | 90 | 99.764723 | 9953 | 508259 |
| 1 | 47 | 88 | 99.769735 | 9954 | 508475 |
| 3 | 45 | 89 | 99.774746 | 9955 | 508523 |
| 8 | 26 | 96 | 99.779757 | 9956 | 508589 |
| 2 | 47 | 88 | 99.784768 | 9957 | 508703 |
| 3 | 43 | 90 | 99.789779 | 9958 | 508757 |
| 8 | 50 | 86 | 99.799800 | 9960 | 508805 |
| 4 | 12 | 99 | 99.804810 | 9961 | 508901 |
| 3 | 47 | 88 | 99.809819 | 9962 | 509027 |
| 1 | 41 | 91 | 99.814829 | 9963 | 509105 |
| 6 | 18 | 98 | 99.819838 | 9964 | 509141 |
| 4 | 43 | 90 | 99.824847 | 9965 | 509237 |
| 1 | 19 | 98 | 99.829855 | 9966 | 509393 |
| 2 | 19 | 98 | 99.844880 | 9969 | 509483 |
| 5 | 12 | 99 | 99.849887 | 9970 | 509543 |
| 1 | 13 | 99 | 99.854895 | 9971 | 509678 |
| 8 | 38 | 92 | 99.859902 | 9972 | 509720 |
| 1 | 54 | 84 | 99.864909 | 9973 | 509786 |
| 1 | 57 | 82 | 99.869915 | 9974 | 510041 |

Table A.4: Number of distinct states for $9976 \leqslant n^2 \leqslant 10000$

| $n_1$ | $n_2$ | $n_3$ | $n$ | $n^2$ | $k$ |
|---|---|---|---|---|---|
| 2 | 54 | 84 | 99.879928 | 9976 | 510071 |
| 2 | 57 | 82 | 99.884934 | 9977 | 510185 |
| 4 | 41 | 91 | 99.889939 | 9978 | 510275 |
| 3 | 13 | 99 | 99.894945 | 9979 | 510335 |
| 3 | 54 | 84 | 99.904955 | 9981 | 510557 |
| 1 | 66 | 75 | 99.909959 | 9982 | 510605 |
| 2 | 66 | 75 | 99.924972 | 9985 | 510695 |
| 1 | 24 | 97 | 99.929975 | 9986 | 510788 |
| 1 | 31 | 95 | 99.934979 | 9987 | 510866 |
| 4 | 54 | 84 | 99.939982 | 9988 | 510908 |
| 2 | 24 | 97 | 99.944985 | 9989 | 511070 |
| 2 | 31 | 95 | 99.949987 | 9990 | 511166 |
| 8 | 18 | 98 | 99.959992 | 9992 | 511223 |
| 1 | 34 | 94 | 99.964994 | 9993 | 511301 |
| 3 | 24 | 97 | 99.969995 | 9994 | 511439 |
| 3 | 31 | 95 | 99.974997 | 9995 | 511559 |
| 2 | 34 | 94 | 99.979998 | 9996 | 511613 |
| 4 | 66 | 75 | 99.984999 | 9997 | 511661 |
| 1 | 14 | 99 | 99.989999 | 9998 | 511763 |
| 36 | 48 | 80 | 100.000000 | 10000 | 511775 |

# APPENDIX B

# NUMBER OF DISTINCT STATES IN $2D$

Table B.1: Number of distinct states for $5 \leqslant n^2 \leqslant 58$

| $n_1$ | $n_2$ | $n$ | $n^2$ | $k$ | $n_1$ | $n_2$ | $n$ | $n^2$ | $k$ |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 2.236067977 | 5 | 2 | 4 | 4 | 5.656854249 | 32 | 19 |
| 2 | 2 | 2.828427125 | 8 | 3 | 3 | 5 | 5.830951895 | 34 | 21 |
| 1 | 3 | 3.16227766 | 10 | 5 | 1 | 6 | 6.08276253 | 37 | 23 |
| 2 | 3 | 3.605551275 | 13 | 7 | 2 | 6 | 6.32455532 | 40 | 25 |
| 1 | 4 | 4.123105626 | 17 | 9 | 4 | 5 | 6.403124237 | 41 | 27 |
| 3 | 3 | 4.242640687 | 18 | 10 | 3 | 6 | 6.708203932 | 45 | 29 |
| 2 | 4 | 4.472135955 | 20 | 12 | 5 | 5 | 7.071067812 | 50 | 32 |
| 3 | 4 | 5 | 25 | 14 | 4 | 6 | 7.211102551 | 52 | 34 |
| 1 | 5 | 5.099019514 | 26 | 16 | 2 | 7 | 7.280109889 | 53 | 36 |
| 2 | 5 | 5.385164807 | 29 | 18 | 3 | 7 | 7.615773106 | 58 | 38 |

