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Physics Letters A 332 (2004) 54–59
PHYSICS LETTERS A
www.elsevier.com/locate/pla

Rigorous lower bounds for the ground state energy of matter

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Received 27 May 2004; received in revised form 23 August 2004; accepted 16 September 2004

Available online 2 October 2004

Communicated by B. Fricke

Abstract

Rigorous lower bounds are derived for the exact ground state energy of neutral matter of bosonic and fermionic types with Coulomb interactions with fixed positive charges by using, in the process, lower bounds for the kinetic energies as some power of an integral of ρ^2 rather than of the familiar $\rho^{5/3}$, where ρ is the particle density. This method, while it leads to a weakening of the bound for fermions, it improves the one for bosons from those in the literature. The bounds for fermionic matter lead to the inescapable conclusion that as more and more matter is put together, thus increasing the number N of electrons, the number k of nuclei, as separate clusters, would necessarily increase and not arbitrarily fuse together, and their individual charges remain bounded. That is, technically, as $N \to \infty$, then *stability* implies that $k \to \infty$ as well, and no nuclei may be found in matter that would carry arbitrarily large portions of the total positive charge available.

The Hamiltonian under study is given by

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

where

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

$$V_2 = \sum_{i<j}^{k} Z_i Z_j e^2 |\mathbf{R}_i - \mathbf{R}_j|^{-1}, \qquad \sum_{i=1}^{k} Z_i = N, \quad k \geqslant 2, \tag{3}$$

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0375-9601/$ – see front matter
doi:10.1016/j.physleta.2004.09.040

with fixed positive charges, and $\mathbf{x}_i$, $\mathbf{R}_j$ refer to the negative and positive charges, respectively. We note that for $k = 1$, the V_2 term in (3) will be absent in the expression for H and one would be dealing with an atom. Throughout, we are interested in the case for which $k \neq 1$ relevant to matter.

A rigorous study of the instability and stability of such systems for bosons and fermions, respectively, began several years ago in some remarkable work of Dyson and Lenard [1] giving rise to the respective famous $N^{5/3}$ and N power laws for the ground state energy. Much simplified derivations with tremendous improvements of the corresponding estimates have been given for the fermionic and bosonic cases notably by Lieb and Thirring in [2–4]. A power law behaviour such as N^α, with $\alpha > 1$, implies the instability of such a system, 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, in the formation of the former system, being proportional to $[(2N)^\alpha - 2(N)^\alpha]$ will be overwhelmingly large for realistic N, e.g., $N \sim 10^{23}$.

In the present work, we are interested in lower bounds for the exact ground state energies of the above systems and we present some new ideas on the construction of such bounds. The well-known estimates for these bounds are [2], respectively,

$$-c_F N\left[1 + \left(\sum_{i=1}^{k} \frac{Z_i^{7/3}}{N}\right)^{1/2}\right]^2, \tag{4}$$

$$-c_B N^{5/3}\left[1 + \left(\sum_{i=1}^{k} \frac{Z_i^{7/3}}{N}\right)^{1/2}\right]^2, \tag{5}$$

in units of $me^4/2\hbar^2$, for the fermionic and bosonic cases, respectively, where c_F and c_B are some positive constants.

The physically important question then arises as to what happens if matter could arrange itself in such a manner as the positive charges form large clusters (heavy nuclei) carrying large portions of the total positive charge available constrained, of course, by the neutrality of matter. In particular, if, say, $Z_1 = Z_2 = \cdots = Z_g = N/q$, $Z_{q+1} = 0, \ldots, Z_k = 0$ for some $2 \leqslant q \ll N$, i.e., the q nuclei carry large portions of the total positive charge $N|e|$, then (4), (5) lead to the respective behaviours $N^{7/3}/q^{4/3}$ and $N^3/q^{4/3}$, for sufficiently large N, for fermionic and bosonic systems. Motivated by the lower bound of the repulsive part [5] of the Coulomb potential derived below, rigorous lower bounds are derived for the ground state energies of the above systems by using, in the process, lower bounds for the kinetic energies as some power of an integral of ρ^2 rather than of the familiar $\rho^{5/3}$, where ρ is the particle density. The physical relevance of the our derived bounds in conjunction with the bounds given above to the question raised in the beginning of this paragraph will be elaborated upon below. For a recent review on most of the fine technical aspects in the problem of the stability of matter, on lower bounds of kinetic energies for multi-particle systems and related problems see [6] and references therein.

