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The $N^{7/5}$ Law for Charged Bosons

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Abstract. Non-relativistic bosons interacting with Coulomb forces are unstable, as Dyson showed 20 years ago, in the sense that the ground state energy satisfies $E_0 \leqq -AN^{7/5}$. We prove that 7/5 is the correct power by proving that $E_0 \geqq -BN^{7/5}$. For the non-relativistic bosonic, one-component jellium problem, Foldy and Girardeau showed that $E_0 \leqq -CN\rho^{1/4}$. This 1/4 law is also validated here by showing that $E_0 \geqq -DN\rho^{1/4}$. These bounds prove that the Bogoliubov type paired wave function correctly predicts the order of magnitude of the energy.

I. Introduction and Background

Twenty years ago Dyson and Lenard [5] proved the stability of ordinary non-relativistic matter with Coulomb forces, namely that the ground state energy, E_0, of an N-particle system satisfies $E_0 \geqq -A_1 N$ for some universal constant A_1. In ordinary matter, the negative particles (electrons) are fermions. At the same time, Dyson [4] proved that bosonic matter is definitely not stable; if all the particles (positive as well as negative) are bosons then $E_0 \leqq -A_2 N^{7/5}$ for some $A_2 > 0$. Dyson and Lenard [5] did prove, however, that $E_0 \geqq -A_3 N^{5/3}$ in the boson case, and thus the open problem was whether the correct exponent for bosons is 5/3 or 7/5 or something in between.

In this paper we prove that the $N^{7/5}$ law is correct for bosons by obtaining a lower bound $E_0 \geqq -A_4 N^{7/5}$. As is well known, the bosonic energy is the absolute lowest energy when no symmetry restriction is imposed.

It may appear that the difference between 5/3 and 7/5 is insignificant, especially since bosonic matter does not exist experimentally, but that impression would fail to take into account the essential difference between the ground states implied by

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the two laws. The $-A_3N^{5/3}$ lower bound can be derived by using a semiclassical estimate which leads to a Thomas–Fermi type theory. This estimate is the same as that used by Lieb and Thirring [15] to give a simple proof of the stability of matter in the fermion case. Correlations are unimportant in this estimate. The $N^{7/5}$ law, on the other hand, is much more subtle. To get the upper bound, $-A_2N^{7/5}$, Dyson had to use an extremely complicated variational function which contains delicate correlations. It is the same kind of function proposed by Bogoliubov [1] (see also [10] for a review) in his theory of the many-boson system and in which particles of equal and opposite momenta are paired. It is also very similar to the Bardeen–Cooper–Schrieffer pair function of superconductivity. Since this kind of wave function plays such an important role in physics, it is important to know whether it is correct, and in proving the $N^{7/5}$ law for the energy we are, in a certain sense, validating this function.

The Hamiltonian to be considered is

$$H_N = -\sum_{i=1}^{N} \Delta_i + \sum_{1 \leqq i < j \leqq N} e_i e_j |x_i - x_j|^{-1}, \tag{1.1}$$

which is relevant for N charged particles with coordinates labeled $x_1, \dots, x_N \in \mathbf{R}^3$. The charges satisfy $e_i = \pm 1$, all i and $\hbar^2/2m = 1$. The neutral case is $\sum e_i = 0$. In Sect. II we shall prove the $N^{7/5}$ lower bound for H_N which is stated precisely in Theorem 1.2 below. The neutrality condition is not imposed in this theorem. If, however, the system is very non-neutral, with N_- negative and N_+ positive particles with $N_- + N_+ = N$ and $N_+ \gg N_-$, we expect that the bounds (1.7) and (1.8) are not optimal. One should have $E_0 \geqq -A_5 N_-^{7/5}$ instead; this is indeed true but, for simplicity of exposition, this generalization is deferred to Sect. V, Theorem 5.1.

A closely related system that we shall consider in Sect. III is jellium. In this case there is a domain Λ, in which there is a fixed constant density, ρ_B, of positive charge called the background. There are also N negative particles of charge -1 and the jellium Hamiltonian is

$$H^J_{N\Lambda} = -\sum_{i=1}^{N} \{\Delta_i + V(x_i)\} + \sum_{1 \leqq i < j \leqq N} |x_i - x_j|^{-1} + \tfrac{1}{2}\rho_B \int_\Lambda V(x)dx, \tag{1.2}$$

where $V(x) = \rho_B \int_\Lambda |x-y|^{-1} dy$ is the potential generated by the background. We do *not* restrict ourselves to the neutral case, $N = \rho_B L^3$, in Sect. III. As boundary conditions we can take either $\psi \in L^2(\mathbf{R}^{3N})$ or else $\psi \in L^2(\Lambda^N)$ with Dirichlet Boundary conditions. Clearly E_0 for the former is less than E_0 for the latter. In the physics literature one usually imposes neutrality and takes Λ to be a cube, $\psi \in L^2(\Lambda^N)$ with periodic boundary conditions and, in addition, the potential is replaced by an interaction solely among the negative particles in which the $k=0$ Fourier component of the $1/r$ potential is omitted. It is not a trivial matter to show rigorously that this periodic problem is the same, in the thermodynamic limit, as the more physical problem (1.2) which we consider here—even in the neutral case. Here, again, the bosonic energy is the absolute lowest.

Let us briefly review what is known rigorously about these two problems.

A. Jellium. Foldy [7] was the first to apply Bogoliubov's method to the neutral bosonic jellium problem (with the periodic boundary conditions mentioned above) and obtained, for large ρ_B and in the thermodynamic limit,

$$E_0 \approx -1.933 N \rho_B^{1/4}. \tag{1.3}$$

A proof of (1.3) was, and is lacking, but later, Girardeau [8] proved that (1.3) is an upper bound to E_0 (for large ρ_B and with the same conditions). Another non-rigorous derivation of (1.3) that does not use Bogoliubov's method was given by Lieb and Sakakura [13]. In Sect. III we shall derive the following lower bound for the real problem (1.2).

Theorem 1.1. *With $H_{N\Lambda}^J$ given by (1.2) on $L^2(\mathbf{R}^{3N})$, the ground state energy satisfies, for all N and Λ*

$$E_0 \geqq -A_6 N \rho_B^{1/4}, \tag{1.4}$$

for some universal constant A_6. A bound for A_6 is given in (3.19); In the limit $\rho_B \to \infty$ we can take $A_6 = 8.57$.

Theorem 1.1 is generalized in Theorem 3.1. Note that our lower bound (1.4) is close to the upper bound (1.3) (with a factor about 4.5).

The existence of the thermodynamic limit for jellium was proved by Lieb and Narnhofer [12]. This limit will not concern us here, but a useful result in the appendix of [12] contains a lower bound to the potential energy terms in (1.2), and hence to the ground state energy of (1.2) for all N. This bound is

$$E_0 \geqq -(0.9)(4\pi/3)^{1/3} N \rho_B^{1/3}. \tag{1.5}$$

A result similar to (1.5) is given in [3].

It is not easy to give a heuristic derivation of the $\rho_B^{1/4}$ law. Dyson [4] gives one, but we prefer the following point of view. The reason that $E_0 < 0$ is that the negative particles stay away from each other. If λ is the correlation length (i.e. the radius of a ball surrounding any one particle in which there is, on the average, an absence of one particle) then the potential energy, P, is roughly $P \approx -N/\lambda$. On the other hand, let us study the kinetic energy, K. Most of the particles will be in the zero momentum state. A correlation length λ can be achieved by decomposing Λ into $n \equiv (L/\lambda)^3$ boxes of size λ. If there is one single particle wave function in each box, with Dirichlet boundary conditions, its kinetic energy will be λ^{-2} and thus $K = n\lambda^{-2} = L^3\lambda^{-5}$. Minimization of $K + P = -N\lambda^{-1} + L^3\lambda^{-5}$ with respect to λ (recalling $N = \rho_B L^3$ for neutrality) yields $\lambda^4 = 5/\rho_B$ and $E_0 = -\frac{4}{5}N\lambda^{-1} = -\frac{4}{5}N(\rho_B/5)^{1/4}$. In addition we learn that $K/P = -1/5$, which is very different from the usual virial theorem value $-1/2$.

The difficulty with the above argument is its apparent inconsistency. If we put n particles into boxes, as stated above, then K will be $n\lambda^{-2}$ but also P will be $-n\lambda^{-1}$, not $N\lambda^{-1}$. Nevertheless, it is true that the Bogoliubov pair wave function has the properties $K \approx n\lambda^{-2}$ and $P = -N\lambda^{-1}$ mentioned above. How it achieves this is not easy to understand; one *must*, apparently, study the problem in momentum space.

If the kinetic energy were $|p|^\alpha$ with $1 \leqq \alpha < 2$, instead of p^2, we would predict, by the same argument, that E_0 would then be of the order $-N\rho_B^{1/(2+\alpha)}$ and $\lambda \approx \rho_B^{-1/(2+\alpha)}$. This conclusion does indeed agree with what is obtained from an appropriately modified Bogoliubov function. When $\alpha = 1$ (the relativistic case) we get $-N\rho_B^{1/3}$ which agrees with the lower bound (1.5).

B. The Two-Component System. For simplicity let us consider the neutral system with N bosons of each charge. In [5] and [15] it is proved that $E_0 \geqq -A_3 N^{5/3}$. Indeed, if one kind of particle is infinitely massive then the $N^{5/3}$ law is correct—as proved by Lieb [9]. Moreover, the $N^{5/3}$ upper bound in [9] is very simple and semiclassical—correlations are unnecessary.

The $N^{7/5}$ result for particles all of finite mass is subtle. For (1.1) Dyson obtained (for large N and $\sum e_i = 0$)

$$E_0 \leqq -5.001 \times 10^{-7} N^{7/5}. \tag{1.6}$$

Surely, the coefficient in (1.6) is too small. Our lower bound for the energy, proved in Sect. II, is the following:

Theorem 1.2. *Let H_N be given by (1.1) with $e_i = \pm 1$. Neutrality is not assumed. Then, on $L^2(\mathbf{R}^{3N})$*

$$H_N \geqq -0.30 N^{7/5} \tag{1.7}$$

for sufficiently large N.

Generalizations of Theorem 1.2 are given in Theorems 2.1 and 5.1. The former is a generalization to the Yukawa potential while the latter treats the nonneutral case $N_- \ll N_+$,

$$E_0 \geqq -A_7 N^{7/5} \tag{1.8}$$

for some constant A_7.

Let us recall Dyson's heuristic derivation [4] of (1.7) from (1.4). There are two parts to the energy: (i) a local kinetic energy and electrostatic correlation energy and (ii) a global kinetic energy needed to localize the system in a region of radius R. The latter is approximately $K_{\text{global}} \approx N/R^2$. The former is approximately $E_{\text{local}} \approx -A_5 N \rho^{1/4}$ with $\rho = N/R^3$. Here we have taken over the one-component jellium result (1.4) even though we are considering a two-component system; the reason is that the electrostatic correlation energy comes primarily from the fact, as we said, that particles of like charge stay away from each other and therefore the energy in the two-component and one-component systems are comparable. If we now minimize $E = E_{\text{global}} + E_{\text{local}}$ with respect to R we find $R \approx N^{-1/5}$ and $E \approx -N^{7/5}$. A check on the consistency of this is that the correlation length satisfies $\lambda \approx \rho^{-1/4} = (N/R^3)^{-1/4} = N^{-2/5} \ll R$.

In the present paper we begin with the $N^{7/5}$ problem and prove (1.7) in Sect. II. Our analysis is based on Conlon's paper [2] in which the following was proved about the two-component system in a box. A symmetric wave function connotes a function that is separately symmetric in the positive and negative charge spatial variables, i.e. a bosonic function.

Theorem 1.3. *Let Λ be a cube in $\mathbf{R}^3$ and suppose that $\psi(x_1, \ldots, x_N)$ is any symmetric, infinitely differentiable, $L^2(\mathbf{R}^{3N})$ normalized function with support in Λ^N. Let*

$$K(\psi) \equiv \sum_{i=1}^{N} \langle \psi, -\Delta_i \psi \rangle \equiv \langle \psi, T\psi \rangle \tag{1.9}$$

be the kinetic energy and define γ_ψ by

$$K(\psi) = N\gamma_\psi^2/L^2, \tag{1.10}$$

where L is the length of Λ. Let H_N^ν be the two-component Hamiltonian analogous to (1.1) but with the Coulomb potential replaced by the Yukawa potential $Y_\nu(x) = |x|^{-1}\exp(-\nu|x|)$, namely

$$H_N^\nu = -\sum_{i=1}^{N} \Delta_i + \sum_{1 \leqq i < j \leqq N} e_i e_j Y_\nu(x_i - x_j).$$

The $e_i = \pm 1$ as before and neutrality is not assumed. Then, if $\gamma_\psi \leqq N^{1/3}$,

$$\langle \psi, H_N^\nu \psi \rangle \geqq -A_8 N^{7/5} \tag{1.11}$$

for some constant A_8, which is independent of ν, N and L.

Theorem 1.3 is proved in [2] by a succession of inequalities that turn the Bogoliubov ansatz [1] into a rigorous bound (with a different constant, of course). It concerns the local energy and, being intrinsically quantum-mechanical, has no classical, analogue. The reason that Theorem 1.3 does not imply the $N^{7/5}$ law, Theorem 1.2, is the condition that $\gamma_\psi \leqq N^{1/3}$ (alternatively, $K(\psi) \leqq N^{5/3}/L^2$). We do not know in advance what the radius, R, is for an energy minimizer. If, for example, $K(\psi) = N^{5/3}$ and $R \gg 1$, we could not use Theorem 1.3. Thus, we are faced with what might be called an infrared problem which our analysis in Sect. II solves.

To get the constant in (1.7) we need a good value for A_8 in (1.11). A value can be deduced from [2], but the constant there is not optimum. It turns out that restricting $\gamma_\psi \leqq N^{1/3-\delta}$ for some $\delta > 0$ is sufficient for the analysis in Sect. II. Under this condition the following improvement of Theorem 1.3 is possible, and is proved in Sect. IV.