Table B.2: Number of distinct states for $61 \leqslant n^2 \leqslant 178$

| $n_1$ | $n_2$ | $n$ | $n^2$ | $k$ | $n_1$ | $n_2$ | $n$ | $n^2$ | $k$ |
|---|---|---|---|---|---|---|---|---|---|
| 5 | 6 | 7.810249676 | 61 | 40 | 6 | 9 | 10.81665383 | 117 | 82 |
| 4 | 7 | 8.062257748 | 65 | 44 | 1 | 11 | 11.04536102 | 122 | 84 |
| 2 | 8 | 8.246211251 | 68 | 46 | 5 | 10 | 11.18033989 | 125 | 88 |
| 6 | 6 | 8.485281374 | 72 | 47 | 8 | 8 | 11.3137085 | 128 | 89 |
| 3 | 8 | 8.544003745 | 73 | 49 | 7 | 9 | 11.40175425 | 130 | 93 |
| 5 | 7 | 8.602325267 | 74 | 51 | 6 | 10 | 11.66190379 | 136 | 95 |
| 4 | 8 | 8.94427191 | 80 | 53 | 4 | 11 | 11.70469991 | 137 | 97 |
| 1 | 9 | 9.055385138 | 82 | 55 | 8 | 9 | 12.04159458 | 145 | 101 |
| 6 | 7 | 9.219544457 | 85 | 59 | 5 | 11 | 12.08304597 | 146 | 103 |
| 5 | 8 | 9.433981132 | 89 | 61 | 2 | 12 | 12.16552506 | 148 | 105 |
| 3 | 9 | 9.486832981 | 90 | 63 | 7 | 10 | 12.20655562 | 149 | 107 |
| 4 | 9 | 9.848857802 | 97 | 65 | 3 | 12 | 12.36931688 | 153 | 109 |
| 7 | 7 | 9.899494937 | 98 | 66 | 6 | 11 | 12.52996409 | 157 | 111 |
| 6 | 8 | 10 | 100 | 68 | 4 | 12 | 12.64911064 | 160 | 113 |
| 1 | 10 | 10.04987562 | 101 | 70 | 9 | 9 | 12.72792206 | 162 | 114 |
| 2 | 10 | 10.19803903 | 104 | 72 | 8 | 10 | 12.80624847 | 164 | 116 |
| 5 | 9 | 10.29563014 | 106 | 74 | 5 | 12 | 13 | 169 | 118 |
| 3 | 10 | 10.44030651 | 109 | 76 | 7 | 11 | 13.03840481 | 170 | 122 |
| 7 | 8 | 10.63014581 | 113 | 78 | 2 | 13 | 13.15294644 | 173 | 124 |
| 4 | 10 | 10.77032961 | 116 | 80 | 3 | 13 | 13.34166406 | 178 | 126 |

# APPENDIX C

# THE MANOUKIAN-SIRININLAKUL LOWER BOUND FOR THE GROUND-STATE ENERGY FOR BOSONIC MATTER

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 their derivation of the lower bound.

The Hamiltonian in question is given by

$$H' = \sum_{i=1}^{N} \frac{\mathbf{P}_i^2}{2M} + \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} - \sum_{j=1}^{N}\sum_{i=1}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{R}_j|} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{C.1}$$

where the $\mathbf{x}_i$ denote the positions of the negatively charged particles, and the $\mathbf{R}_j$ those of the positive charges.

Since $\dfrac{\mathbf{P}_i^2}{2M} \geqslant 0$ is a *positive* operator, $H'$ is bounded from below by the Hamiltonian

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} - \sum_{j=1}^{N}\sum_{i=1}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{R}_j|} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|} + \sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|} \tag{C.2}$$

which is the *same* Hamiltonian used in Chapter IV, V and VI. For any positive real numbers $A_1, \ldots, A_k$ they derive the following lower bound for the repulsive parts of the Coulomb potentials

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

$$\sum_{i<j}^{k} \frac{e^2 A_i A_j}{|\mathbf{R}_i - \mathbf{R}_j|} \geqslant \sum_{j=1}^{k} e^2 A_j \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}_j|} - \frac{2\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{\lambda e^2}{2} \sum_{j=1}^{k} A_j^2 - \frac{e^2}{2} \int \mathrm{d}^3\mathbf{x}\, \mathrm{d}^3\mathbf{x}'\, \rho(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \rho(\mathbf{x}') \tag{C.4}$$

Here

$$\rho(\mathbf{x}) = N \int \mathrm{d}^3\mathbf{x}_2 \ldots \mathrm{d}^3\mathbf{x}_N \, \big|\psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)\big|^2 \tag{C.5}$$

This is a generalization of an inequality derived by Hertel, Lieb and Thirring (1975).

In particular for $k = N$, $A_1 = \ldots = A_N = 1$, (C.2), (C.3) and (C.4) lead to

$$\langle \psi | H | \psi \rangle \geqslant T - \frac{4\pi e^2}{\lambda^2} \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{\lambda e^2}{2}\,(2N) \tag{C.6}$$

where $T = \left\langle \psi \middle| \sum_j \frac{\mathbf{p}_j^2}{2m} \middle| \psi \right\rangle$. Optimizing over $\lambda$, this gives the remarkably simple bound

$$\langle \psi | H | \psi \rangle \geqslant T - \frac{3\pi^{1/3} e^2}{2^{2/3}}\,(2N)^{2/3} \left( \int \mathrm{d}^3\mathbf{x}\, \rho^2(\mathbf{x}) \right)^{1/3} \tag{C.7}$$

[It is of utmost importance that $k \geqslant 2$, otherwise the $\sum_{i<j}^{N} \frac{e^2}{|\mathbf{R}_i - \mathbf{R}_j|}$ term will be absent in the expression for $H$ in (C.2), and there will be an additional term $-e^2 N \int \mathrm{d}^3\mathbf{x}\, \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{R}|}$ on the right-hand side of the inequality in (C.7), after having

omitted the positive term $\frac{e^2}{2}\int \mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{x}'\,\rho(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\rho(\mathbf{x}')$. 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 an integral of $\rho^2$.