Consider a real function $v(\mathbf{x}) \geqslant 0$ such that $v(0) < \infty$, and its Fourier transform $\tilde{v}(\mathbf{p}) \geqslant 0$ as well. Let $\phi(\mathbf{x})$ be a real function, and $A_1, \ldots, A_k$ $(k \geqslant 2)$ be real and positive number. Then we may write

$$\sum_{j=1}^{k} A_j \phi(\mathbf{x}_j) = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{\tilde{\phi}(\mathbf{p})}{\sqrt{\tilde{v}(\mathbf{p})}} \left(\sum_{j=1}^{k} A_j \sqrt{\tilde{v}(\mathbf{p})} e^{i\mathbf{p}\cdot\mathbf{x}_j}\right), \tag{6}$$

which upon using the Cauchy–Schwartz inequality, we obtain

$$\frac{(\sum_{j=1}^{k} A_j \phi(\mathbf{x}_j))^2}{\int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{|\tilde{\phi}(\mathbf{p})|^2}{\tilde{v}(\mathbf{p})}} \leqslant \sum_{i,j=1}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j). \tag{7}$$

For any real number a, b such that $b > 0$, we have $a^2/2b \geqslant a - b/2$. Hence with $a = \sum_j A_j \phi(\mathbf{x}_j)$, $b = \int d^3\mathbf{p}\, |\tilde{\phi}(\mathbf{p})|^2/(2\pi)^3 \tilde{v}(\mathbf{p})$ used on the left-hand side of the inequality in (7), the latter leads to

$$\frac{1}{2}\sum_{i,j=1}^{k} A_i A_j v(\mathbf{x}_i - \mathbf{x}_j) \geqslant \sum_{j=1}^{k} A_j \phi(\mathbf{x}_j) - \frac{1}{2}\int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{|\tilde{\phi}(\mathbf{p})|^2}{\tilde{v}(\mathbf{p})}. \tag{8}$$

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

$$\phi(\mathbf{x}) = \int d^3\mathbf{x}'\, \rho(\mathbf{x}') V(\mathbf{x}' - \mathbf{x}), \tag{9}$$

which upon substituting in (8), we obtain

$$\sum_{i,j=1}^{k} A_i A_j V(\mathbf{x}_i - \mathbf{x}_j) \geqslant \sum_{j=1}^{k} A_j \int d^3\mathbf{x}\, \rho(\mathbf{x}) V(\mathbf{x} - \mathbf{x}_j) - \frac{1}{2}\int d^3\mathbf{x}\, d^3\mathbf{x}'\, \rho(\mathbf{x}) V(\mathbf{x} - \mathbf{x}')\rho(\mathbf{x}') - \frac{1}{2} v(0) \sum_{j=1}^{k} A_j^2$$
$$- \frac{1}{2}\int \frac{d^3\mathbf{p}}{(2\pi)^3} \left|\tilde{\rho}(\mathbf{p})\right|^2 \left[\frac{|\tilde{V}(\mathbf{p})|^2}{\tilde{v}(\mathbf{p})} - \tilde{V}(\mathbf{p})\right], \tag{10}$$

where, needless to say, $\int d^3\mathbf{p}\, |\tilde{\rho}(\mathbf{p})|^2 \tilde{V}(\mathbf{p})$ is real. In particular for $V(\mathbf{x}) = e^2/|\mathbf{x}| \geqslant v(\mathbf{x}) = e^2(1 - e^{-\lambda|\mathbf{x}|})/|\mathbf{x}|$, $\lambda > 0$, $v(0) = e^2\lambda$, $\tilde{V}(\mathbf{p}) = 4\pi e^2/\mathbf{p}^2$, $\tilde{v}(\mathbf{p}) = 4\pi\lambda^2/\mathbf{p}^2(\mathbf{p}^2 + \lambda^2)$, and (10) gives the bound ($k \geqslant 2$)