Theorem 1.4. *Assume the hypotheses of Theorem 1.3 except that $\gamma_\psi \leqq N^{1/3}$ is replaced by $\gamma_\psi \leqq N^{1/3-\delta}$ for some fixed $\delta > 0$. The parameters ν and L can depend on N, but we assume that $N^{-1/5}\nu L$ stays bounded as $N \to \infty$. Then, for sufficiently large N,*

$$\langle \psi, H_N^\nu \psi \rangle \geqq -0.30 N^{7/5}. \tag{1.12}$$

The analysis in Sect. III of the jellium problem, leading to (1.4), uses the $N^{7/5}$ result of Sect. II. This may seem a bit odd in view of Dyson's heuristic discussion in which one uses the jellium result to understand the $N^{7/5}$ theorem. Our procedure is to bound the jellium energy in arbitrarily large boxes in terms of the energy in a box of size $l = \rho_B^{-1/8}$. In such a box the particle number (with neutrality) is $n = \rho_B l^3 = \rho_B^{5/8}$. But then, by the $N^{7/5}$ theorem (with the background being thought of as N particles in a simple, smeared out state), $E_{\text{box}} \geqq -An^{7/5} = -A\rho_B^{7/8} = -An\rho_B^{1/4}$. By adding up the boxes we obtain $E_0 \geqq -AN\rho_B^{1/4}$.

Our work here leads to many questions, of which the following are a few.

Open Problems

(1) Find the correct coefficient in (1.4) for large ρ_B in the jellium problem. Is Foldy's constant in (1.3) correct?

(2) Find the correct coefficient A_7 in (1.8) as $N \to \infty$ for the two-component

problem. The bound in Theorem 1.4 is within a factor of 11 of what one would get heuristically from a calculation using the Bogoliubov function. This is discussed in Sect. IV. This bound translates into the bound (1.7) of Theorem 1.2. We should emphasize, however, that Bogoliubov's method does not predict an exact value for the asymptotic constant in Theorem 1.2. The reason for this is that in the Bogoliubov method one is forced to work in cubes and, in the Bogoliubov function, most particles are in the lowest momentum mode of the cube. The size of the cube can be taken to be the size of the system, namely $N^{-1/5}$. Thus the energy depends critically on the lowest eigenvalue of the Laplacian in a cube and this depends on boundary conditions. The lowest eigenvalue will be uncertain because of the boundary conditions and will be of order $N^{2/5}$. The uncertainty in the energy will be of order $N^{7/5}$.

(3) What can be said about the correlation functions at high density? Is Bogoliubov's ansatz really correct or does it merely give a good account of the energy?

(4) As shown in Sect. II, the statement $E_0 \geqq -AN^{7/5}$ for the two-component system is equivalent, via the virial theorem, to $-P(\psi) \leqq 2A^{1/2}N^{7/10}K(\psi)^{1/2}$ for all ψ. Here $K(\psi)$ is the kinetic energy and $P(\psi)$ the potential energy of ψ. Now let us replace p^2 by $|p|^\alpha$ in the kinetic energy. In the heuristic discussion above we surmised that the jellium energy should be $-C_\alpha \rho_B^{1/(2+\alpha)}$. Then, by the uncertainty principle argument relating the jellium energy to the two-component energy given before, we would have (with $K_{\text{global}} \approx NR^{-\alpha}$) $R \approx N^{-1/(\alpha-1)(\alpha+3)}$ and $E_0 = -A_\alpha N^{(\alpha^2+3\alpha-3)/(\alpha^2+2\alpha-3)}$. This statement about E_0 is equivalent, via the virial theorem, to

$$-P(\psi) \leqq \alpha[A_\alpha/(\alpha-1)]^{1-1/\alpha} N^{(\alpha^2+3\alpha-3)/\alpha(\alpha+3)} K(\psi)^{1/\alpha}. \tag{1.13}$$

We conjecture that these formal calculations are correct as $N \to \infty$. If so, it is interesting to look at the $\alpha = 1$ case (relativistic bosons). In this case, $E_0 = -\infty$ for large enough N, which is correct, but (1.13) continues to make sense. Namely, for $\alpha = 1$,

$$-P(\psi) \leqq CN^{1/4}K(\psi). \tag{1.14}$$

We conjecture that (1.14) is true for large N and we remark that in [3] it is proved that (1.14) holds with $N^{1/4}$ replaced by $N^{1/3}$. Since the bosonic energy is the absolute lowest, (1.13) and (1.14) are independent of statistics.

II. The $N^{7/5}$ Theorem

Our strategy to prove Theorem 1.2 is to decompose $\mathbf{R}^3$ into cubic boxes of size $l = N^{-\varepsilon}$ with ε some small number less than 1/5. This l is large compared to the expected size of the system, $N^{-1/5}$, but we do not know this fact in advance. It will be necessary to localize H_N in these boxes and to control the interaction between boxes.

The main difficulty in localizing the Hamiltonian (1.1) comes from the localization of the Coulomb potential. The effects of localization on the kinetic energy can be easily computed to be of order Nl^{-2}, where l is the cutoff length. For the potential energy, however, even a small amount of net charge will produce enormous potential energies, and therefore charge neutrality must be preserved very carefully. Our basic strategy is first to replace the Coulomb potential by a Yukawa cutoff and then, by averaging over all possible box locations, the errors can be controlled.

For $\mu > 0$, let

$$Y_\mu(r) \equiv r^{-1} e^{-\mu r} \tag{2.1}$$

be the Yukawa potential with range μ^{-1}. For $\kappa > 0$ and N a positive integer, let

$$H_{\kappa N}^{\mu l} \equiv -\sum_{i=1}^{N} \Delta_i + \kappa \sum_{1 \leqq i < j \leqq N} e_i e_j Y_\mu(x_i - x_j) \tag{2.2}$$

be the Hamiltonian of N charged bosons interacting pairwise by the Yukawa potential with coupling constant κ. As before, $e_i = \pm 1$ but neutrality is not assumed. $H_{\kappa N}^{\mu l}$ is defined as a quadratic form on $L^2([0,l]^{3N})$ with Dirichlet boundary conditions. We shall drop μ or l or κ whenever they are equal to $0, \infty$ or 1 respectively. Since the Hamiltonian (2.2) is symmetric under permutations separately on positive or negative particles, the ground state automatically obeys Bose statistics, and we shall assume this henceforth. Let

$$E_{\kappa N}^{\mu l} = \inf \operatorname{spec} H_{\kappa N}^{\mu l} \tag{2.3}$$

be the ground state energy. Then a trivial scaling yields, for the Coulomb Hamiltonian in all of $\mathbf{R}^3$,

$$E_{\kappa N} = \kappa^2 E_N. \tag{2.4}$$

To fix a partition, let g be a piecewise C^1 function on $\mathbf{R}$ defined by

$$g(t) = \cos(\pi t/2), \quad -1 \leqq t \leqq 1 \tag{2.5}$$

and zero otherwise. Then $\sum_{j \in \mathbf{Z}} g^2(t+j) = 1$ for all $t \in \mathbf{R}$. Let $\chi(x) \equiv g(x^1) g(x^2) g(x^3)$, with $x = (x^1, x^2, x^3)$ and let $\chi_{u\lambda}(x) \equiv \chi(x + u + \lambda)$. Here $\lambda \in \mathbf{Z}^3$ and $u \in [0,1]^3 \equiv \Gamma$. Then

$$\sum_{\lambda \in \mathbf{Z}^3} \chi_{u\lambda}^2(x) = 1 \quad \forall x \in \mathbf{R}^3, \quad u \in \Gamma. \tag{2.6}$$

A function h which is of central importance in our localization is defined by

$$h(x,y) \equiv \int_\Gamma du \sum_{\lambda \in \mathbf{Z}^3} \chi_{u\lambda}^2(x) \chi_{u\lambda}^2(y). \tag{2.7}$$

Then h depends only on the difference $z \equiv x - y$ and

$$\begin{aligned} h(z) \equiv h(x-y) &= \int_\Gamma du \sum_{\lambda \in \mathbf{Z}^3} \chi^2(x+u+\lambda) \chi^2(y+u+\lambda) \\ &= \int_{\mathbf{R}^3} du \, \chi^2(x+u) \chi^2(y+u) = (\chi^2 * \chi^2)(z). \end{aligned} \tag{2.8}$$

An easy computation shows that

$$\begin{aligned} (g^2 * g^2)(t) &= \frac{1}{8}\left[4 - 2|t| + \frac{3}{\pi} \sin \pi |t| + (2 - |t|) \cos \pi t\right], \quad |t| \leqq 1 \\ &\sim \tfrac{3}{4} - \tfrac{1}{8}\pi^2 t^2 + O(t^4) \end{aligned} \tag{2.9}$$

and zero otherwise. Hence $h(z)$ is a C^4 function and

$$|h(z) - a_0 - a_1|z|^2| \leqq a_2|z|^4 \tag{2.10}$$

with $a_0 = (3/4)^3, a_1 = -(\frac{3}{4})^2(\pi^2/8)$ and a_2 some constant of order 1.

Let $h_l(x) \equiv h(x/l)$.

We now define localized kinetic and potential energies. Let $\alpha = (u, \alpha_1, \ldots, \alpha_N) \in \Gamma \times \mathbf{Z}^{3N}$ be a multi-index and let $\int d\alpha \equiv \int_\Gamma du \sum_{\alpha_1 \in \mathbf{Z}^3} \cdots \sum_{\alpha_N \in \mathbf{Z}^3}$. If $\beta = (v, \beta_1, \ldots, \beta_N)$ is another multi-index, denote $\delta(u-v) \prod_{i=1}^N \delta_{\alpha_i \beta_i}$ by $\delta_{\alpha\beta}$. (Here, $\delta(u-v)$ is the Dirac δ-function and $\delta_{\alpha_i\beta_i}$ is the Kronecker delta.) For any $l > 0$, let

$$\psi_\alpha^l(x_1, \ldots, x_N) \equiv \prod_{k=1}^N \chi_{u\alpha_k}(x_k/l)\psi(x_1, \ldots, x_N), \tag{2.11}$$

$$V_\alpha^\mu \equiv \sum_{1 \leqq i < j \leqq N} e_i e_j Y_\mu(x_i - x_j)\delta_{\alpha_i, \alpha_j}. \tag{2.12}$$

Then by using (2.6) and (2.7) one has the identity

$$\int d\alpha \langle \psi_\alpha^l, V_\alpha^\mu \psi_\alpha^l \rangle = \sum_{1 \leqq i < j \leqq N} e_i e_j \int dX \int d\alpha \prod_{k=1}^N \chi_{u\alpha_n}^2(x_k/l)\psi^2(x_1, \ldots, x_N) Y_\mu(x_i - x_j)\delta_{\alpha_i\alpha_j}$$

$$= \left\langle \psi, \sum_{1 \leqq i < j \leqq N} e_i e_j Y_\mu(x_i - x_j) h_l(x_i - x_j)\psi \right\rangle. \tag{2.13}$$

Similarly, since for any $f \in C_0^\infty(\mathbf{R}^3)$

$$\langle f\chi, -\Delta(f\chi) \rangle = \langle f, -\Delta(\chi^2 f) \rangle + \langle f, |\nabla\chi|^2 f \rangle,$$

one has the following estimate for the kinetic energy with $C_0 = \sup_x |\nabla\chi|^2(x) < 3(\pi/2)^2$ (and recalling (1.9)):

$$\int d\alpha \langle \psi_\alpha^l, T\psi_\alpha^l \rangle \leqq \langle \psi, T\psi \rangle + C_0 N l^{-2}. \tag{2.14}$$

We emphasize that, definition (2.12), particles in different boxes *do not interact*. Hence

$$\left\langle \psi, \left[T + \sum_{1 \leqq i < j \leqq N} e_i e_j Y_\mu(x_i - x_j) h_l(x_i - x_j) \right] \psi \right\rangle + C_0 N l^{-2}$$

$$\geqq \int d\alpha \langle \psi_\alpha^l, (T + V_\alpha^\mu)\psi_\alpha^l \rangle \geqq \left(\int d\alpha \|\psi_\alpha^l\|_2^2\right) \inf_{\sum n_\sigma = N} \sum_{\sigma \in \mathbf{Z}^3} E_{n_\sigma}^{\mu l}$$

$$= \inf_{\sum n_\sigma = N} \sum_{\sigma \in \mathbf{Z}^3} E_{n_\sigma}^{\mu l}. \tag{2.15}$$

Here $E_{n_\sigma}^{\mu l}$ is the ground state energy of a n_σ-particle system with Yukawa cutoff μ in a box of size l (see (2.2)). The sub-systems need to be neutral.

To complete the localization, one has to relate the potential $Y_\mu(z)h_l(z)$ to the Coulomb potential. Let

$$f_{\mu l}(z) \equiv a_0|z|^{-1} - Y_\mu(z)h_l(z). \tag{2.16}$$

The coefficient a_0 in front of r^{-1} is added for the purpose of normalization. Clearly, $f_{\mu l}(0) = a_0 \mu$. It will be shown in Lemma 2.1 below that $f_{\mu l}$ has a positive Fourier transform if $\mu l \geqq C_3$ for some fixed constant C_3. Hence by (2.15), (2.4) and (2.20)

$$E_N = a_0^{-2} E_{a_0,N} \geqq a_0^{-2}\left[-C_0 N l^{-2} - \tfrac{1}{2} a_0 \mu N + \inf_{\sum n_\sigma = N} \sum_{\sigma \in \mathbf{Z}^3} E_{n_\sigma}^{\mu l} \right]. \tag{2.17}$$

Equation (2.17) is the localization estimate which we need to prove Theorem 1.2. Note that the correction terms are remarkably simple.

Let $l = N^{-\varepsilon}$ with ε some small number ($\varepsilon < 1/5$) and $\mu = C_3 N^{\varepsilon}$. Our goal is to apply Theorem 1.4 in each box.

Let ϕ be a n-particle wave function satisfying $\langle \phi, H_n^{\mu l} \phi \rangle \leqq 0$. Then one has the trivial estimate (recall definition (2.2))

$$\tfrac{1}{2}\langle \phi, T\phi \rangle \leqq -\tfrac{1}{2}\langle \phi, H_{2,n}^{\mu l}\phi \rangle \leqq -\tfrac{1}{2}\inf\operatorname{spec} H_{2,n}^{\mu l}. \tag{2.18}$$

But $H_{2,n}^{\mu l}$ can be bounded below by $-C_5 n^{5/3}$ [see (A.23) which is the stability of matter bound with Yukawa cutoff derived in the Appendix]. Hence the hypothesis of Theorem 1.4 is satisfied for each box with $l = N^{-\varepsilon}$ and $\gamma_\psi = N^{1/3-\varepsilon}$. We also have that $\sum_{\sigma \in \mathbf{Z}^3} (n_\sigma)^{7/5} \leqq \left(\sum_{\sigma \in \mathbf{Z}^3} n_\sigma \right)^{7/5} = N^{7/5}$.