To the above end, given a function $g(\mathbf{x}) \geqslant 0$, the Schwinger bound (Schwinger, 1961) for the number of eigenvalues (counting degeneracy) $\leqslant -\xi$, (if any) of a Hamiltonian $\frac{\mathbf{p}^2}{2m} - g(\mathbf{x})$, for $\xi > 0$, satisfies the inequality

$$N_{-\xi}\left(\frac{\mathbf{p}^2}{2m} - g(\mathbf{x})\right) \leqslant \left(\frac{m}{2\hbar^2}\right)^{3/2}\frac{1}{\pi\sqrt{\xi}}\int \mathrm{d}^3\mathbf{x}\; g^2(\mathbf{x}). \tag{C.8}$$

Hence for any $\delta > 0$, we may choose

$$-\xi = -\frac{(1+\delta)}{\pi^2}\left(\frac{m}{2\hbar^2}\right)^3\left(\int \mathrm{d}^3\mathbf{x}\; g^2(\mathbf{x})\right)^2, \tag{C.9}$$

so that $N_{-\xi}\left(\frac{\mathbf{p}^2}{2m} - g(\mathbf{x})\right) < 1$, which implies that $N_{-\xi}\left(\frac{\mathbf{p}^2}{2m} - g(\mathbf{x})\right) = 0$, and the right-hand side of (C.9) provides a lower bound to the spectrum of $\left(\frac{\mathbf{p}^2}{2m} - g(\mathbf{x})\right)$ since its spectrum would then be empty for energies $\leqslant -\xi$.

Accordingly, with

$$g(\mathbf{x}) = \frac{4}{3}T\frac{\rho(\mathbf{x})}{\left(\int \mathrm{d}^3\mathbf{x}\;\rho^2(\mathbf{x})\right)}, \tag{C.10}$$

we obtain from (C.9), the following inequality involving $T$, by noting, in the process, that for bosons, we may put all of the $N$ particles at the bottom of the spectrum of $\left(\frac{\mathbf{p}^2}{2m} - g(\mathbf{x})\right)$,

$$T \geqslant \frac{3\hbar^2}{2mN^{1/3}}\left(\frac{\pi}{2}\right)^{2/3}\frac{1}{1+\varepsilon}\left(\int \mathrm{d}^3\mathbf{x}\;\rho^2(\mathbf{x})\right)^{2/3}, \tag{C.11}$$

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

Upon setting $\left(\int \mathrm{d}^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{1/3} \equiv A$ and $\dfrac{3\hbar^2}{2m}\left(\dfrac{\pi}{2}\right)^{2/3}\dfrac{1}{1+\varepsilon} \equiv c$, (C.7), (C.11) lead to ($k \geqslant 2$)

$$\begin{aligned}
\langle\psi|H|\psi\rangle &\geqslant \frac{c}{N^{1/3}}A^2 - \frac{3}{2^{2/3}}e^2\pi^{1/3}(2N)^{2/3}A \\
&= \frac{c}{N^{1/3}}\left(A - \frac{3e^2\pi^{1/3}N^{1/3}}{2^{5/3}c}(2N)^{2/3}\right)^2 - \frac{9}{8}\frac{e^4}{2^{1/3}}\frac{\pi^{2/3}}{c}N^{1/3}(2N)^{4/3} \\
&> -\frac{9}{8}\frac{e^4}{2^{1/3}}\frac{\pi^{2/3}}{c}N^{1/3}(2N)^{4/3} \\
&= -1.89\left(\frac{me^4}{2\hbar^2}\right)N^{1/3}(2N)^{4/3}\,.
\end{aligned} \tag{C.12}$$

Then,

$$\begin{aligned}
\langle\psi|H|\psi\rangle &\geqslant -1.89\left(\frac{me^4}{2\hbar^2}\right)N^{1/3}(2N)^{4/3} \\
&= -4.7625\left(\frac{me^4}{2\hbar^2}\right)N^{5/3}
\end{aligned} \tag{C.13}$$

where we have taken $\varepsilon$ arbitrarily small for $N$ sufficiently large to be used below.

From Chapter IV, we have the upper bound for the ground-state energy for $N \sim 10^{23}$ or larger

$$E_{N,N} \leqslant -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{5/3}}{27\pi^2} \tag{C.14}$$

Then for the exact ground-state energy of bosonic system corresponding to our Hamiltonian, with a common mass $m$ of negatively charged particles, we have the following range

$$-4.7625\left(\frac{me^4}{2\hbar^2}\right)N^{5/3} \leqslant E_{N,N} \leqslant -\left(\frac{me^4}{2\hbar^2}\right)\frac{N^{5/3}}{27\pi^2}$$

or

$$-4.7625\left(\frac{me^4}{2\hbar^2}\right)N^{5/3} \leqslant E_{N,N} \leqslant -0.0038\left(\frac{me^4}{2\hbar^2}\right)N^{5/3} \tag{C.15}$$

Therefore the energy released upon collapse of two bodies each containing $(N+N)$ particles will be between $0.0038\left(\frac{me^4}{2\hbar^2}\right)\left[(2N)^{5/3}-2(N)^{5/3}\right]$ and $4.7625\left(\frac{me^4}{2\hbar^2}\right)\left[(2N)^{5/3}-2(N)^{5/3}\right]$.