$$\sum_{i,j=1}^{k} \frac{e^2 A_i A_j}{|\mathbf{x}_i - \mathbf{x}_j|} \geqslant \sum_{j=1}^{k} e^2 A_j \int d^3\mathbf{x} \frac{\rho(\mathbf{x})}{|\mathbf{x} - \mathbf{x}_j|} - \frac{2\pi e^2}{\lambda^2} \int d^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{\lambda e^2}{2} \sum_{j=1}^{k} A_j^2$$
$$- \frac{e^2}{2}\int d^3\mathbf{x}\, d^3\mathbf{x}'\, \rho(\mathbf{x}) |\mathbf{x} - \mathbf{x}'|^{-1} \rho(\mathbf{x}'), \tag{11}$$

generalizing a result in [5].

For the bosonic case (of spin 0 for simplicity), for example, we may take

$$\rho(\mathbf{x}) = N \int d^3\mathbf{x}_2 \cdots d^3\mathbf{x}_N \left|\psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)\right|^2, \tag{12}$$

where ψ is an N boson symmetric normalized wavefunction. It is then straightforward to use (11) twice, once for $A_j = 1, k \to N$ and then again for $A_j = Z_j, \mathbf{x}_j \to \mathbf{R}_j$ *for* $k \geqslant 2$, for the repulsive potentials in (2), (3), respectively, to obtain from (12) and (1) the bound

$$\langle\psi|H|\psi\rangle \geqslant T - \frac{4\pi e^2}{\lambda^2} \int d^3\mathbf{x}\, \rho^2(\mathbf{x}) - \frac{\lambda e^2}{2}\left(N + \sum_{i=1}^{k} Z_i^2\right), \tag{13}$$

where $T = \langle\psi| \sum_j \mathbf{p}_j^2/2m |\psi\rangle$. Optimizing over λ, this gives the remarkably simple bound

$$\langle\psi|H|\psi\rangle \geqslant T - \frac{3e^2}{2^{2/3}} \pi^{1/3} \left(N + \sum_{i=1}^{k} Z_i^2\right)^{2/3} \left(\int d^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^{1/3}. \tag{14}$$

It is of utmost importance that $k \geqslant 2$, otherwise the V_2 term will be absent in the expression for H in (1), and there will be an additional term $-e^2 N \int d^3\mathbf{x}\, \rho(\mathbf{x})/|\mathbf{x} - \mathbf{R}|$ on the right-hand side of the inequality in (14), after having omitted the positive term $e^2 \int d^3\mathbf{x}\, d^3\mathbf{x}'\, \rho(\mathbf{x}) |\mathbf{x} - \mathbf{x}'|^{-1} \rho(\mathbf{x}')/2$. The numerical factor 3 would be also replaced by $3/2$. This suggests to use a lower bound to T which is some power of an integral of ρ^2.

To the above end, given a function $g(\mathbf{x}) \geqslant 0$, the Schwinger bound [7] for the number of eigenvalues (counting degeneracy) $\leqslant -\xi$, (if any) of a Hamiltonian $\mathbf{p}^2/2m - g(\mathbf{x})$, for $\xi > 0$, satisfies [2] the inequality

$$N_{-\xi}\left(\frac{\mathbf{p}^2}{2m} - g(\mathbf{x})\right) \leqslant \left(\frac{m}{2\hbar^2}\right)^{3/2} \frac{1}{\pi\sqrt{\xi}} \int d^3\mathbf{x}\, g^2(\mathbf{x}). \tag{15}$$

Hence for any $\delta > 0$, we may choose

$$-\xi = -\frac{(1+\delta)}{\pi^2}\left(\frac{m}{2\hbar^2}\right)^3 \left(\int d^3\mathbf{x}\, g^2(\mathbf{x})\right)^2, \tag{16}$$

so that $N_{-\xi}(\mathbf{p}^2/2m - g(\mathbf{x})) < 1$, which implies that $N_{-\xi}(\mathbf{p}^2/2m - g(\mathbf{x})) = 0$, and the right-hand side of (16) provides a lower bound to the spectrum of $[\mathbf{p}^2/2m - g(\mathbf{x})]$ since its spectrum would then be empty for energies $\leqslant -\xi$.