Let us now combine Theorem 1.4 with (2.17), temporarily ignoring the possibility that the particle number in some boxes may not be large. This yields

$$E_N \geqq -0.30 a_0^{-2} N^{7/5} - a_0^{-2} C_0 N^{1+2\varepsilon} - C_3 a_0^{-1} N^{1+\varepsilon}. \tag{2.19}$$

To eliminate the last two terms as $N \to \infty$ we simply take $\varepsilon < 1/5$.

Despite the aforementioned problem about the particle number in each box, (2.19) is correct as $N \to \infty$. To prove this, note that in any box we can use $E_\sigma \geqq -C_5 n_\sigma^{5/3}$. However, $\sup\{\sum n_\sigma^{5/3} | \sum n_\sigma \leqq N \text{ and } n_\sigma < N^p\} \leqq N^{2p/3} \sum n_\sigma = N^{1+2p/3}$. If we take $0 < p < 3/5$, this shows that boxes with small particle number can be neglected.

Finally, to complete the proof of Theorem 1.2 we have to eliminate the a_0^{-2} factor in the first term in (2.19). This can be done as follows. Note that $a_0 = h(0)^3 = (\int g^4)^3$ with g given in (2.5), and g satisfies $\int g^2 = 1$. If g is replaced by $\eta(t) = 1$ for $|t| \leqq \frac{1}{2}$ and $\eta(t) = 0$ otherwise, we would have $a_0 = 1$. But we cannot do this because $\int |\nabla g|^2$, the coefficient of the l^{-2} term in (2.14), would be infinite. Since $N l^{-2}$ is small on a scale of $N^{7/5}$, the remedy is to take $g \approx \eta$ and $\int |\nabla g|^2$ finite, but large. As $N \to \infty, g \to \eta$ and $a_0 \to 1$. Note that Lemma 2.1 does not depend on the special choice (2.5) we made for g.

This concludes the proof of Theorem 1.2 and we turn to Lemma 2.1.

Lemma 2.1. *Let $K: \mathbf{R}^3 \to \mathbf{R}$ be given by*

$$K(z) = r^{-1}\{e^{-\nu r} - e^{-\omega r} h(z)\}$$

with $r = |z|$ and $\omega > \nu \geqq 0$. Let h satisfy (i) *h is a C^4 function of compact support;* (ii) *$h(z) = 1 + ar^2 + O(r^3)$ near $z = 0$. Let $h(z) = h(-z)$, so that K has a real Fourier transform. Then there is a constant C_3 (depending on h) such that if $\omega - \nu \geqq C_3$ then*

K has a positive Fourier transform and, moreover,

$$\sum_{1 \leqq i < j \leqq N} e_i e_j K(x_i - x_j) \geqq \tfrac{1}{2}(v - \omega)N \tag{2.20}$$

for all $x_1, \ldots, x_N \in \mathbf{R}^3$ *and* $e_i = \pm 1$.

Proof. Let $F(z) = [h(z) - 1 - ar^2]r^{-1}(1 + r^5)^{-1}$. $K(z)$ can thus be decomposed as

$$K(z) = Y_v(z) - Y_\omega(z) - are^{-\omega r} - (1 + r^5)e^{-\omega r}F(z).$$

The Fourier transforms of the first three terms are $4\pi/(p^2 + v^2)$, $-4\pi/(p^2 + \omega^2)$ and $-8\pi a(3\omega^2 - p^2)(p^2 + \omega^2)^{-3}$ respectively. For the last term note that $F(z)$ is of order r^2 and r^{-4} near the origin and near infinity, respectively and $\Delta^2 F(z)$ is of order r^{-2} and r^{-8} near the origin and near infinity, respectively. Therefore, ΔF and $\Delta^2 F \in L^1(\mathbf{R}^3)$ and hence (with ^ denoting Fourier transform)

$$|(1 + p^2)^2 \hat{F}(p)| \leqq 4\pi C_1$$

for some constant C_1. But the Fourier transform of $(1 + r^5)e^{-\omega r}$ can be shown to satisfy $|((1 + r^5)e^{-\omega r})\hat{}\,| \leqq 16\pi\omega(\omega^2 + p^2)^{-2}$ if $\omega \geqq C_2$ for some constant C_2. Hence

$$\begin{aligned} |[(1 + r^5)e^{-\omega r}F(z)]\hat{}\,| &= C_1[8\pi\omega(\omega^2 + p^2)^{-2}] * [8\pi(1 + p^2)^{-2}] \\ &= C_1[e^{-\omega r} \cdot e^{-r}]\hat{} = 8\pi C_1(\omega + 1)[(\omega + 1)^2 + p^2]^{-2}. \end{aligned}$$

We can now put all these Fourier transform together to yield the estimate

$$\hat{K}(p) \geqq 4\pi[(p^2 + v^2)^{-1} - (p^2 + \omega^2)^{-1} - 6|a|(p^2 + \omega^2)^{-2} - 2C_1(\omega + 1)(\omega^2 + p^2)^{-2}].$$

Hence $\hat{K}(p) \geqq 0$ for all p if $\omega - v$ is large enough. To conclude the proof of Lemma 2.1, one only has to note the identity

$$\sum_{1 \leqq i < j \leqq N} e_i e_j K(x_i - x_j) = \tfrac{1}{2}\int \hat{K}(p) \left[\left| \sum_{j=1}^{N} e_j e^{ipx_j} \right|^2 - N \right] dp$$

which implies (2.20) since $\int \hat{K} = K(0) = \omega - v$. □

Lemma 2.1 is applied to (2.16) with $v = 0$ and the requirement is that $\mu l \geqq C_3$. However, our energy bound does not depend on the fact that we started with a Coulomb potential in (1.1). By the foregoing construction and Lemma 2.1 we have the following generalization of Theorem 1.2.

Theorem 2.1. *Let* $e_i = \pm 1$ *and let*

$$H_N^v = -\sum_{i=1}^{N} \Delta_i + \sum_{1 \leqq i < j \leqq N} e_i e_j Y_v(x_i - x_j) \tag{2.21}$$

be defined on $L^2(\mathbf{R}^{3N})$ *with* $Y_v(x) = |x|^{-1}\exp(-v|x|)$. *v can depend on N, but suppose that as* $N \to \infty$, $N^{-2/5}v \to 0$. *Then, for sufficiently large N,*

$$H_N^v \geqq -0.30 N^{7/5}. \tag{2.22}$$

Proof. As in (2.16), we write $f_{\mu l} = a_0 Y_v - Y_\mu h_l$. In order to apply our foregoing construction, the assumptions of Lemma 2.1 and Theorem 1.4 must be satisfied, namely $l(\mu - v) \geqq C_3$, $l^{-1} \geqq N^\varepsilon$ and $l\mu N^{-1/5} < \infty$ as $N \to \infty$. On the other hand, the correction terms resulting from the localization (cf. (2.17)) should be of lower order. Hence we must have $l^{-1} \leqq o(N^{1/5})$ and $(\mu - \nu) \leqq o(N^{2/5})$. It is easy to check that $\mu = \max(N^{1/5+\varepsilon}, 2\nu)$ and $l = N^{1/5}\mu^{-1}$ satisfy all the requirements. □

Returning to the Coulomb case, (1.1), we note the following *virial type theorem.*

Theorem 2.2 *Let the hypotheses be as in Theorem 1.2 and let ψ be any normalized (not necessarily symmetric) function in $L^2(\mathbf{R}^{3N})$. Let $K(\psi)$ and $P(\psi)$ denote the kinetic and potential energies of ψ (see (1.9) and $P(\psi) = \langle \psi, \sum e_i e_j |x_i - x_j|^{-1} \psi \rangle$). Then*

$$-P(\psi) \leqq 2A^{1/2} N^{7/10} K(\psi)^{1/2}, \tag{2.23}$$

where $A = -N^{-7/5} \inf \operatorname{spec}(H_N)$.

Proof. Replacing $\psi(x_i)$ by $\lambda^{3N/2}\psi(\lambda x_i)$ we find that $\lambda^2 K(\psi) + \lambda P(\psi) \geqq -AN^{7/5}$. Then $-P(\psi) \geqq \lambda^{-1} AN^{7/5} + \lambda K(\psi)$. Optimizing this with respect to λ yields (2.23). □

III. The $\rho^{1/4}$ Law for Jellium

We shall prove Theorem 1.1 in this section by localizing the jellium Hamiltonian to a box of size $l = \rho_B^{-1/8}$. The localized Hamiltonian can thus be estimated by relating it to Theorem 2.1. In localizing the jellium Hamiltonian (1.2), one should be cautious about the fact that, after averaging over all translations, the coupling constant in the two-particle Coulomb interactions changes from 1 to a_0 [see (2.9)–(2.16)], while that of the particle-background remains unchanged. A straightforward localization as in Sect. II will fail to preserve the charge neutrality. We shall solve this difficulty by replacing the uniform background charge density, ρ_B, in each small box by a *non-uniform* background charge density which depends on the cutoff functions.

Let χ_Λ be the characteristic function of the big domain, Λ. For $\tau \in \mathbf{Z}^3$, $l > 0$, $\mu > 0$ and $\alpha = (u, \alpha_1, \ldots, \alpha_N)$, and recalling (2.6), (2.7), *et.seq.*, let

$$\rho_{B\tau}^{lu}(y) \equiv \chi_\Lambda(y) \chi_{u\tau}^2(y/l) \rho_B, \tag{3.1}$$

$$V_{B\tau\mu}^{lu}(x) \equiv \int Y_\mu(x-y) \rho_{B\tau}^{lu}(y)\, dy, \tag{3.2}$$

$$V_{B\mu}^{l}(x) \equiv \rho_B \int_\Lambda Y_\mu(x-y) h_l(x-y)\, dy. \tag{3.3}$$

Then using (2.11) one has the following definitions of $\mathscr{L}(\psi)$ and $\mathscr{R}(\psi)$ and localization estimate:

$$\begin{aligned}
\mathscr{L}(\psi) \equiv \int d\alpha \Big\langle \psi_\alpha^l, \Big[-\sum_{i=1}^N \Big\{ \Delta_i + \sum_{\tau \in \mathbf{Z}^3} V_{B\tau\mu}^{lu}(x_i) \delta_{\alpha_i,\tau} \Big\} \\
+ \sum_{1 \leqq i < j \leqq N} Y_\mu(x_i - x_j) + \sum_{\tau \in \mathbf{Z}^3} \tfrac{1}{2} \int \rho_{B\tau}^{lu}(y) V_{B\tau\mu}^{lu}(y)\, dy \Big] \psi_\alpha^l \Big\rangle \\
\leqq \Big\langle \psi, \Big[-\sum_{i=1}^N \{ \Delta_i + V_{B\mu}^l(x_i) \} + \sum_{1 \leqq i < j \leqq N} Y_\mu(x_i - x_j) h_l(x_i - x_j) \\
+ \tfrac{1}{2} \rho_B \int_\Lambda V_{B\mu}^l(y)\, dy \Big] \psi \Big\rangle + C_0 N l^{-2} \equiv \mathscr{R}(\psi).
\end{aligned} \tag{3.4}$$

Equation (3.4) may appear to be complicated, but the proof is just a reordering of indices. Recall Eq. (2.6),

$$\int d\alpha \left\langle \psi_\alpha^l, \sum_{j=1}^N \sum_{\tau \in Z^3} V_{B\tau\mu}^{lu}(x_j) \delta_{\alpha_j,\tau} \psi_\alpha^l \right\rangle$$

$$= \sum_{j=1}^N \left\langle \psi, \left[\rho_B \int_A dy \int d\alpha \sum_{\tau \in Z^3} \delta_{\alpha_j,\tau} Y_\mu(x_j - y) \chi_{u\tau}^2(y/l) \prod_{i=1}^N \chi_{u\alpha_i}^2(x_i/l) \right] \psi \right\rangle$$

$$= \sum_{j=1}^N \left\langle \psi, \rho_B \int_A dy\, Y_\mu(x_j - y) \left[\int_\Gamma du \sum_{\alpha_j} \chi_{u\alpha_j}^2(y/l) \chi_{u\alpha_j}^2(x_j/l) \right] \psi \right\rangle$$

$$= \sum_{j=1}^N \langle \psi, V_{B\mu}^l(x_j) \psi \rangle,$$

$$\int d\alpha \left\langle \psi_\alpha^l, \sum_{j=1}^N \sum_{\tau \in Z^3} \iint \rho_{B\tau}^{lu}(y) \rho_{B\tau}^{lu}(y') Y_\mu(y - y') dy dy' \psi_\alpha^l \right\rangle$$

$$= \left\langle \psi, \rho_B^2 \int_A dy \int_A dy' \left\{ \int du \sum_{\tau \in Z^3} \chi_{u\tau}^2(y/l) \chi_{u\tau}^2(y'/l) \right\} \sum_{\alpha_1, \dots, \alpha_N \in Z^3} \prod_{j=1}^N \chi_{u\alpha_j}^2(x_j/l) \psi \right\rangle$$

$$= \rho_B \int_A V_{B\mu}^l(y) dy.$$

For the other terms in (3.4) one can use (2.13) and (2.14).

As in Sect. II, one can use the positive definiteness of $f_{\mu l}$ (Lemma 2.1) to yield the bound

$$\mathcal{R}(\psi) \leqq \langle \psi, H_{NA}^J(a_0, \rho_B) \psi \rangle + C_0 N l^{-2} + N \mu a_0. \tag{3.5}$$

In (3.5) $H_{NA}^J(a_0, \rho_B)$ is the jellium Hamiltonian (1.2) but with all the potential energy terms multiplied by a_0. To utilize (3.5) we have to relate the energy of $H_{NA}^J(a_0, \rho_B)$ to that of H_{NA}^J. By simple scaling this is given by

$$\inf \operatorname{spec} H_{N, a_0 A}^J(1, \rho_B) = a_0^{-2} \inf \operatorname{spec} H_{NA}^J(a_0, \rho_B a_0^3). \tag{3.6}$$

Let $l = \rho_B^{-1/8}$ and $\mu = C_6 \rho_B^{1/8}$. Then the last two terms in (3.5) are of order at most $N\rho_B^{1/4}$. To complete the proof of Theorem 1.1, one only has to show that $\mathcal{L}(\psi) \geqq -C_7 N \rho_B^{1/4}$.