To obtain an order of magnitude estimate suppose that $N \sim 10^{23}$. For definiteness consider the minimum energy release and take $m$ to be of the order of the magnitude of the mass of the electron. A larger mass will lead even to a larger energy release. This leads to an energy release about $2.095 \times 10^{18}$ J. We recall that this energy bound is based on fixed positive charges, i.e., with corresponding *arbitrary large* masses. The rest mass energy of the total system of positively and negatively charged bosons is $\sum_{i=1}^{2N} M_i c^2$. This is to be compared with our binding energy estimate $0.0038\left(\frac{me^4}{2\hbar^2}\right)N^{5/2}$, where $m$ is the smallest mass of the negatively charged bosons. Accordingly, the total rest mass energy will be greater than our binding energy estimate for $\frac{1}{m}\sum_{i=1}^{2N} M_i \geqslant \frac{\alpha^2 N^{5/3}}{526.4}$, where $\alpha$ is the fine-structure constant. For $N \sim 10^{23}$, this gives the lower bound $\frac{1}{m}\sum_{i=1}^{2N} M_i \geqslant 2 \times 10^{31}$ as a *sufficiency* condition.

In terms of TNT units, (1 kiloton of TNT $= 4.184 \times 10^{12}$ J)*), the energy released is between

$$5.007 \times 10^5 \text{ kilotons of TNT and } 6.2767 \times 10^8 \text{ kilotons of TNT} \tag{C.16}$$

This is to be compared with the Hiroshima bomb which was about 13 kilotons of TNT, and the Nagasaki bomb which was about 20 kilotons of TNT which much smaller than the minimum energy estimate in (C.16). The energy content of the Tsunami disaster off west coast of northern Sumatra on December 26, 2004 was about $4.75 \times 10^5$ kilotons of TNT.

---

*) cf. Wikipedia (2005)

# APPENDIX D

# SOME BASIC INTEGRALS AND SUMS ENCOUNTERED IN THIS THESIS

In this appendix, we spell out details of computations of some integrals and sums used in this thesis :

$$\int \mathrm{d}^3\mathbf{x}\ \left|\phi(\mathbf{x})\right|^2 = \left(\frac{1}{L}\right)^3 \int_{-L}^{L}\mathrm{d}x_1 \int_{-L}^{L}\mathrm{d}x_2 \int_{-L}^{L}\mathrm{d}x_3\ \cos^2\left(\frac{\pi x_1}{2L}\right)\cos^2\left(\frac{\pi x_2}{2L}\right)\cos^2\left(\frac{\pi x_3}{2L}\right)$$

$$= \left(\frac{1}{L}\right)^3 \left[\int_{-L}^{L}\mathrm{d}x\ \cos^2\left(\frac{\pi x}{2L}\right)\right]^3$$

$$= \left(\frac{1}{L}\right)^3 \left[\frac{1}{2}\int_{-L}^{L}\mathrm{d}x\left(1+\cos\left(\frac{\pi x}{L}\right)\right)\right]^3$$

$$= \left(\frac{1}{2L}\right)^3 \left[2L + \frac{L}{\pi}\sin\left(\frac{\pi x}{L}\right)\Big|_{x=-L}^{L}\right]^3$$

$$= \left(\frac{1}{2L}\right)^3 \left[2L + \frac{L}{\pi}\left(\sin(\pi) - \sin(-\pi)\right)\right]^3$$

$$= \left(\frac{1}{2L}\right)^3 (2L)^3$$

$$\int \mathrm{d}^3\mathbf{x}\ \left|\phi(\mathbf{x})\right|^2 = 1 \tag{D.1}$$

For

$$a_i = L_{ji} + L_0$$

$$b_i = L_{ji} - L_0 \tag{D.2}$$

then, we have

$$\begin{aligned}
\int_{a_i}^{b_i} \mathrm{d}x_i \; \sin^2\left(\frac{\pi(x_i - L_{ji})}{2L_0}\right) &= \frac{1}{2}\int_{a_i}^{b_i} \mathrm{d}x_i \; \left[1 - \cos\left(\frac{\pi(x_i - L_{ji})}{L_0}\right)\right] \\
&= \frac{1}{2}\left[\int_{a_i}^{b_i} \mathrm{d}x_i - \int_{a_i}^{b_i} \mathrm{d}x_i \; \cos\left(\frac{\pi(x_i - L_{ji})}{L_0}\right)\right] \\
&= \frac{1}{2}\left[\big(b_i - a_i\big) - \frac{L_0}{\pi}\sin\left(\frac{\pi(x_i - L_{ji})}{L_0}\right)\Bigg|_{x_i = a_i}^{b_i}\right] \\
&= \frac{1}{2}\big(L_{ji} + L_0 - L_{ji} + L_0\big) \\
&\quad - \frac{1}{2}\frac{L_0}{\pi}\left[\sin\left(\frac{\pi(L_{ji} + L_0 - L_{ji})}{L_0}\right)\right. \\
&\quad \left. - \sin\left(\frac{\pi(L_{ji} - L_0 - L_{ji})}{L_0}\right)\right] \\
&= \frac{1}{2}(2L_0) - \frac{1}{2}\frac{L_0}{\pi}\left[\sin(\pi) - \sin(-\pi)\right]
\end{aligned}$$