Accordingly, with

$$g(\mathbf{x}) = \frac{4}{3} \frac{T\rho(\mathbf{x})}{\int d^3\mathbf{x}\, \rho^2(\mathbf{x})}, \tag{17}$$

we obtain from (16), 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 $[\mathbf{p}^2/2m - g(\mathbf{x})]$,

$$T \geqslant \frac{3\hbar^2}{2mN^{1/3}}\left(\frac{\pi}{2}\right)^{2/3} \frac{1}{1+\varepsilon}\left(\int d^3\mathbf{x}\, \rho^2(\mathbf{x})\right)^{2/3}, \tag{18}$$

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

Upon setting $(\int d^3\mathbf{x}\, \rho^2(\mathbf{x}))^{1/3} = A$, $3\hbar^2(\pi/2)^{2/3}/2m(1+\varepsilon) = c$, (14), (18) lead to $(k \geqslant 2)$

$$\begin{aligned} \langle\psi|H|\psi\rangle &\geqslant \frac{c}{N^{1/3}}A^2 - \frac{3}{2^{2/3}}e^2\pi^{1/3}\left(N + \sum_{i=1}^k Z_i^2\right)^{2/3} A \\ &= \frac{c}{N^{1/3}}\left(A - \frac{3e^2\pi^{1/3}N^{1/3}}{2^{5/3}c}\left(N + \sum_{i=1}^k Z_i^2\right)^{2/3}\right)^2 - \frac{9}{8}\frac{e^4}{2^{1/3}}\frac{\pi^{2/3}}{c}N^{1/3}\left(N + \sum_{i=1}^k Z_i^2\right)^{4/3} \\ &> -\frac{9}{8}\frac{e^4}{2^{1/3}}\frac{\pi^{2/3}}{c}N^{1/3}\left(N + \sum_{i=1}^k Z_i^2\right)^{4/3} \\ &= -1.89\left(\frac{me^4}{2\hbar^2}\right)N^{1/3}\left(N + \sum_{i=1}^k Z_i^2\right)^{4/3}, \end{aligned} \tag{19}$$

where we have taken ε arbitrarily small for N sufficiently large. It is interesting to note that even if $Z_1 = \cdots = Z_N = 1$ in (5), the coefficient of $N^{5/3}$ in (5) is of the order 8.71, and the new estimate in (19) improves this numerical estimate by a factor of about two. For $Z_1 = \cdots = Z_q = N/q$, $N_{q+1} = \cdots = N_k = 0$, $2 \leqslant q \ll N$, i.e., $N \ll N^2/q$, the N dependence of the right-hand side of (19) is $N^3/q^{4/3}$ coinciding with that obtained from (5). Such N dependences alone with $N^{5/3}$ for $Z_1 = \cdots = Z_N = 1$ and $N^3/q^{4/3}$ for the case just discussed imply *physically* that for no arrangements of the positive charges corresponding to light or heavy nuclei, bosonic matter may be stable. The situation with fermionic matter is quite different as discussed below.

For the fermionic case, we may use a Lieb–Thirring inequality for the kinetic energy [8, Eg. (3.7), $p=2, n=3$]: $T \geqslant b(\int d^3\mathbf{x}\,\rho^2(\mathbf{x}))^{2/3}\hbar^2/2m$ where b is *independent* of N, which from (14) leads to $k \geqslant 2$

$$\langle\psi|H|\psi\rangle \geqslant \frac{\hbar^2}{2m}b\left(A - \frac{3me^2}{2^{2/3}b\hbar^2}\pi^{1/3}\left(N + \sum_{i=1}^{k} Z_i^2\right)^{2/3}\right)^2 - \frac{9}{2^{4/3}}\frac{\pi^{2/3}}{b}\left(N + \sum_{i=1}^{k} Z_i^2\right)^{4/3}\frac{me^4}{2\hbar^2}$$
$$> -\frac{9}{2^{4/3}}\frac{\pi^{2/3}}{b}\left(N + \sum_{i=1}^{k} Z_i^2\right)^{4/3}\frac{me^4}{2\hbar^2}. \tag{20}$$