For each fixed τ and multi-index α, consider the localized Hamiltonian

$$-\sum_{j=1}^N [\Delta_j \delta_{\tau\alpha_j} + V_{B\tau\mu}^{lu}(x_j) \delta_{\tau\alpha_j}] + \sum_{i<j} \delta_{\tau\alpha_i} \delta_{\tau\alpha_j} Y_\mu(x_i - x_j) + \tfrac{1}{2} \int \rho_{B\tau}^{lu}(y) V_{B\tau\mu}^{lu}(y) dy. \tag{3.7}$$

Our goal is to estimate the ground state of (3.7). Suppose $\alpha_1 = \alpha_2 = \dots = \alpha_M = \tau$ and $\alpha_j \neq \tau$ for $j > M$. Let $\rho_{B\tau}^{lu}(y) \equiv \tilde{\rho}_B(y)$ and $\tilde{V}_B^\mu \equiv Y_\mu * \tilde{\rho}_B$. Then (3.7) becomes

$$H_{BM}^\mu \equiv -\sum_{j=1}^M \{\Delta_j + \tilde{V}_B^\mu(x_j)\} + \sum_{i<j}^M Y_\mu(x_i - x_j) + \tfrac{1}{2} \int \tilde{\rho}_B(y) \tilde{V}_B^\mu(y) dy. \tag{3.8}$$

Note that, by definition (3.1),

$$n_B \equiv \int \tilde{\rho}_B(y) dy \leqq l^3 \rho_B. \tag{3.9}$$

Recall that the density function ρ_ϕ for an M-particle normalized wave function,

ϕ, is defined by

$$\rho_\phi(x) = M \int |\phi(x, x_2, \ldots, x_M)|^2 dx_2 \cdots dx_M.$$

Therefore, if one defines

$$D_\mu(f) \equiv \tfrac{1}{2} \iint f(x) f(y) Y_\mu(x-y) dx dy, \tag{3.10}$$

and

$$\Omega(\phi) \equiv \left\langle \phi, \left[-\sum_{j=1}^{M} \Delta_j + \sum_{1 \leqq i < j \leqq M} Y_\mu(x_i - x_j) \right] \phi \right\rangle - D_\mu(\rho_\phi),$$

an easy calculation yields

$$\langle \phi, H_{BM}^\mu \phi \rangle = \Omega(\phi) + D_\mu(\rho_\phi - \tilde{\rho}_B). \tag{3.11}$$

Let $Q \equiv \int \rho_\phi - \int \tilde{\rho}_B$ be the value of the total charge in the small box. The following lemma is needed to bound the last term in (3.11).

Lemma 3.1 *Let $U = \{x \mid |x| \leqq d\}$ be a ball of radius d and let $f: U \to \mathbf{R}$ be a (not necessarily positive) density satisfying $\int_U f = Q$. Then*

$$D_\mu(f) \geqq \tfrac{1}{2}(Q^2/d)[1 + \mu d + \mu^2 d^2/3]^{-1}. \tag{3.12}$$

Proof. $D_\mu(f)$ can be written as

$$D_\mu(f) = \sup_h \int_U fh - \frac{1}{8\pi} \int_{\mathbf{R}^3} [|\nabla h|^2 + \mu^2 h^2].$$

To prove (3,10) we merely take (with $r = |x|$) $h(x) = \alpha$ for $r \leqq d$ and $h(x) = \alpha d e^{-\mu(r-d)}/r$ for $r \geqq d$. Then $\int fh = \alpha Q$. The $r < d$ part of the second integral is $\alpha^2 \mu^2 d^3/6$. The $r > d$ part can be calculated by integrating by parts, using $(-\Delta + \mu^2)h = 0$, and $d^2 h h'|_{r=d} = -\alpha^2(\mu d^2 + d)$. This $r > d$ part is $\frac{1}{2}\alpha^2 d(1 + d\mu)$. Maximizing with respect to α yields (3.12). □

Remark. Equation (3.12) is sharp when $\mu = 0$ or $\mu \to \infty$ with fixed d.

Returning to (3.11), recall that $l = \rho_B^{-1/8}$ and $\mu = C_6 \rho_B^{1/8}$. The $l \times l \times l$ cube fits into a ball of radius $d = 3^{1/2} l/2$. Applying (3.12) with $\mu d = \sqrt{3} C_6/2 \equiv C_7$ we find that, with $C_8 = 3^{-1/2}[1 + C_7 + C_7^2/3]^{-1}$,

$$D_\mu(\rho_\phi - \tilde{\rho}_B) \geqq C_8 (M - n_B)^2 \rho_B^{1/8}. \tag{3.13}$$

Finally, we have to estimate $\Omega(\phi)$. For this purpose we introduce a "duplication of variables" trick. Consider the Hamiltonian on $L^2(\mathbf{R}^{3M})$.

$$H_{2M}^\mu = -\sum_{j=1}^{2M} \Delta_i + \sum_{1 \leqq i < j \leqq 2M} e_i e_j Y_\mu(x_i - x_j), \tag{3.14}$$

where $e_i = 1$ for $i \leqq M$ and $e_i = -1$ for $i > M$. Let Φ be a normalized trial function defined by

$$\Phi(x_1, \ldots, x_{2M}) = \phi(x_1, \ldots, x_M)\phi(x_{M+1}, \ldots, x_{2M}).$$

A simple calculation yields

$$\Omega(\phi) = \tfrac{1}{2}\langle \Phi, H_{2M}^\mu \Phi \rangle. \tag{3.15}$$

By (A.23) in the appendix,

$$\Omega(\phi) \geqq -\tfrac{1}{2}(4.016)(2M)^{5/3}. \tag{3.16}$$

Let us divide the possible values of M into two cases.

(a) $M \leqq \rho_B^{11/32}$. Here we use (3.11), (3.16) and $D_\mu(\rho_\phi - \tilde{\rho}_B) \geqq 0$ to conclude that

$$\langle \phi, H_{BM}^{\mu} \phi \rangle \geqq -(6.375)M^{5/3} \geqq -(6.375)M\rho_B^{11/48}. \tag{3.17}$$

(b) $M > \rho_B^{11/32}$. Here we use Theorem 2.1, (3.11), (3.13) and (3.15) to conclude that for large enough ρ_B

$$\langle \phi, H_{BM}^{\mu} \phi \rangle \geqq -C_9(\rho_B)M^{7/5} + C_8(M - n_B)^2 \rho_B^{1/8}, \tag{3.18}$$

where $C_9(\rho_B) \to (0.30)2^{2/5}$ as $\rho_B \to \infty$. The statement "large enough ρ_B" comes from the condition in Theorem 2.1 that $\mu M^{-2/5} \to 0$ as $M \to \infty$. By our assumption $\mu M^{-2/5} \leqq C_6 \rho_B^{-1/80}$, and this goes to zero as $\rho_B \to \infty$. If, in (3.18), we recall that $n_B \leqq \rho_B l^3 = \rho_B^{5/8}$ and $M > \rho_B^{11/32}$, it is easy to see that the right side of (3.18) is bounded below by $-C_{10}(\rho_B)M\rho_B^{1/4}$ and that $C_{10}(\rho_B) \to (0.30)2^{2/5}$ as $\rho_B \to \infty$.

Using these results (a) and (b), and summing over boxes, and recalling (3.6), we conclude that

$$E_0 \geqq -[C_{11}(\rho_B)a_0^{-5/4} + C_0]N\rho_B^{1/4} \tag{3.19}$$

with $C_{11}(\rho_B) \to (0.30)2^{2/5}$ as $\rho_B \to \infty$. Recall from Sect. II that $a_0 = (3/4)^3$ and $C_0 < 3(\pi/2)^2$. Note that (3.19) holds for all N; we did not take the limit $N \to \infty$ in deriving (3.19). With the bounds just given, the factor [ ] in (3.19) is 8.57 when $\rho_B \to \infty$.

This completes the proof of Theorem 1.1. This theorem can be generalized to the case of Yukawa potentials as in Theorem 2.1. It can also be generalized in another direction as follows.

Theorem 3.1. *Consider the modified jellium Hamiltonian with variable background charge density*

$$H_N^J = -\sum_{i=1}^{N} \{\Delta_i + V(x_i)\} + \sum_{1 \leqq i < j \leqq N} |x_i - x_j|^{-1} + \tfrac{1}{2}\int \rho(x)\rho(y)|x-y|^{-1} dx dy, \tag{3.20}$$

with $V(x) = \int \rho(y)|x-y|^{-1} dy$. The density ρ satisfies $-\infty < \rho(x) \leqq \rho_B$ with $\rho_B \geqq 0$. Then the ground state energy satisfies

$$E_0 \geqq -A_9 N \rho_B^{1/4} \tag{3.21}$$

and A_9 satisfies the same bound as A_6, given in Theorem 1.1.

The proof is an easy generalization of the one for constant $\rho(x) = \rho_B$ in Λ just given.

IV. Computation of Constants

Our main goal in this section is to obtain the constant 0.30 in the inequality (1.12). The calculation will consist of optimizing the methodology of [2]. We shall first make a heuristic calculation of the ground state energy E_0 of the Hamiltonian H_N

in (1.1) by using a modification of Bogoliubov's method, and will return to a proper proof of Theorem 1.4 later after Eq. (4.23). We find heuristically that $E_0 \sim -0.028N^{7/5}$ but we are not conjecturing that this constant is sharp. In the following we shall closely follow the notation of [2].

Heuristic Calculations. We consider the case $v = 2\pi/L$ (essentially the Coulomb case) and introduce periodic boundary conditions on Λ for the Hamiltonian H_N. Thus we have

$$\langle \psi, H_N^v \psi \rangle = \langle \psi, T\psi \rangle + \tfrac{1}{2} \sum_{k \in \mathbf{Z}^3} v(k) [\langle \psi, A_k^* A_k \psi \rangle - N]. \tag{4.1}$$

The operator T is the kinetic energy operator, which we write in the second quantized form (see [10] or [7], for example) as

$$T = L^{-2} 4\pi^2 \sum_{k \in \mathbf{Z}^3} k^2 [a_k^* a_k + b_k^* b_k]. \tag{4.2}$$

Here L is the length of a side of Λ. The operators a_k, b_k are annihilation operators corresponding to the two species of bosons and $k \in \mathbf{Z}^3$. The charge density operator A_k is given by

$$A_k = \sum_{n \in \mathbf{Z}^3} a_{n+k}^* a_n - b_{n+k}^* b_n. \tag{4.3}$$

The $v(k)$ is just the Fourier transform of the Yukawa potential Y_v (with $v = 2\pi/L$) divided by the volume of Λ. We take this value of $v > 0$ to avoid the singularity at $k = 0$. Thus $v(k)$ is given by

$$v(k) = [\pi L(|k|^2 + 1)]^{-1}. \tag{4.4}$$

In Bogoliubov's approximation one makes the ansatz

$$A_k \simeq \sum_{|m| \leqq D\gamma} [S_{k,m}^* + T_{k,m}]. \tag{4.5}$$

Here, D and γ are constants which will be defined later in (4.14) and (4.23). The operators $S_{k,m}, T_{k,m}$ are defined as in (2.8) of [2] by

$$S_{k,m} = \begin{cases} a_n^* a_{n+k} & \text{if } m = (n, 1) \\ -b_n^* b_{n+k} & \text{if } m = (n, -1) \end{cases},$$
$$T_{k,m} = \begin{cases} a_n^* a_{n-k} & \text{if } m = (n, 1) \\ -b_n^* b_{n-k} & \text{if } m = (n, -1) \end{cases}. \tag{4.6}$$

In (4.6) $n \in \mathbf{Z}^3$ and ± 1 indicates the charge species; $|m|$ is defined to be $|n|$. The operators $a_n^\#, b_n^\#$ with $|n| \leqq D\gamma$ are to be thought of as scalars subject to the constraint

$$\sum_{|n| \leqq D\gamma} a_n^* a_n = \sum_{|n| \leqq D\gamma} b_n^* b_n = \frac{N}{2}. \tag{4.7}$$

Hence if $|m| \leqq D\gamma$ and $|k| > 2D\gamma$ the $S_{k,m}$ and $T_{k,m}$ are just annihilation operators. The expression (4.1) then becomes quadratic in creation and annihilation operators. One can compute its ground state energy exactly in the case when $D\gamma = 0$ but also to a good approximation when $D\gamma > 0$. We do this by writing (4.1) as

$$\langle \psi, H_N^v \psi \rangle = 4\pi^2 L^{-2} \sum_{|k| \leqq D\gamma} k^2 \langle \psi, [a_k^* a_k + b_k^* b_k] \psi \rangle$$

$$+ \tfrac{1}{2} \sum_{|k| > D\gamma N^\delta} v(k) I_k(\varepsilon_k, \psi) + \text{lower order terms}, \tag{4.8}$$

where $\delta > 0$ is a small positive number. The expression $I_k(\varepsilon, \psi)$ is given, for general ε, by

$$I_k(\varepsilon, \psi) = \left\langle \psi, \left[\varepsilon \sum_{|m| \leqq D\gamma} [S_{k,m}^* S_{k,m} + T_{k,m}^* T_{k,m}] \right.\right.$$

$$\left.\left. + \left(\sum_{|m| \leqq D\gamma} S_{k,m}^* + T_{k,m} \right)^* \left(\sum_{|m| \leqq D\gamma} S_{k,m}^* + T_{k,m} \right) - N \right] \psi \right\rangle. \tag{4.9}$$

The number ε_k is given by the formula

$$\varepsilon_k = 8\pi^2 k^2 [NL^2 v(k)]^{-1}. \tag{4.10}$$

One can compute exactly the ground state energy of $I_k(\varepsilon, \psi)$. It is given in [2] as

$$I_k(\varepsilon, \psi) \geqq N \left\{ \left[\left(\frac{\varepsilon}{n_0} \right)^2 + 2 \left(\frac{\varepsilon}{n_0} \right) \right]^{1/2} - 1 - \frac{\varepsilon}{n_0} \right\}, \tag{4.11}$$

where

$$n_0 = \sum_{|m| \leqq D\gamma} 1. \tag{4.12}$$

The right-hand side of (4.11) can be achieved if the numbers a_n, b_n satisfy

$$a_n^* a_n = b_n^* b_n = \frac{N}{n_0}, \quad |n| \leqq D\gamma. \tag{4.13}$$

We shall take γ to be large, $\gamma \geqq N^\delta$, and fix D to be the finite number

$$D = \pi^{-1} (5/12)^{1/2} = 0.645/\pi. \tag{4.14}$$

Then, to leading order of magnitude the ground state energy of the second sum in (4.8) is given by

$$\frac{-2N}{L} \left(\frac{NLn_0}{8\pi^3} \right)^{1/4} I, \tag{4.15}$$

where I is the integral

$$I = \int_0^\infty [1 + \xi^4 - (\xi^8 + 2\xi^4)^{1/2}] d\xi. \tag{4.16}$$

Observe that

$$0 < I < J = \int_0^\infty \frac{d\xi}{1 + 2\xi^4}. \tag{4.17}$$

Numerical values for I, J are given by

$$I = .806, \quad J = \pi 2^{1/4}/4 = 0.934. \tag{4.18}$$

The integral I can be expressed exactly in terms of elliptic integrals [7]. Since γ is large n_0 is given to leading order as

$$n_0 = 2 \int_{|x| \leqq D\gamma} dx = \frac{8\pi}{3}(D\gamma)^3. \tag{4.19}$$

Hence (4.15) is given by

$$-B_0 \frac{N}{L}(NL\gamma^3)^{1/4}, \tag{4.20}$$

where

$$B_0 = 2(3\pi^2)^{-1/4} D^{3/4} I. \tag{4.21}$$

The formula (4.20) gives the second sum in (4.8) to leading order of magnitude. Next we need to calculate the first sum in (4.8) which is the macroscopic kinetic energy of the low lying occupied states subject to (4.13). This is clearly given to leading order of magnitude by

$$\begin{aligned}\frac{2N}{n_0} \sum_{|k| \leqq D\gamma} \frac{4\pi^2}{L^2}|k|^2 &= \frac{2N}{n_0}\frac{4\pi^2}{L^2} \int_{|x| \leqq D\gamma} |x|^2 dx \\ &= \left(\frac{12D^2\pi^2}{5}\right)\frac{N\gamma^2}{L^2} = \frac{N\gamma^2}{L^2}.\end{aligned} \tag{4.22}$$

The total energy of the system then, according to this calculation, is

$$\frac{12\pi^2}{5} N\left(\frac{D\gamma}{L}\right)^2 - 2(3\pi^2)^{-1/4} I N^{5/4}\left(\frac{D\gamma}{L}\right)^{3/4}. \tag{4.23}$$

If we minimize this expression with respect to $D\gamma/L$ we obtain the value $-0.028N^{7/5}$.