$$\int_{a_i}^{b_i} \mathrm{d}x_i \; \sin^2\left(\frac{\pi(x_i - L_{ji})}{2L_0}\right) = L_0 \tag{D.3}$$

and

$$\begin{aligned}
\int_{a_i}^{b_i} \mathrm{d}x_i \; \cos^2\left(\frac{\pi(x_i - L_{ji})}{2L_0}\right) &= \frac{1}{2}\int_{a_i}^{b_i} \mathrm{d}x_i \; \left[1 + \cos\left(\frac{\pi(x_i - L_{ji})}{L_0}\right)\right] \\
&= \frac{1}{2}\left[\int_{a_i}^{b_i} \mathrm{d}x_i + \int_{a_i}^{b_i} \mathrm{d}x_i \; \cos\left(\frac{\pi(x_i - L_{ji})}{L_0}\right)\right] \\
&= \frac{1}{2}\left[\big(b_i - a_i\big) + \frac{L_0}{\pi}\sin\left(\frac{\pi(x_i - L_{ji})}{L_0}\right)\Bigg|_{x_i = a_i}^{b_i}\right]
\end{aligned}$$

$$= \frac{1}{2}\left(L_{ji} + L_0 - L_{ji} + L_0\right)$$

$$+ \frac{1}{2}\frac{L_0}{\pi}\left[\sin\left(\frac{\pi(L_{ji} + L_0 - L_{ji})}{L_0}\right)\right.$$

$$\left. - \sin\left(\frac{\pi(L_{ji} - L_0 - L_{ji})}{L_0}\right)\right]$$

$$= \frac{1}{2}\left(2L_0\right) + \frac{1}{2}\frac{L_0}{\pi}\left[\sin\left(\pi\right) - \sin\left(-\pi\right)\right]$$

$$\int_{a_i}^{b_i} \mathrm{d}x_i \ \cos^2\left(\frac{\pi(x_i - L_{ji})}{2L_0}\right) = L_0 \tag{D.4}$$

$$\frac{e^2}{D}\sum_{i<j}^{N-k} 1 = \frac{e^2}{D}\sum_{j=2}^{N-k}\sum_{i=1}^{j-1} 1$$

$$= \frac{e^2}{D}\sum_{j=2}^{N-k}(j-1)$$

$$= \frac{e^2}{D}\left[\sum_{j=1}^{N-k}(j-1) - \sum_{j=1}^{1}(j-1)\right]$$

$$= \frac{e^2}{D}\left[\sum_{j=1}^{N-k} j - \sum_{j=1}^{N-k} 1\right]$$

$$= \frac{e^2}{D}\left[\frac{(N-k)(N-k+1)}{2} - (N-k)\right]$$

$$= \frac{e^2}{D}(N-k)\left[\frac{(N-k+1)}{2} - 1\right]$$

$$\frac{e^2}{D}\sum_{i<j}^{N-k} 1 = \frac{e^2(N-k)(N-k-1)}{2D} \tag{D.5}$$

For

$$\boldsymbol{\nabla}\phi(\mathbf{x}) = \frac{1}{L^{\nu/2}}\left[\hat{\mathbf{j}}_1\frac{\partial}{\partial x_1}\cos\left(\frac{\pi x_1}{2L}\right)\ldots\cos\left(\frac{\pi x_\nu}{2L}\right)\right.$$
$$+$$
$$\vdots$$
$$\left.+\,\hat{\mathbf{j}}_\nu\frac{\partial}{\partial x_\nu}\cos\left(\frac{\pi x_1}{2L}\right)\ldots\cos\left(\frac{\pi x_\nu}{2L}\right)\right]$$
$$= -\frac{\pi}{2L}\frac{1}{L^{\nu/2}}\left[\hat{\mathbf{j}}_1\sin\left(\frac{\pi x_1}{2L}\right)\cos\left(\frac{\pi x_2}{2L}\right)\ldots\cos\left(\frac{\pi x_\nu}{2L}\right)\right.$$
$$+$$
$$\vdots$$
$$\left.+\,\hat{\mathbf{j}}_\nu\cos\left(\frac{\pi x_1}{2L}\right)\cos\left(\frac{\pi x_2}{2L}\right)\ldots\sin\left(\frac{\pi x_\nu}{2L}\right)\right] \tag{D.6}$$

then

$$\left|\boldsymbol{\nabla}\phi(\mathbf{x})\right|^2 = \left(\frac{\pi}{2L}\right)^2\left(\frac{1}{L}\right)^\nu\left[\sin^2\left(\frac{\pi x_1}{2L}\right)\cos^2\left(\frac{\pi x_2}{2L}\right)\ldots\cos^2\left(\frac{\pi x_\nu}{2L}\right)\right.$$
$$+$$
$$\vdots$$
$$\left.+\cos^2\left(\frac{\pi x_1}{2L}\right)\cos^2\left(\frac{\pi x_2}{2L}\right)\ldots\sin^2\left(\frac{\pi x_\nu}{2L}\right)\right] \tag{D.7}$$