(As a rough estimate obtained from [8], the numerical factor $9\pi^{2/3}/2^{4/3}b$ is of the order 1.5.) For $Z_1 = \cdots = Z_q = N/q$, $2 \leqslant q \ll N$, the N dependence on the right-hand side of (20) is $N^{8/3}/q^{4/3}$ and does not improve the bound obtained from (4) which has the N dependence on $N^{7/3}/q^{4/3}$. On the other hand, for $Z_1 = \cdots = Z_N = 1$, or more generally for bounded Z_i the right-hand side of (4) grows with a single power of N. One may consider the situation of having q separate ions, each in its ground state with nuclear charges $|e|Z_1, \ldots, |e|Z_q$ having each only one electron and having separately $(N-q)$ "free" electrons with arbitrarily small kinetic energies with all the N entities, i.e., the q ions and the $(N-q)$ "free" electrons being infinitely separated from each other. This leads to an upper bound for the ground state energy of such matter given by the well know expression $-\sum_i Z_i^2 me^4/2\hbar^2$ (which incidently is bounded above by $-Nme^4/2\hbar^2$ for $\sum_i Z_i = N$). From this and (4)/(20), we conclude that for $Z_1 = \cdots = Z_q = N/q$, $Z_{q+1} = \cdots = Z_k = 0$, $2 \leqslant q \ll N$, the ground state energy for fermionic matter will grow not slower than $-N^2$ and is obviously quite relevant physically to the *stability* of matter. It leads to the conclusion that as more and more matter is put together, thus increasing the number N of electrons, the number k of nuclei in such matter, as separate clusters, would necessarily increase and not arbitrarily fuse together and their individual charges remain *bounded*. That is, as $N \to \infty$, then stability implies that $k \to \infty$ as well, and no nuclei may be found in matter that would carry arbitrarily large portions of the total charge available.

Finally we note that our new estimates (obtained by somewhat simpler methods) and the other well known ones in the literature [2] for the bosonic case are comparable leading to the $N^{5/3}$ law and, as expected, two different methods of estimation lead, in general, to different multiplicative numerical factors to $N^{5/3}$ with some improvement in our case. The situation for the fermionic case is, however, more critical and deserves some comments. The lower bound for the ground state energy arises as a competition between the kinetic energy and the interaction parts in (1) contributing, respectively, with positive and negative signs. A lower bound corresponding to the repulsive part of the potential in (11) based on the so-called "no-binding theorem" (see [2,3] for detail), based on the $5/3$ power of ρ, is expected to be a better one than the one given in (11) based only on positivity arguments and hence the former will contribute more optimally to the lower bound of the ground state energy being sought. Also the extra $N^{1/3}$ multiplicative factor arising in the second term on the right-hand side of (20) may presumably be accounted for by an application of Hölder's inequality relating our integral of ρ^2 and the familiar one of the integral of $\rho^{5/3}$ of the density ρ. In this case, it reads

$$\int d^3\mathbf{x}\,\rho^{5/3}(\mathbf{x}) \leqslant \left(\int d^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3}\left(\int d^3\mathbf{x}\,\rho(\mathbf{x})\right)^{1/3} \tag{21}$$

or

$$\left(\int d^3\mathbf{x}\,\rho^2(\mathbf{x})\right)^{2/3} \geqslant \frac{1}{N^{1/3}}\int d^3\mathbf{x}\,\rho^{5/3}(\mathbf{x}), \tag{22}$$

which upon comparison with the known method, using the $5/3$ power of the density, would provide a weaker contribution to (a lower bound to) the kinetic energy in an estimation of the ground state energy.

Acknowledgements

One of the authors (E.B.M.) acknowledges useful communications with Prof. Walter E. Thirring which have much clarified some of the technical details used in this work. The authors would like to thank the referees for their very incisive comments and recommendations, and also thank one of the referees for kindly pointing out an error in the original version of the inequality in (10) which after having been corrected, while weakening the energy bound for fermions, has improved the one for bosons.

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