Proof of Theorem 1.4. In the following calculation we shall ignore all terms of lower order then $N^{7/5}$ since we are only concerned with proving the inequality (1.12) for $N \to \infty$. Let γ be the γ_ψ defined by (1.10). We can assume without loss of generality (by changing Λ to be a sufficiently large cube) that the δ in Theorem 1.4 is less than $\frac{1}{6}$ and that $\gamma \geqq N^\delta$. Define μ by $\mu L = \max(N^{1/10}, \nu L)$ so that $\mu L \to \infty$ and $N^{-1/5}\mu L < \infty$ as $N \to \infty$. If $\nu L < N^{1/10}$, let us write $Y_\nu = (Y_\nu - Y_\mu) + Y_\mu$ and write

$$\langle \psi, H_N^\nu \psi \rangle = N^{-1/10} K(\psi) + P_\nu(\psi) - P_\mu(\psi) + (1 - N^{-1/10})K(\psi) + P_\mu(\psi). \tag{4.24}$$

Here, $P_\nu(\psi)$ denotes the potential energy terms in H_N^ν with the Yukawa potential Y_ν. Since $Y_\nu - Y_\mu$ is positive definite, $P_\nu(\psi) - P_\mu(\psi) \geqq -\frac{1}{2}(\mu - \nu)N \geqq -\frac{1}{2}\mu N \geqq -\frac{1}{2}N^{11/10}/L$. By the uncertainty principle in a box, $K(\psi) \geqq CN/L^2$, whence the first three terms on the right side of (4.24) are at least $CN^{9/10}/L^2 - \frac{1}{2}N^{11/10}/L$. Minimizing this with respect to L, we find that these terms are bounded below by $-CN^{13/10} \gg -N^{7/5}$. For the last two terms on the right side of (4.24) we can clearly replace $N^{-1/10}$ by zero in the limit $N \to \infty$. Thus we need prove Theorem 1.4 only under the condition $\nu L \geqq N^{1/10}$ and $N^{-1/5}\nu L$ bounded.

By taking Λ to be four times as big, we can suppose that ψ is supported in Q^N, where Q is a smaller cube of size $L/4$. We can then replace $Y_\nu(x)$ in H_N^ν by its periodic extension

$$Y_\nu^L(x) = \sum_{n \in \mathbf{Z}^3} Y_\nu(x + nL), \tag{4.25}$$

because the difference in the two potential energies is at most $W(N) = N^2 L^{-1} e^{-\nu L/2}$ (with the factor N^2 coming from the number of interaction terms). Since $\nu L \geqq N^{1/10}$, $W(N) < N^\varepsilon/L$ as $N \to \infty$ for every $\varepsilon > 0$. As before, we can borrow $N^{-1/10} K(\psi) \geqq N^{9/10}/L^2$ to control $W(N)$.

Using Y_ν^L in H_N^ν, we then have that (4.1) is an identity provided that H_N^ν is now understood to contain Y_ν^L and provided (4.4) is replaced by

$$\nu(k) = [\pi L\{k^2 + (\nu L/2\pi)^2\}]^{-1}. \tag{4.26}$$

Clearly, $\nu(k) \geqq [\pi L(|k|^2 + 1)]^{-1}$. Now we are ready to bound the various terms in (4.1).

First we bound the potential energy terms for $|k| < N^\delta D\gamma$ from below by

$$-\tfrac{1}{2}N \sum_{|k| \leqq N^\delta D\gamma} \nu(k) \geqq -CN^{1+\delta} D\gamma/L. \tag{4.27}$$

If, as before, we combine a small portion of the kinetic energy with (4.27) we obtain a lower bound which is lower order than $N^{7/5}$.

Next consider terms in the potential energy which have $|k| > N^\delta D\gamma$. We define $S_{k,m}$, and $T_{k,m}$ again as in (4.6) but this time for all m with $|m| \leqq |k|/N^\delta$. Let us assume for the moment that the system is neutral so that the number of negative particles is $N/2$. We shall return to the nonneutral case after Eq. (4.68). Since $\gamma \leqq N^{1/3-\delta}$, Lemma 2.2 of [2] becomes

$$\langle \psi, T\psi \rangle \geqq \frac{4\pi^2}{NL^2} \sum_{|k| > N^\delta D\gamma} [1 - CN^{-\delta}] k^2 C_k(\psi), \tag{4.28}$$

and $C_k(\psi)$ is given by

$$C_k(\psi) = \sum_{r=0}^{\infty} 2^{-4r} \sum_{|m|}^{r} \langle \psi | S_{k,m}^* S_{k,m} + T_{k,m}^* T_{k,m} | \psi \rangle, \tag{4.29}$$

where $\sum_{|m|}^{r}$ is a sum over $(2^r - 1)N^{1/3-\delta/2} \leqq |m| < (2^{r+1} - 1)N^{1/3-\delta/2}$. Note that the constant $4\pi^2/NL^2$ in (4.28) is better than that in [2]. This is due to the improved summation procedure in (4.29). Hence we have

$$\langle \psi, H_N^\nu \psi \rangle \geqq \tfrac{1}{2} \sum_{|k| > N^\delta D\gamma} \nu(k) I_k(\varepsilon_k, \psi), \tag{4.30}$$

where

$$I_k(\varepsilon, \psi) = \varepsilon C_k(\psi) + \langle \psi | A_k^* A_k - N | \psi \rangle, \tag{4.31}$$

$$\varepsilon_k = 8\pi^2 k^2 [1 - CN^{-\delta}][NL^2 \nu(k)]^{-1}. \tag{4.32}$$

Since the term $CN^{-\delta}$ in (4.32) is lower order, we shall ignore it in future computations.

Now let $a > 1$ be a positive number which we shall fix later. We define

$$n_0 = \#\{m : |m| \leqq D\gamma\},$$
$$n_r = \#\{m : a^{r-1} D\gamma < |m| \leqq a^r D\gamma\}, \quad r = 1, 2, 3, \ldots. \tag{4.33}$$

Evidently we have, to leading order,

$$n_0 = \frac{8\pi}{3}(D\gamma)^3,$$

$$n_r = \frac{8\pi}{3}(D\gamma)^3 a^{3(r-1)}[a^3 - 1]. \tag{4.34}$$

We define N_r, $r = 1, 2, \ldots$, to be the maximum possible number of particles, consistent with the given $K(\psi)$, such that $|k| > a^{r-1} D\gamma$. Thus we have

$$4\pi^2 N_r (a^{r-1} D\gamma)^2 L^{-2} = N\gamma^2 L^{-2}, \tag{4.35}$$

which yields

$$N_r = N[4\pi^2 (a^{r-1} D)^2]^{-1}. \tag{4.36}$$

We define $N_0 = N$.

The key inequality in [2] is

$$I_k(\varepsilon, \psi) \geqq \sum_{r=0}^{\infty} [\alpha_r - (1 + \eta_r) N_r] + E_k. \tag{4.37}$$

The term E_k is a constant times the number of particles with momentum n satisfying $|n| \geqq C|k|/N^\delta$. It follows that the expression

$$\sum_k v(k) E_k \tag{4.38}$$

can be combined with a small portion of the kinetic energy to yield a lower order term. We shall therefore concentrate on the sum on the right-hand side of (4.37). The η_r are defined as

$$\eta_r = \varepsilon / [n_r p_r], \tag{4.39}$$

and

$$p_r = 2^{4t} \quad \text{if} \quad (2^t - 1) N^{1/3 - \delta} \leqq a^r D\gamma < (2^{t+1} - 1) N^{1/3 - \delta/2}. \tag{4.40}$$

The α_r are the positive roots of the polynomial equation (in μ)

$$1 + \sum_{r=0}^{\infty} N_r [\eta_r N_r - \mu]^{-1} + N_r [\eta_r N_r + \mu]^{-1} = 0. \tag{4.41}$$

We order the roots α_r in the following manner: Let α_0 be the unique root of (4.41) which has $\alpha_0 > \eta_0 N_0$. The roots $\alpha_r, r = 1, 2, \ldots$, are the unique roots of (4.41) which satisfy $\eta_{r-1} N_{r-1} > \alpha_r > \eta_r N_r$. We define $\beta_r(k)$ by

$$-\beta_r(k) = \alpha_r - (1 + \eta_r) N_r, \tag{4.42}$$

where α_r is determined from (4.41) after setting $\varepsilon = \varepsilon_k$ in the definition, (4.39), of η_r.

Let us define

$$\tfrac{1}{2} \sum_{|k| > N^\delta D\gamma} v(k) \beta_r(k) = B_r N (N L \gamma^3)^{1/4} / L. \tag{4.43}$$

Note that B_r is a constant plus correction terms which tend to zero as $NL\gamma^3 \to \infty$. In the following computation (cf. (4.66)), it will be found that $NL\gamma^3$ indeed tends to infinity, and thus we are able to neglect these correction terms.

If we define B by

$$B = \sum_{r=0}^{\infty} B_r, \tag{4.44}$$

we have that

$$\langle \psi, H_N^\nu \psi \rangle \geqq -BN(NL\gamma^3)^{1/4}/L. \tag{4.45}$$

We need then to estimate β_r and B_r, for $r = 0, 1, 2, \ldots$. We first consider the case $r = 0$. The root α_0 of (4.41) is clearly bounded below by the unique positive root of the equation

$$N_0[\eta_0 N_0 - \mu]^{-1} + N_0[\eta_0 N_0 + \mu]^{-1} + 1 = 0. \tag{4.46}$$

Hence we obtain

$$\beta_0 \leqq N_0\{1 + \eta_0 - [\eta_0^2 + 2\eta_0]^{1/2}\}. \tag{4.47}$$

Now substituting the values for $\beta_0(k)$ and performing the sum in (4.43) we obtain

$$B_0 = 2(3\pi^2)^{-1/4} D^{3/4} I. \tag{4.48}$$

In the calculation for (4.48) we have used the fact that $p_0 = 1$ in (4.39). In fact $p_r = 1$ provided $r \leqq C \log N$, since $\gamma \leqq N^{1/3-\delta}$. Note that (4.48) and (4.21) are identical.

Next, we wish to estimate β_r and B_r when $r = 1, 2, \ldots$. Now α_r is bounded below by the unique root, μ, of the equation

$$1 + \sum_{j=0}^{r} N_j[\eta_j N_j - \mu]^{-1} + N_j[\eta_j N_j + \eta_r N_r]^{-1} = 0, \tag{4.49}$$

which lies in the interval $\eta_{r-1} N_{r-1} > \mu > \eta_r N_r$. Let $\alpha_{r,1}$ be the root of the polynomial equation which is the same as (4.49) except that the terms $N_j/(\eta_j N_j - \mu)$, $j = 0, \ldots, r-1$ are replaced by $N_j/(\eta_j N_j - \eta_r N_r)$, $j = 0, \ldots, r-1$. Thus $\alpha_{r,1}$ is *larger* than the corresponding root of (4.49). Next, let $\alpha_{r,2}$ be the root of the polynomial equation which is the same as (4.49) except that the terms $N_j/(\eta_j N_j - \mu)$, $j = 0, \ldots, r-1$ are replaced by $N_j/(\eta_j N_j - \alpha_{r,1})$. It is clear that $\alpha_{r,2}$ is *smaller* than the corresponding root of (4.49). We can define the quantities $\beta_{r,1}, B_{r,1}, B^1$ and $\beta_{r,2}, B_{r,2}, B^2$ to correspond to the roots $\alpha_{r,1}, \alpha_{r,2}$ respectively in exactly the some manner as β_r, B_r, B correspond to α_r.