and then we obtain,

$$\int \mathrm{d}^\nu\mathbf{x}\;\left|\boldsymbol{\nabla}\phi(\mathbf{x})\right|^2$$
$$= \left(\frac{\pi}{2L}\right)^2\left(\frac{1}{L}\right)^\nu\left[\int_{-L}^{L}\mathrm{d}x_1\ldots\int_{-L}^{L}\mathrm{d}x_\nu\;\sin^2\left(\frac{\pi x_1}{2L}\right)\cos^2\left(\frac{\pi x_2}{2L}\right)\ldots\cos^2\left(\frac{\pi x_\nu}{2L}\right)\right.$$
$$+$$

$$\vdots$$

$$+ \int_{-L}^{L} \mathrm{d}x_1 \ldots \int_{-L}^{L} \mathrm{d}x_\nu \; \cos^2\left(\frac{\pi x_1}{2L}\right) \cos^2\left(\frac{\pi x_2}{2L}\right) \ldots \sin^2\left(\frac{\pi x_\nu}{2L}\right)\Bigg]$$

$$= \nu \left(\frac{\pi}{2L}\right)^2 \left(\frac{1}{L}\right)^\nu \int_{-L}^{L} \mathrm{d}x_1 \ldots \int_{-L}^{L} \mathrm{d}x_\nu \; \sin^2\left(\frac{\pi x_1}{2L}\right) \cos^2\left(\frac{\pi x_2}{2L}\right) \ldots \cos^2\left(\frac{\pi x_\nu}{2L}\right)$$

$$= \nu \left(\frac{\pi}{2L}\right)^2 \left(\frac{1}{L}\right)^\nu \left[\int_{-L}^{L} \mathrm{d}x_1 \; \sin^2\left(\frac{\pi x_1}{2L}\right)\right] \left[\int_{-L}^{L} \mathrm{d}x_2 \; \cos^2\left(\frac{\pi x_2}{2L}\right)\right]^{\nu-1}$$

$$= \nu \left(\frac{\pi}{2L}\right)^2 \left(\frac{1}{L}\right)^\nu L^\nu$$

$$= \nu \left(\frac{\pi}{2L}\right)^2$$

or

$$\int \mathrm{d}^\nu \mathbf{x} \; \left|\boldsymbol{\nabla} \phi(\mathbf{x})\right|^2 = \frac{\nu \pi^2}{4L^2}. \tag{D.8}$$

# APPENDIX E

# SOME TRIAL WAVEFUNCTIONS FOR THE BOSONIC SYSTEMS INVESTIGATED

1. Let

$$f_1(x) = \sum_{n=1}^{2} \left[ \frac{2}{n\pi} \sin\left(\frac{n\pi x}{2}\right) \cos\left(\frac{n\pi x}{2}\right) \right] \tag{E.1}$$

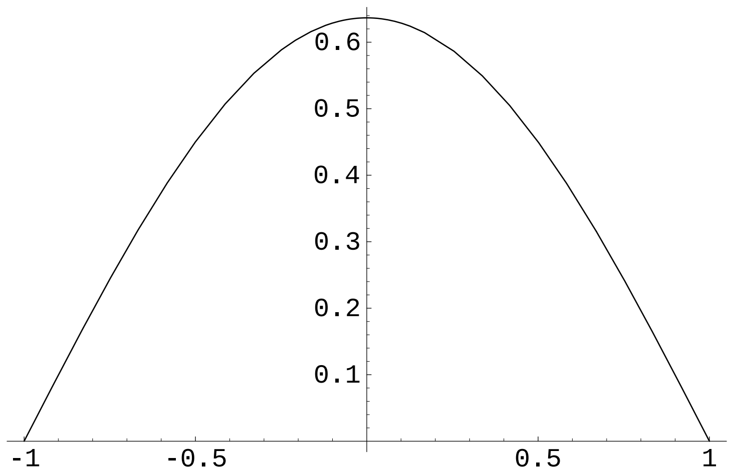


Figure E.1: The figure displays plot of $f_1(x)$

For

$$A = \int_{-1}^{1} \mathrm{d}x \; \left|f_1(x)\right|^2 \equiv \left\|f_1(x)\right\|^2 \tag{E.2}$$

then, we have

$$T = \frac{3}{\left\|f_1(x)\right\|^2} \int_{-1}^{1} \mathrm{d}x \; \left|\frac{\mathrm{d}}{\mathrm{d}x} f_1(x)\right|^2 = 7.4022 \tag{E.3}$$

2. Let

$$f_2(x) = \sum_{n=1}^{4} \left[ \frac{2}{n\pi} \sin\left(\frac{n\pi x}{2}\right) \cos\left(\frac{n\pi x}{2}\right) \right] \tag{E.4}$$