We calculate $\alpha_{r,1}$. To do this we write the corresponding polynomial equation in the form

$$N_r[\eta_r N_r - \mu]^{-1} + 1 + h_{r,1}/(2\eta_r) = 0, \tag{4.50}$$

where $h_{r,1}$ is given by the equation

$$h_{r,1} = 1 + 2\sum_{j=0}^{r-1} [\eta_j/\eta_r + N_r/N_j]^{-1} + [\eta_j/\eta_r - N_r/N_j]^{-1}. \tag{4.51}$$

From (4.50) it follows that

$$\beta_{r,1} = (1 + \eta_r) N_r - \alpha_{r,1} = N_r[1 + 2\eta_r/h_{r,1}]^{-1}. \tag{4.52}$$

We wish now to fix the values of a and D in an optimal way. We do this by making the approximation $h_{r,1} \simeq 1$ and optimizing the value of B^1 based on this. With this approximation we have, then, an approximate value for $B_{r,1}$ obtained by summing (4.52),

$$B_{r,1} \simeq \tfrac{1}{2} J [\pi(a^{r-1} D)]^{-2} \left[\frac{1}{3\pi^2} D^3 a^{3(r-1)}(a^3 - 1) \right]^{1/4}. \tag{4.53}$$

Summing (4.53) from $r = 1, \ldots, \infty$ we have

$$\sum_{r=1}^{\infty} B_{r,1} \simeq \tfrac{1}{2}(3\pi^2)^{-1/4} \pi^{-2} J D^{-5/4} g(a), \tag{4.54}$$

where $g(a)$ is the function of a given by

$$g(a) = (a^3 - 1)^{1/4} a^{5/4} [a^{5/4} - 1]^{-1}. \tag{4.55}$$

We shall take $a = 2$, which is close to the minimum for g, and the corresponding value for g is $g(2) = 2.81$. From (4.48) and (4.54) we then have

$$B_0 + \sum_{r=1}^{\infty} B_{r,1} \simeq \tfrac{1}{2}(3\pi^2)^{-1/4} [4ID^{3/4} + 2.81\pi^{-2} J D^{-5/4}]. \tag{4.56}$$

The value of D is chosen to minimize the right side of (4.56). This yields the value

$$D = (1/\pi)[14.05J/12I]^{1/2} = 1.16/\pi. \tag{4.57}$$

It is of some interest to compare this value of D with the value of D given in (4.14), namely $D = .645/\pi$, which was used in the previous heuristic calculation. With D chosen as in (4.57), Eq. (4.56) yields

$$B_0 + \sum_{r=1}^{\infty} B_{r,1} \simeq 0.53. \tag{4.58}$$

Having fixed a and D we obtain an upper bound for B. The expression $h_{r,1}$ is given from (4.51) and (4.34), (4.36) as

$$\begin{aligned} h_{r,1} = 1 &+ 2 \sum_{j=1}^{r-1} \{[a^{3(r-j)} + a^{2(j-r)}]^{-1} + [a^{3(r-j)} - a^{2(j-r)}]^{-1}\} \\ &+ 2\left[a^{3(r-1)}(a^3 - 1) + \frac{a^{2(1-r)}}{4\pi^2 D^2} \right]^{-1} + 2\left[a^{3(r-1)}(a^3 - 1) - \frac{a^{2(1-r)}}{4\pi^2 D^2} \right]^{-1}. \end{aligned} \tag{4.59}$$

It is easy to see from (4.59) that

$$1 < h_{r,1} < 5/3. \tag{4.60}$$

If we use the lower bound in (4.60) we obtain from (4.50) an upper bound on $\alpha_{r,1}$,

$$\alpha_{r,1} < \eta_r N_r + (1 + 1/2\eta_r)^{-1} N_r = \eta_r N_r [1 + 2(1 + 2\eta_r)^{-1}] \leqq 3\eta_r N_r. \tag{4.61}$$

We may now use the upper bound (4.61) to obtain a *lower* bound on $\alpha_{r,2}$. In view of (4.61), $\alpha_{r,2}$ is bounded below by the root of the equation

$$N_r [\eta_r N_r - \mu]^{-1} + 1 + h_{r,2}/(2\eta_r) = 0, \tag{4.62}$$

where $h_{r,2}$ is given by the equation

$$h_{r,2} = 1 + 2\sum_{j=0}^{r-1} [\eta_j/\eta_r + N_r/N_j]^{-1} + [\eta_j/\eta_r - 3N_r/N_j]^{-1}. \tag{4.63}$$

If we express $h_{r,2}$ in a similar fashion to (4.59) it is easy to conclude that $h_{r,2} < 5/3$. We conclude then that

$$\beta_{r,2} \leqq N_r\left[1 + \frac{6\eta_r}{5}\right]^{-1}. \tag{4.64}$$

Hence from (4.58) we have

$$B \leqq 0.53(5/3)^{1/4} = 0.60. \tag{4.65}$$

Thus (4.45) and (4.65) yield a lower bound on the energy, $\langle\psi, H_N^\nu\psi\rangle$, of the wave function, ψ, in terms of $\gamma = \gamma_\psi$ and L.

To obtain a lower bound on the energy in terms of N alone, we have to use the fact that γ, L and N are not really independent when the energy is negative and when the hypotheses of Theorem 1.4 are satisfied. To see this let us divide the kinetic energy into two parts. One part is estimated by using the definition of γ as $N\gamma^2/L^2$. The other part is put together with the potential energy and use is made of (4.45). In all, then, we have for any $\lambda, 0 < \lambda < 1$, the inequality

$$\langle\psi, H_N^\nu\psi\rangle \geqq \frac{\lambda N\gamma^2}{L^2} - \frac{B}{(1-\lambda)^{1/4}} N^{5/4}\left(\frac{\gamma}{L}\right)^{3/4}. \tag{4.66}$$

The factor $(1-\lambda)^{-1/4}$ in (4.66) is obtained by applying scaling to (4.45). Minimizing (4.66) with respect to γ/L yields

$$\langle\psi, H_N^\nu\psi\rangle \geqq -(5/8)(3/8)^{3/5} B^{8/5} N^{7/5} \lambda^{-3/5}(1-\lambda)^{-2/5}. \tag{4.67}$$

The maximum value of $h(\lambda) = \lambda^{3/5}(1-\lambda)^{2/5}$ for $0 < \lambda < 1$ is obtained at $\lambda = 3/5$ with $h(3/5) = .510$. Hence (4.67) yields

$$\langle\psi, H_N^\nu\psi\rangle \geqq -0.30 N^{7/5}. \tag{4.68}$$

We have proven (4.68) under the assumption that H_N^ν is the Hamiltonian of a *neutral* system. However for the argument of Sect. II to be valid we need to know that (4.68) holds even for nonneutral systems. The neutrality assumption entered in our calculations only in the inequality (4.28) and it did so in the following way. The estimate in Lemma 2.2 of [2] leads to a denominator $2\max(N_+, N_-)$ instead of N in (4.28). It is only when $N_+ = N_- = N/2$ that we get (4.28). If the system is not neutral and the ratio of negative particles to the total number of particles is given by

$$\frac{N_-}{N} = \frac{(1-\xi)}{2}, \quad 0 \leqq \xi \leqq 1, \tag{4.69}$$

then the coefficient $4\pi^2/NL^2$ of the sum in (4.28) must be decreased to $4\pi^2/(1+\xi)NL^2$, which in turn leads to the inequality

$$\langle\psi, H_N^\nu\psi\rangle \geqq -0.30(1+\xi)^{2/5} N^{7/5}. \tag{4.70}$$

The inequality (4.70) gives an $N^{7/5}$ lower bound for a nonneutral system which has a slightly larger constant than the constant 0.30 for the neutral case. We wish to show that the constant 0.30 still holds for the nonneutral case in the situation where we apply this inequality in Sect. II. The Hamiltonian H_N^ν can be written as

$$H_N^\nu = W_N^\nu + H_N^\omega, \tag{4.71}$$

where W_N^ν is the N-body potential energy obtained from the function

$$r^{-1}(e^{-\nu r} - e^{-\omega r}) = \int_\nu^\omega e^{-ur} du. \tag{4.72}$$

We choose $\omega = \nu + N^{1/5}$. The inequality (4.70) applies to H_N^ω. In fact, the inequality becomes better since $\omega > \nu$, which implies that $\nu(k)$ becomes smaller. Our bound (4.70) is monotone in $\nu(k)$.

To bound W_N^ν from below, let us suppose the particles are fixed at points $x_1, \ldots, x_N$ with the negative particles being at $x_i, i = 1, \ldots, N_-$. We define a density $\rho(x)$, by

$$\rho(x) = \sum_{i=1}^N e_i \delta(x - x_i). \tag{4.73}$$

It is clear that

$$W_N^\nu = \frac{1}{2}\int_\nu^\omega du \int e^{-u|x-y|} \rho(x)\rho(y) dx dy - \tfrac{1}{2} N^{6/5}. \tag{4.74}$$

The following lemma and proof is due to Federbush [6, 3]. It can also be proved by the method of Lemma 3.1.

Lemma 4.1. *Let $\Lambda \subset \mathbf{R}^3$ be a cube of side length L. Let $f: \Lambda \to \mathbf{R}$ be a (not necessarily positive) density with $Q = \int_\Lambda f dx$. Let $\mu \geqq 0$. Then there is a constant C_{14} independent of μ, f, L such that*

$$D_\mu(f) \equiv \tfrac{1}{2}\int f(x) f(y) \exp[-\mu|x-y|] dx dy \geqq C_{14} Q^2 \mu L (1 + \mu^2 L^2)^{-2}.$$

Proof. Assume $f \in L^2(\Lambda)$ and write

$$\begin{aligned} D_\mu(f) &= \tfrac{1}{2}\langle f, e^{-\mu|x-y|} f\rangle = 4\pi\mu \langle f, (-\Delta + \mu^2)^{-2} f\rangle \\ &= 4\pi\mu \|(-\Delta + \mu^2)^{-1} f\|_2^2 \geqq 4\pi\mu |\langle g, (-\Delta + \mu^2)^{-1} f\rangle|^2 / \|g\|_2^2 \\ &\geqq 4\pi\mu |\langle h, f\rangle|^2 / \|(-\Delta + \mu^2) h\|_2^2, \end{aligned}$$

where g is any function in $L^2(\mathbf{R}^3)$ and where $g = (-\Delta + \mu^2)h$. Let H be a C^∞ function with $H(x) = 1$ for $|x| \leqq 2$ and $H(x) = 0$ for $|x| \geqq 3$. Finally, take $h(x) = H(x/L)$. □

From (4.70) to (4.74) and Lemma 4.1 we conclude that

$$\langle \psi, H_N^\nu \psi\rangle \geqq C_{14} \nu L (1 + \nu^2 L^2)^{-2} \xi^2 N^{11/5} - \tfrac{1}{2} N^{6/5} - 0.30(1 + \xi)^{2/5} N^{7/5}. \tag{4.75}$$

The inequality (4.75) shows that (4.68) holds for large N, even in the nonneutral case, provide $\nu L N^{-1/5} < \infty$ as $N \to \infty$. (Recall that, as stated in the beginning, it is only necessary to prove Theorem 1.4 when $\nu L > N^{1/10}$.) This concludes the proof of Theorem 1.4.

V. The Nonneutral Case

Consider the Hamiltonian H_N of (1.1) and its generalization H_N^ν of Theorem 2.1 or (2.21) acting on N_- negative particles and N_+ positive particles with $N_- \leqq N_+, N_- + N_+ = N$. Our goal here is to generalize Theorems 1.2 and 2.1 as follows.

Theorem 5.1. *Let H_N^ν be as in Theorem 2.1, and let there be N_- negative and N_+ positive particles with $N_- \leqq N_+$. The parameter ν can depend on N_- and N_+ but we suppose that $N_-^{-2/15}\nu \to 0$ as $N_- \to \infty$. (Note the difference from Theorem 2.1.) Then*

$$H_N^\nu \geqq -A_5 N_-^{7/5} \tag{5.1}$$

for some constant, A_5.

The proof follows the same lines as in Sect. II. One must modify it in two respects, however. First, it is necessary to prove that the interaction energy depends only on the number of negative particles. Second, we need to localize the kinetic energy in a somewhat different way than in Sect. II. Basically we only want to localize the kinetic energy of a positive particle if it lies in a box containing a negative particle. If we were to localize the kinetic energy of all positive particles, the cost in energy would be proportional to the number of positive particles and this of course could be much larger than $N_-^{7/5}$.

We solve the problem of the interaction energy in Lemma 5.3 below, but first we require the two preliminary Lemmas 5.1 and 5.2. The first is independently interesting.

Lemma 5.1. *Suppose that K and $L:\mathbf{R}^3 \to \mathbf{R}^+$ are two nonnegative functions (not necessarily symmetric) that satisfy the following (5.2), for some fixed, positive integer s,*

$$sL(x) \geqq K(y) \quad \text{whenever} \quad |x| \leqq |y|. \tag{5.2}$$

Let $x_1, \ldots, x_{N_-}$ and $y_1, \ldots, y_{N_+}$ be points in $\mathbf{R}^3$ that satisfy

$$\sum_{i=1}^{N_-} K(y_j - x_i) - \sum_{1 \leqq k \leqq N_+, k \neq j} L(y_j - y_k) > 0 \tag{5.3}$$

for each $j = 1, \ldots, N_+$. Then $N_+ \leqq CsN_-$, where C is some universal geometric constant (60 will suffice).

Proof. We shall use the following geometric fact. There exists a finite set of closed, solid, circular cones in $\mathbf{R}^3$, each with apex at the origin and each with solid angle $\pi/3$ such that their union is all of $\mathbf{R}^3$. The minimum number of cones required for this is some integer C, and it is easy to see that $C \leqq 60$. Denote these cones by $B_1, \ldots, B_C$. Let Y denote the set of y_i points.

Now, without loss of generality, assume $x_1 = 0$. Let $Y_1 = \{y_i | y_i \in B_1\}$ be the points in B_1, and let Z_1 be those s points in Y_1 which are closest to x_1. (If there is an ambiguity, make an arbitrary choice; if Y_1 has fewer than s points then $Z_1 \equiv Y_1$.) Next, apply this process to the remainder $Y \setminus Y_1$ and thereby obtain Z_2 with respect to B_2. Continuing in this way we obtain $Z_1, \ldots, Z_C$ and $Y_1, \ldots, Y_C$. Let $Z = \bigcup_{i=1}^{C} Z_i$, whence Z has at most sC points.

Take $y_j \notin Z$ and consider the contribution to the left side of (5.3) coming from x_1 and Z. This contribution is

$$A_j = K(y_j) - \sum_{y_k \in Z} L(y_j - y_k).$$

We claim that $A_j \leqq 0$. If $y_j \in B_\alpha$ then the second sum in A_j is not less than $\sum_{y_k \in Z_\alpha} L(y_j - y_k)$. But $|y_j - y_k|^2 = |y_j|^2 + |y_k|^2 - 2y_j \cdot y_k \leqq |y_j|^2 + |y_k|^2 - |y_j|\,|y_k| \leqq |y_j|^2$, since $|y_k| \leqq |y_j|$. Thus, $|y_j - y_k| \leqq |y_j|$ and thus $sL(y_j - y_k) \geqq K(y_j)$. Given that $y_j \in B_\alpha$, Z_α has s points and thus $A_j \leqq 0$.

If we now remove x_1 and Z from the system we obtain a reduced system with a new $N_- = N_- - 1$ and with a new $N_+ \geqq N_+ - sC$, and that satisfies (5.3) for all y_j in the new system. The construction can now be repeated with x_2 and then x_3 and so on until we obtain a final system with $N_- = 0$ and a final $\tilde{N}_+ \geqq N_+ - sCN_-$. This clearly cannot satisfy (5.3) if $\tilde{N}_+ > 0$. □

Lemma 5.2. *Let $K: \mathbf{R}^3 \to \mathbf{R}^+$ be given as in Lemma 2.1 by*

$$K(x) = r^{-1}\{e^{-\nu r} - e^{-\omega r} h(x)\}$$

with $r = |x|$ and $\omega > \nu \geqq 0$. Here we assume only that $h: \mathbf{R}^3 \to \mathbf{R}$ satisfies (i) $-H \leqq h(x) \leqq 1$ *for all x and some finite $H \geqq 0$;* (ii) *h is continuous in some neighborhood of $x = 0$. Then there is a positive integer s such that*

$$sK(x) \geqq K(y) \quad \textit{whenever} \quad |x| \leqq |y|. \tag{5.4}$$

The integer s depends only on $\omega - \nu \equiv \rho$ and on h. For fixed h, s is a nonincreasing function of ρ.

Proof. For (5.4) we can restrict our attention to the case $\nu = 0, \omega = \rho$ because multiplication of this K by $e^{-\nu r}$ only makes inequality (5.4) stronger. There is an $R > 0$ such that h is continuous in $B_R = \{x \mid |x| \leqq R\}$. Since $K(x) \geqq r^{-1}\{1 - e^{-\rho r}\}$, which is decreasing in r and since $K(x) \leqq r^{-1}\{1 + He^{-\rho r}\}$, we have that $K(y)/K(x) \leqq (1 + He^{-\rho r})/(1 - e^{-\rho r})$ with $r = |y|$. The maximum of this ratio for $r \geqq R$ occurs at $r = R$ and is $s_1 = (1 + He^{-\rho R})/(1 - e^{-\rho R})$. Thus $s_1 K(y) \geqq K(x)$ when $|x| \leqq |y|$ and $|y| \geqq R$. On the other hand, when $|x| \leqq |y| \leqq R$, consider the function $F_R(x, y) \equiv K(y)/K(x)$ defined in the closed set $T = \{(x, y): |x| \leqq |y| \leqq R\}$. There are 2 cases. Case (i): $h(0) = 1$. Then K is continuous on B_R with $K(0) = \rho$. Moreover, $K(x) \geqq r^{-1}(1 - e^{-\rho r})$ on B_R. Thus $F_R(x, y)$ is continuous and so has a maximum on T. Case (ii): $h(0) < 1$. Then $|x|K(x)$ is a continuous function on B_R and it is never zero, so $|x|K(x) \geqq t$ for some $t > 0$. Hence, $F_R(x, y) \leqq t^{-1}|x|K(y) \leqq t^{-1}(1 + H)$. Thus, (5.4) is satisfied for any integer $s \geqq \max\{s_1, \max_T F_R(x, y)\}$. To prove the monotonicity of s, consider $K(x)$ with $\nu \geqq 0$ and $\omega = \nu + \rho$. Let $F(x, y) = K(y)/K(x)$. Since $s \geqq 1$, we only consider x, y such that $F(x, y) \geqq 1$. Hence $(\partial F/\partial \rho)(x, y) = [(\partial K/\partial \rho)(y) - F(\partial K/\partial \rho)(x)]/K(x) = -[|y|K(y) - e^{-\nu|y|} - |x|K(y) + Fe^{-\nu|x|}]/K(x)$. One concludes that $(\partial F/\partial \rho)(x, y) \leqq 0$ if $|x| \leqq |y|$ and if $F(x, y) \geqq 1$. Hence s is monotone in ρ. □

Lemma 5.3. *Suppose $\nu, \rho, l \geqq 0$ and let*

$$f(x) = a_0 Y_\nu(x) - Y_{\rho+\nu}(x) h_l(x)$$

with $h_l(0) = a_0, h_l(x) = h(x/l)$ *and with* $h(x)$ *given by (2.8). This* f *is a generalization of* $f_{\mu l}$ *given in (2.16). Given* $x_1, \ldots, x_N \in \mathbf{R}^3$ *and* $e_i = \pm 1$, *let* N_- *(respectively* N_+*) be the number of* e_i *which are* -1 *(respectively* $+1$*). Assume that* $N_- \leqq N_+$. *Finally, suppose that* $\rho l \geqq C_3$ *(which is defined in Lemma 2.1 and which depends only on* h*), so that* $\hat{f} \geqq 0$. *Then there is a constant* C_{13} *depending only on* h *and not on* v, ρ, l, *such that*

$$\sum_{i<j} e_i e_j f(x_i - x_j) \geqq -C_{13} \rho N_- . \tag{5.5}$$

Proof. Let W denote the left side of (5.5). Combining Lemmas 5.1 and 5.2, there is an s (which depends on h and on ρl (by scaling)) so that whenever $N_+ \geqq CsN_-$ we can eliminate $N_+ - CsN_-$ positive particles without increasing W. Thus we can assume $N_+ \leqq CsN_-$. Furthermore, this s can only decrease when ρl increases, so we can take s to be the value it has when $\rho l = C_3$ (which depends only on h). Thus s depends only on h. Now since $\hat{f} \geqq 0$, we have $W \geqq -\frac{1}{2}(N_+ + N_-) f(0) = -\frac{1}{2}(N_+ + N_-)\rho a_0 \geqq -\frac{1}{2}(Cs+1)\rho a_0 N_-$. □

We return next to the problem of localizing the kinetic energy similarly to Sect. II. For any $\alpha = (u, \alpha_1, \ldots, \alpha_N) \in \Gamma \times \mathbf{Z}^{3n}$ we define ψ_α^l as in (2.11). We adopt the convention that the negative particles are labelled $1, \ldots, N_-$ and the positive particles are labelled $N_- + 1, \ldots, N$. Let S_α be the α_i which correspond to the negative particles,

$$S_\alpha = \{\alpha_1, \ldots, \alpha_{N_-}\}. \tag{5.6}$$

We denote by $\bar{S}_\alpha$ the set of nearest neighbors in $\mathbf{Z}^3$ of S_α, so

$$\bar{S}_\alpha = \{m \in \mathbf{Z}^3 \mid |m - \alpha_i| \leqq \sqrt{3} \text{ for some } \alpha_i \in S_\alpha\}. \tag{5.7}$$

Let N_α be "the number of positive particles which lie in a box occupied by a negative particle" and $\bar{N}_\alpha$ "the number of positive particles which lie in the same box as a negative particle or a nearest neighbor of such box." By this is meant

$$\begin{aligned} N_\alpha &= \#\{j > N_- \mid \alpha_j \in S_\alpha\}, \\ \bar{N}_\alpha &= \#\{j > N_- \mid \alpha_j \in \bar{S}_\alpha\}. \end{aligned} \tag{5.8}$$

The definition of $S_\alpha, \bar{S}_\alpha, N_\alpha, \bar{N}_\alpha$ depend only on $\alpha \in \mathbf{Z}^{3N}$. Finally we define the kinetic energy operator T_α (which also depends only on α) to be the kinetic energy of the negative particles plus the kinetic energy of "the positive particles which lie in a box occupied by a negative particle," namely

$$T_\alpha = \sum_{i=1}^{N_-} -\Delta_i + \sum_{\{j > N_- \mid \alpha_j \in S_\alpha\}} -\Delta_j . \tag{5.9}$$

We then have the following lemma:

Lemma 5.4. *Let* C_0 *be the constant in (2.14). The kinetic energy is bounded below (recalling the definition of* $\int d\alpha$ *before (2.11)) as*

$$\langle \psi, T\psi \rangle \geqq \tfrac{1}{2} \int d\alpha \langle \psi_\alpha^l, T_\alpha \psi_\alpha^l \rangle - C_0 l^{-2} [N_- + 27 \int \bar{N}_\alpha \|\psi_\alpha^l\|^2 d\alpha]. \tag{5.10}$$

Proof. We use (2.14) to bound $\langle \psi, -\Delta_i \psi \rangle$ below for $i \leqq N_-$, namely

$$\left\langle \psi, \sum_{i=1}^{N_-} -\Delta_i \psi \right\rangle \geqq \int d\alpha \left\langle \psi_\alpha^l, \sum_{i=1}^{N_-} -\Delta_i \psi_\alpha^l \right\rangle - C_0 l^{-2} N_- .$$

Now suppose $i > N_-$ and consider a fixed α. Then we have the inequality

$$\tfrac{1}{2}\int dx_i |\nabla_i(\chi_{u\alpha_i}(x_i/l)\psi)|^2 \leqq \int dx_i |\nabla_i \chi_{u\alpha_i}(x_i/l)|^2 |\psi|^2 + \int dx_i \chi^2_{u\alpha_i}(x_i/l)|\nabla_i \psi|^2. \quad (5.11)$$

Now use the fact that

$$|\nabla_i \chi_{u\alpha_i}(x_i/l)|^2 \leqq C_0 l^{-2} \sum_{\lambda \in \mathbf{Z}^3} g(\lambda - \alpha_i)\chi^2_{u\alpha_i}(x_i/l), \quad (5.12)$$

where $g(z)$ is the function $g(z) = 1$ if $|z| \leqq \sqrt{3}, g(z) = 0$ if $|z| > \sqrt{3}$. Hence we have for all $i > N_-$,

$$\tfrac{1}{2}\langle \psi^l_\alpha, -\Delta_i \psi^l_\alpha \rangle \leqq \int \prod_{j=1}^{N} \chi^2_{u\alpha_j}(x_j/l)|\nabla_i \psi|^2 dx + C_0 l^{-2} \sum_{\lambda \in \mathbf{Z}^3} g(\lambda - \alpha_i)\| \psi^l_{\alpha_1, \dots, \lambda, \dots, \alpha_N} \|^2, \quad (5.13)$$

with λ being in the i^{th} position in the last sum. For $i > N_-$ let T^i_α be the i^{th} term in the kinetic energy T_α in (5.9), namely $T^i_\alpha = -\Delta_i$ if $\alpha_i \in S_\alpha$, and $T^i_\alpha = 0$ otherwise. We have then from (5.13),

$$\tfrac{1}{2} \sum_{\alpha_i \in \mathbf{Z}^3} \langle \psi^l_\alpha, T^i_\alpha \psi^l_\alpha \rangle \leqq \sum_{\alpha_i \in \mathbf{Z}^3} \int \prod_{j=1}^{N} \chi^2_{u\alpha_j}(x_j/l)|\nabla_i \psi|^2 dx + 27 C_0 l^{-2} \sum_{\alpha_i \in \bar{S}_\alpha} \| \psi^l_\alpha \|^2. \quad (5.14)$$

The number 27 is the number of nearest neighbors of a point in $\mathbf{Z}^3$. If we sum (5.14) with respect to all α_j for $j \neq i$, and then sum over i, and then integrate over $u \in \Gamma$, we obtain the inequality (5.10). □

The following lemma is also needed for the proof of Theorem 5.1.

Lemma 5.5. *Let ψ^l_α be the localized wave function (2.11). Let V^μ_α be given by (2.12) and T_α by (5.9). Assume that $1 \leqq \mu \leqq N_-^{2/15}$. Then there is a constant $C = C(\mu l)$, depending only on μl such that, with the notation of (5.8), there is the estimate*

$$\tfrac{1}{2}\langle \psi^l_\alpha, T_\alpha \psi^l_\alpha \rangle + \langle \psi^l_\alpha, V^\mu_\alpha \psi^l_\alpha \rangle - 27 C_0 l^{-2} \bar{N}_\alpha \| \psi^l_\alpha \|^2 \geqq -C(\mu l) N_-^{7/5} \| \psi^l_\alpha \|^2. \quad (5.15)$$

Proof. We analyze the left side of (5.15) similarly to (2.15). Since there is no interaction between boxes, the left-hand side of (5.15) is bounded below by

$$\left[\sum_{\sigma \in \mathbf{Z}^3} E_\sigma \right] \| \psi^l_\alpha \|^2, \quad (5.16)$$

where E_σ is the ground state energy of the following Hamiltonian, H_σ, depending on σ. There are three cases: $\sigma \in S_\alpha$, $\sigma \in \bar{S}_\alpha \backslash S_\alpha$ and $\sigma \notin \bar{S}_\alpha$. If $\sigma \in S_\alpha$ and n_σ of the i, $1 \leqq i \leqq N$, have $\alpha_i = \sigma$ with n^-_σ of these satisfying $i \leqq N_-$, then H_σ is the Hamiltonian

$$H_\sigma = \tfrac{1}{2} T + V^\mu - 27 C_0 l^{-2} n^+_\sigma \quad (5.17)$$

acting on n_σ particles in a box of size l, n^-_σ of which are negative, n^+_σ positive. Here, $V^\mu = \sum_{i<j} e_i e_j Y_\mu(x_i - x_j)$. If $\sigma \in \bar{S}_\alpha \backslash S_\alpha$, then $n^-_\sigma = 0$ and H_σ is the Hamiltonian

$$H_\sigma = V^\mu - 27 C_0 l^{-2} n_\sigma \quad (5.18)$$

acting on n_σ positive particles in a box of size l. If $\sigma \notin \bar{S}_\alpha$ then H_σ is

$$H_\sigma = V^\mu \quad (5.19)$$

acting on n_σ positive particles.

We estimate the ground state energies E_σ. In the case of (5.19) we clearly have $E_\sigma \geqq 0$. In the case of (5.17) we use (4.75). Taking into account the factor $\frac{1}{2}$ in (5.17), which gives a factor $2^{1/4}$ in the $N^{7/5}$ law (cf. (4.66)), and with $\tau \equiv \mu l$, (4.75) reads (with $v = \mu$ and $\omega = 2\mu$ instead of $\omega = \mu + N^{1/5}$)

$$H_\sigma = C_{14}\mu\tau(1+\tau^2)^{-2}(n_\sigma^+ - n_\sigma^-)^2 - \tfrac{1}{2}\mu n_\sigma - (0.30)2^{1/4} n_\sigma[\max(2n_\sigma^+, 2n_\sigma^-)]^{2/5} - 27C_0\mu^2\tau^{-2}n_\sigma^+ . \tag{5.20}$$

The quantities in (5.20) satisfy $n_\sigma^- \leqq N_-$, τ is fixed, $1 \leqq \mu \leqq N_-^{2/15}$ and n_σ^+ is arbitrary. We minimize the left side of (5.20) with respect to n_σ^+. One can show that

$$H_\sigma \geqq -A(\tau)[\mu^2 n_\sigma^- + \mu^3 + (n_\sigma^-)^{7/5}] \tag{5.21}$$

for some A depending only on τ.