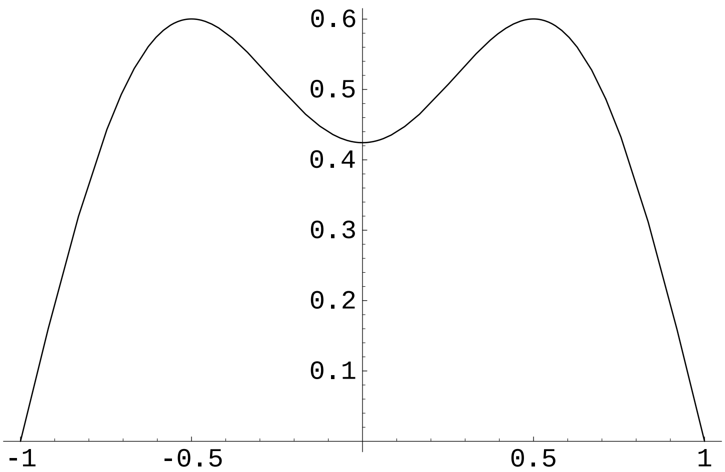


Figure E.2: The figure displays plot of $f_2(x)$

For

$$A = \int_{-1}^{1} \mathrm{d}x \ \left|f_2(x)\right|^2 \equiv \left\|f_2(x)\right\|^2 \tag{E.5}$$

then, we have

$$T = \frac{3}{\left\|f_2(x)\right\|^2} \int_{-1}^{1} \mathrm{d}x \ \left|\frac{\mathrm{d}}{\mathrm{d}x} f_2(x)\right|^2 = 13.324 \tag{E.6}$$

3. Let

$$f_3(x) = \begin{cases} 0, & -\infty \leqslant x \leqslant 1 \\ \dfrac{(1-a)^m}{(1+x)^m} \exp\left[\dfrac{1}{k(1-a)^n} - \dfrac{1}{k(1+x)^n}\right], & -1 < x < -a \\ 1 + \cos\dfrac{\pi x}{2a}, & -a \leqslant x \leqslant a \\ \dfrac{(1-a)^m}{(1-x)^m} \exp\left[\dfrac{1}{k(1-a)^n} - \dfrac{1}{k(1-x)^n}\right], & a < x < 1 \\ 0, & 1 \leqslant x \leqslant \infty \end{cases} \tag{E.7}$$

where $n = 1$, $k = 4$, $m = 1$. We have to find the best value of $a$ which give the smallest minimum of $T$, where

$$T = \frac{3}{\left\|f_3(x)\right\|^2} \int_{-1}^{1} \mathrm{d}x \, \left|\frac{\mathrm{d}}{\mathrm{d}x} f_3(x)\right|^2 \tag{E.8}$$

Table E.1: Values of expectation value of $T$ of the kinetic energy for $0.43 \leqslant a \leqslant 0.58$

| $a$ | $T$ | $a$ | $T$ |
|---|---|---|---|
| 0.58 | 13.391345785413233 | 0.5 | 12.072676208531734 |
| 0.57 | 13.109685669005511 | 0.49 | 12.029862837135562 |
| 0.56 | 12.867383132649215 | 0.48 | 12.00855843556944 |
| 0.55 | 12.660911745442522 | 0.47 | 12.007711480451206 |
| 0.54 | 12.487223544860774 | 0.46 | 12.026442205825708 |
| 0.53 | 12.343682846474547 | 0.45 | 12.064027138233175 |
| 0.52 | 12.228011060315506 | 0.44 | 12.119886499060446 |
| 0.51 | 12.138240581798241 | 0.43 | 12.193574144234809 |

From Table E.1, we see that $T > 12$.

4. Let

$$f_4(x) = -\exp x^2 + \mathrm{e} \tag{E.9}$$

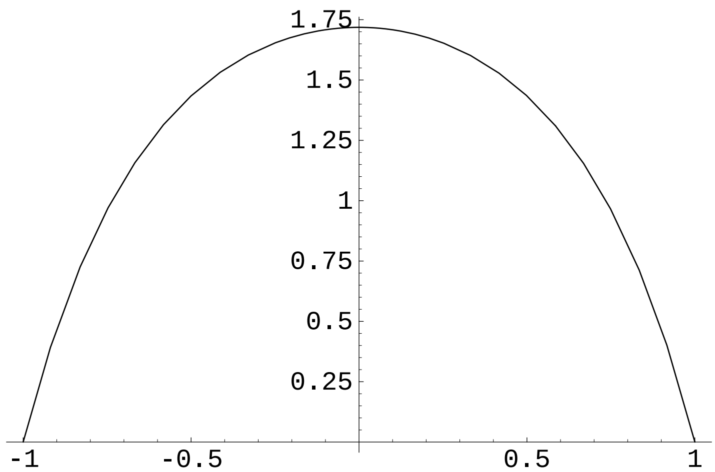


Figure E.3: The figure displays plot of $f_4(x)$

For

$$\int_{-1}^{1} \mathrm{d}x \; \left|f_4(x)\right|^2 \equiv \left\|f_4(x)\right\|^2 \tag{E.10}$$

then, we have

$$T = \frac{2}{\left\|f_4(x)\right\|^2} \int_{-1}^{1} \mathrm{d}x \; \left|\frac{\mathrm{d}}{\mathrm{d}x} f_4(x)\right|^2 = 8.36639 \tag{E.11}$$