To bound (5.18), one simply notes that in this case

$$H_\sigma \geqq \tfrac{1}{2}(\sqrt{3}l)^{-1} n_\sigma(n_\sigma - 1)\exp(-\sqrt{3}\tau) - 27C_0 l^{-2} n_\sigma \geqq -B(\tau)l^{-3}$$

for some $B(\tau)$ independent of n_σ. By using the fact that $1 \leqq \mu \leqq N_-^{2/15}$, one has $H_\sigma \geqq -D(\tau)N_-^{2/5}$.

Now, putting together the bounds for (5.17), (5.18) and (5.19), we conclude that for some $F(\tau)$

$$\sum_{\sigma\in \mathbf{Z}^3} E_\sigma \geqq -F(\tau)\sum_\sigma^{(1)}\{\mu^2 n_\sigma^- + \mu^3 + n_\sigma^{-\,7/5}\} - F(\tau)\sum_\sigma^{(2)} N_-^{2/5},$$

where the first sum is over S_α and the second is over $\bar{S}_\alpha \backslash S_\alpha$. The number of points in S_α is N_- while the number of points in $\bar{S}_\alpha$ is at most 27 N_-. Using the facts that $\mu \leqq N_-^{2/15}$, $\sum^{(1)} n_\sigma^- = N_-$, and the convexity of $n \to n^{7/5}$, the lemma is proved. □

Proof of Theorem 5.1. Step 1. Starting with v, we define $\mu = N_-^{2/15}$, and $l = C_3 N_-^{-2/15}$, where C_3 is given in Lemma 2.1. As in Sect. II we write $a_0 Y_v = f + Y_\mu h_l$, with $f = a_0 Y_v - Y_\mu h_l$ as in Lemma 5.3. By Lemma 5.3, the contribution to the potential energy from f is bounded below by $-C_{13}(\mu - v)N_- \geqq -C_{13}N_-^{17/15}$ for large N. This can be neglected compared to $N_-^{7/5}$.

Step 2. Lemma 5.4 is used to localize the kinetic energy. The term $-C_0 l^{-2} N_-$ in (5.10) can be neglected since $l^{-2} = (C_3)^{-2} N_-^{4/15}$.

Step 3. The first and third terms on the right side of (5.10) is combined with the $Y_\mu h_l$ part of the potential energy. We localize this potential energy as in (2.13). The first and third terms of (5.10) plus the localized potential energy is just the left side of (5.15). To prove the theorem we merely have to sum the right side of (5.15) over α, but this is exactly $-C(C_3)N_-^{7/5}$ by the normalization condition on ψ. □

Appendix: Thomas–Fermi Theory and the Stability of Matter with Yukawa Potentials

Our main goal here is to establish a lower bound to the energy and an upper bound to the kinetic energy for quantum mechanical particles interacting with

Yukawa, instead of Coulomb potentials. We consider N movable particles with charge -1 and coordinates $x_1,\dots,x_N\in\mathbf{R}^3$ and K fixed particles with coordinates $R_1,\dots,R_K\in\mathbf{R}^3$ and charges $z_1,\dots,z_K\geqq 0$. The movable particles will be considered to be fermions with q spin states, so that $q=N$ corresponds to the boson case. The Hamiltonian is

$$H=-\sum_{i=1}^{N}\{\Delta_i+V(x_i)\}+\sum_{1\leqq i<j\leqq N}Y_\mu(x_i-x_j)+U, \tag{A.1}$$

with

$$V(x)=\sum_{j=1}^{K}z_jY_\mu(x-R_j),$$
$$U=\sum_{1\leqq i<j\leqq K}z_iz_jY_\mu(R_i-R_j). \tag{A.2}$$

$Y_\mu(x)=|x|^{-1}\exp\{-\mu|x|\}$ is the Yukawa potential. It is positive definite and satisfies

$$(-\Delta+\mu^2)Y_\mu=4\pi\delta. \tag{A.3}$$

The energy is

$$E=\inf\{(\psi,H_n\psi)|\,\|\psi\|_2=1\text{ and all }R_1,\dots,R_K\}. \tag{A.4}$$

The method of [15] will be used, which means that we first have to examine the Thomas–Fermi (TF) functional

$$\mathscr{E}(\rho)=\tfrac{3}{5}q^{-2/3}\gamma\int\rho^{5/3}(x)dx-\int V(x)\rho(x)dx+\tfrac{1}{2}\int\int\rho(x)\rho(y)Y_\mu(x-y)dxdy+U \tag{A.5}$$

and corresponding energy

$$E^{\mathrm{TF}}=\inf\{\mathscr{E}(\rho)|\rho\in L^{5/3}\cap L^1\}. \tag{A.6}$$

Notice that in (A.6) we do not impose $\int\rho=N$. This constraint could easily be dealt with, but it is not needed in this paper.

One of our results will be that $E^{\mathrm{TF}}-U$ is a monotone decreasing function of μ.

A. The Thomas–Fermi Problem. By the methods of [14], a minimizer exists for (A.6) and satisfies $\gamma q^{-2/3}\rho(x)^{2/3}=\max(\phi(x),0)$ with

$$\phi(x)=V(x)-(Y_\mu*\rho)(x). \tag{A.7}$$

Lemma A.1. $\phi(x)\geqq 0$, *all* x, *and therefore the* TF *equation becomes*

$$\gamma q^{-2/3}\rho(x)^{2/3}=\phi(x). \tag{A.8}$$

Proof. Let $B=\{x|\phi(x)<0\}$. On $B,\rho(x)=0$ and $R_i\notin B$, all i (because $\phi(R_i)=\infty$). Therefore $-\Delta\phi=-\mu^2\phi\geqq 0$ on B, so ϕ is superharmonic on B. Since $\phi=0$ on $\partial B,\phi\geqq 0$ on B which implies that B is empty. □

Lemma A.2. *Let* $z_1,\dots,z_K\geqq 0$ *and* $\tilde z_1,z_2,\dots,z_K>0$ *be two sets of charges with* $\tilde z_1\geqq z_1$. *Then, for all* $x,\tilde\phi(x)\geqq\phi(x)$.

Proof. Let $\psi=\tilde\phi-\phi$ and $B=\{x|\psi<0\}$. Clearly, $R_1\notin B$. On $B,\tilde\rho\leqq\rho$ so $(-\Delta+\mu^2)\psi=4\pi(\rho-\tilde\rho)\geqq 0$. Thus ψ is superharmonic on B and again B is empty. □

Lemma A.3. *Let* $z_1,\dots,z_M>0$ *and* $z_{M+1},\dots,z_K>0$ *be two sets of charges located* *at* $R_1, \ldots, R_K$. *Then*

$$E(z_1, \ldots, z_K) > E(z_1, \ldots, z_M) + E(z_{M+1}, \ldots, z_K). \tag{A.9}$$

Proof. This is Teller's theorem for the Yukawa potential and is proved as in [14] using Lemma A.2. □

Lemma A.3 is given in [16, p. 237].

Next, we turn to the question of monotonicity with respect to μ.

Lemma A.4. *Suppose* $\mu_1 > \mu_2$, *with given fixed charges* $z_i > 0$ *and locations* R_i. *Then* $\phi_2(x) \geqq \phi_1(x)$, *for all* x.

Proof. Let $\psi = \phi_2 - \phi_1$ and $B = \{x | \psi(x) < 0\}$. Then $(-\Delta + \mu_i^2)\phi_i(x) = \sum z_j \delta(x - R_j) - \rho_i(x)$. By subtracting these two equations, and using the fact that $\rho_1 > \rho_2$ on B, we find that $-\Delta\psi > \mu_1^2\phi_1 - \mu_2^2\phi_2 > 0$. Again, B is empty. □

Let us define

$$N^c = \int \rho, \tag{A.10}$$

where ρ is the solution to (A.8). N^c is the maximum negative charge for the TF system (A.5).

Lemma A.5. *If* $\mu_1 > \mu_2$, *with fixed* z_i *and* R_i, *then*

$$N_1^c \leqq N_2^c \quad \text{and} \quad E_1^{\mathrm{TF}} - U_1 \geqq E_2^{\mathrm{TF}} - U_2. \tag{A.11}$$

Proof. $N_1^c \leqq N_2^c$ is a trivial consequence of Lemma A.4 and (A.8). By multiplying (A.8) by ρ and integrating, we have that

$$E - U = -\tfrac{2}{5}\int V\rho - \tfrac{1}{10}\int\int \rho(x)\rho(y)\, Y_\mu(x-y)dxdy. \tag{A.12}$$

Since $\mu_1 > \mu_2, \rho_1(x) \leqq \rho_2(x)$ and $Y_{\mu_1}(x) < Y_{\mu_2}(x)$, for all x. This, together with (A.12), proves the lemma. □

Let us now compare the Yukawa TF problem with the Coulomb TF problem, which corresponds to $\mu = 0$. For the Coulomb problem $N^c = Z \equiv \sum_1^K z_j$ [14]. By Lemmas A.3 and A.5 we have that

$$E^{\mathrm{TF}} \geqq \sum_{j=1}^{K} E^{\mathrm{TF,atom}}(z_j) \geqq \sum_{j=1}^{K} E_{\mathrm{Coulomb}}^{\mathrm{TF,atom}}(z_j). \tag{A.13}$$

The latter inequality follows from the fact that $U = 0$ for an atom. For the TF Coulomb atom [14], $E^{\mathrm{TF}}(z) = -(3.679)\gamma^{-1}q^{2/3}z^{7/3}$. Thus, for the Yukawa problem,

$$E^{\mathrm{TF}} \geqq -(3.679)\gamma^{-1}q^{2/3}\sum_{j=1}^{K} z_j^{7/3}. \tag{A.14}$$

Another lower bound for $E^{\mathrm{TF,atom}}(z)$ can be obtained by dropping the $\rho\rho Y_\mu$ term in (A.5). The resulting minimization problem is trivial: $q^{-2/3}\gamma\rho(x)^{2/3} = V(x) = zY_\mu(x)$ for an atom. Since $\int Y_\mu^{5/2} = 4\pi(2\pi/5\mu)^{1/2}$, (A.13) implies

$$E^{\mathrm{TF}} \geqq -4q\mu^{-1/2}\gamma^{-3/2}(2\pi/5)^{3/2}\sum_{j=1}^{K} z_j^{5/2}. \tag{A.15}$$

B. The Quantum-Mechanical Problem. Returning to the Hamiltonian in (A.1), we want to find a lower bound to $\langle\psi, H\psi\rangle$ for any normalized N-particle function, ψ. The one-particle density of ψ is defined by

$$\rho_\psi(x) = N\int|\psi(x, x_2, \ldots, x_N)|^2 dx_2 \cdots dx_N, \tag{A.16}$$

and $\langle\psi, H\psi\rangle$ will be bounded in terms of ρ_ψ.

To bound the particle-particle energy we use the trick in [15]. Consider (A.5) with $q=1, K=N, \gamma=\delta$ (arbitrary), $R_i = x_i$ and $z_i = 1$ for $i=1,\ldots,N$. Then, inserting ρ_ψ in (A.1) and using (A.14),

$$\sum_{1\leqq i<j\leqq N} Y_\mu(x_i - x_j) \geqq \tfrac{1}{2}\int\int \rho_\psi(x)\rho_\psi(y) Y_\mu(x-y)dxdy - \tfrac{3}{5}\delta\int\rho_\psi^{5/3} - 3.679N/\delta. \tag{A.17}$$

To bound the kinetic energy, we use the bound in [15] (recall that $q=N$ for bosons):

$$K(\psi) = \left\langle \psi, -\sum_{i=1}^{N} \Delta_i\psi \right\rangle \geqq K_3 N^{-2/3}\int\rho_\psi(x)^{5/3}dx. \tag{A.18}$$

In [15], the constant K_3 is given as $\frac{3}{5}(3\pi/2)^{2/3} = 1.69$, but this constant was subsequently improved. The best bound at present is in [11] where it is shown that we can take $K_3 = 2.7709$.

Combining (A.17), (A.18) we have the following bound for any normalized ψ

$$\langle\psi, H\psi\rangle \geqq \mathscr{E}(\rho_\psi) - (3.679)N/\delta, \tag{A.19}$$

with $q=1$ and $\gamma = \frac{5}{3}K_3 N^{-2/3} - \delta$ in (A.5). We choose

$$\delta = \tfrac{5}{3}K_3 N^{-1/6}\left[N^{1/2} + \left(\sum_{j=1}^{K} z_j^{7/3}\right)^{1/2}\right]^{-1}, \tag{A.20}$$

which implies that $\gamma > 0$. Using the bound (A.14) we obtain

Theorem A.1. *With H given by (A.1), the following holds for all normalized ψ:*

$$\langle\psi, H\psi\rangle \geqq -\tfrac{3}{5}(3.679)K_3^{-1}N^{2/3}\left[N^{1/2} + \left(\sum_{j=1}^{K} z_j^{7/3}\right)^{1/2}\right]^2 \tag{A.21}$$

with $K_3 = 2.7709$.

The final task is to apply Theorem A.1 to H_N in (1.1). Suppose that K particles have $e_i = +1$ and M particles have $e_i = -1$ with $K+M=N$. By ignoring the positive kinetic energy of the positive particles, (A.21) can be used with $(N,K)\rightarrow(M,K)$. Alternatively, the roles of positive and negative particles can be interchanged, so we can also replace (N,K) in (A.21) by (K,M). The two bounds can then be averaged and an expression of the form $\frac{1}{2}(K^{2/3}+M^{2/3})(K^{1/2}+M^{1/2})^2$ is obtained. However, given that $K+M=N$, $K^{2/3}+M^{2/3}$ has its maximum at $K=M=N/2$. So does $K^{1/2}+M^{1/2}$. Thus we have

Theorem A.2. *With H_N given by (1.1), the following holds for all normalized ψ.*

$$\langle\psi, H_N\psi\rangle \geqq -1.004N^{5/3}. \tag{A.22}$$

A virial type theorem, analogous to Theorem 2.2, can be obtained from (A.22). Another application is the following.

Theorem A.3. *Suppose ψ is normalized and $\langle \psi, H_N \psi \rangle \leqq 0$. Then*

$$K(\psi) \leqq 4.016 N^{5/3}. \tag{A.23}$$

Proof. $0 \geqq K(\psi) + P(\psi) = \frac{1}{2}K(\psi) + \langle \psi, H_{N,1/2}\psi \rangle$ where $H_{N,1/2}$ is given by (1.1) but with Δ_i replaced by $\frac{1}{2}\Delta_i$. By scaling, the analogue of (A.22) is $\langle \psi, H_{N,1/2}\psi \rangle \geqq -2(1.004)N^{5/3}$. □

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