5. Let

$$f_5(x) = \cos \frac{\pi x}{2} \tag{E.12}$$

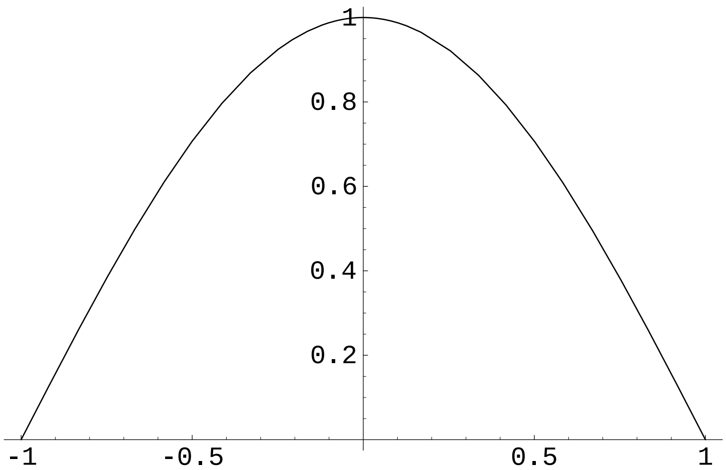


Figure E.4: The figure displays plot of $f_5(x)$

For

$$\int_{-1}^{1} \mathrm{d}x \; \left|f_5(x)\right|^2 \equiv \left\|f_5(x)\right\|^2 \tag{E.13}$$

then, we have

$$T = \frac{3}{\left\|f_5(x)\right\|^2} \int_{-1}^{1} \mathrm{d}x \; \left|\frac{\mathrm{d}}{\mathrm{d}x} f_5(x)\right|^2 = 7.4022 \tag{E.14}$$

6. Let

$$T = \frac{3}{c^2} \frac{\displaystyle\int_1^\infty \mathrm{d}z\ z^{2(\alpha+\beta)} \left[ \frac{c\beta}{z^\alpha} \exp\left( -\frac{2z^\alpha}{c} \right) \right]^2}{\displaystyle\int_1^\infty \mathrm{d}z\ z^{2\beta-2} \exp\left( -\frac{2z^\alpha}{c} \right)} \tag{E.15}$$

By using the elementary computation, we can find the minimum value of $T$, at point $c = 0.01$, $\alpha = 0.051$, $\beta = 4.606$, which gives $T = 7.73152$.

7. Let

$$f_7(x) = \frac{64}{105} P_0(x) - \frac{16}{21} P_2(x) + \frac{32}{385} P_4(x) + \frac{16}{231} P_6(x) \tag{E.16}$$

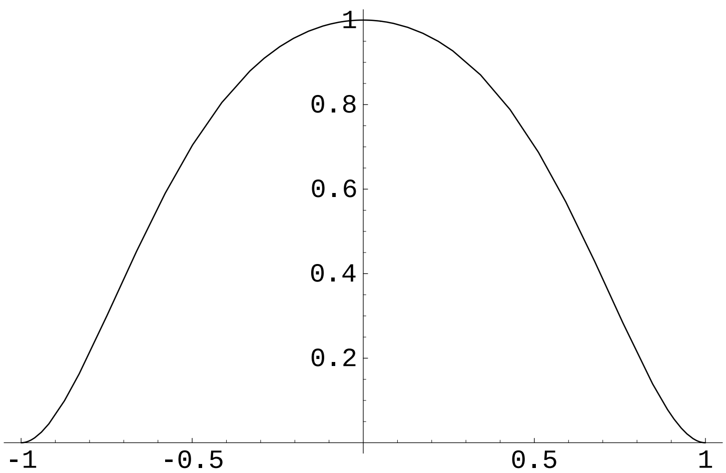


Figure E.5: The figure displays plot of $f_7(x)$

For

$$\int_{-1}^{1} \mathrm{d}x\ \left| f_7(x) \right|^2 \equiv \left\| f_7(x) \right\|^2 \tag{E.17}$$

then, we have

$$T = \frac{3}{\left\| f_7(x) \right\|^2} \int_{-1}^{1} \mathrm{d}x\ \left| \frac{\mathrm{d}}{\mathrm{d}x} f_7(x) \right|^2 = 8.16279 \tag{E.18}$$

# CURRICULUM VITAE

FIRST NAME: Chaiyapoj LAST NAME: Muthaporn

GENDER: Male NATIONALITY: Thai DATE OF BIRTH: 17 August 1976

EDUCATION BACKGROUND:

- Bachelor of Science in Physics, 1999, Khon Kaen University, Khon Kaen, Thailand.

PUBLICATIONS: (All refereed papers)

1. Muthaporn, C. and Manoukian, E. B. (2004). Instability of "bosonic matter" in all dimensions. **Physics Letters A** 321: 152–154.
2. Muthaporn, C. and Manoukian, E. B. (2004). $N^2$ Law for bosons in $2D$. **Report on Mathematical Physics** 53: 415–424.
3. Manoukian, E. B. and Muthaporn, C. (2003). $N^{5/3}$ Law for bosons for arbitrary large $N$. **Progress of Theoretical Physics** 110: 385–391.
4. Manoukian, E. B. and Muthaporn, C. (2003). Is "bosonic matter" unstable in $2D$?. **Journal of Physics A** 36: 653–663.
5. Manoukian, E. B. and Muthaporn, C. (2002). The Collapse of "bosonic matter". **Progress of Theoretical Physics** 107: 927–939.

SCHOLARSHIPS:

1. Royal Golden Jubilee Ph.D. Program, Thailand Research Fund, 2000–2005.
2. DPST Scholarship, The Institute for the Promotion of Teaching Science and Technology, 1992–1998.