On the Dirac and Schwinger Corrections to the Ground-State Energy of an Atom

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Contents

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Introduction

In this article and [FS2, ..., 7] we prove an asymptotic formula for the ground-state energy of a non-relativistic atom. The ground-state energy $E(N,Z)$ for N electrons and a nucleus of charge Z is defined[1] as the infimum of the spectrum of the Hamiltonian

$$H_{NZ} = \sum_{k=1}^{N} \left(-\Delta_{x_k} - Z|x_k|^{-1}\right) + \sum_{1\le j<k\le N} |x_j - x_k|^{-1}, \tag{1}$$

acting on antisymmetric $\Psi(x_1 \dots x_N) \in L^2(\mathbb{R}^{3N})$. The ground-state energy of an atom is then defined as

$$E(Z) = \min_{N\ge 1} E(N,Z), \tag{2}$$

and our problem is to compute $E(Z)$ asymptotically for large Z. Building on the previous work of Thomas, Fermi, Dirac and Scott (see the survey article of Lieb [L2]), Schwinger [S] proposed the refined formula

$$E(Z) \approx -c_0 Z^{7/3} + \frac{1}{8} Z^2 - c_1 Z^{5/3}, \tag{3}$$

for explicit positive constants c_0, c_1. After the early work of Lieb and Simon [LS] on molecules, Hughes and Siedentop-Weikard [H,S-W] gave a rigorous proof of the "Scott conjecture", namely

$$E(Z) = -c_0 Z^{7/3} + \frac{1}{8} Z^2 + O(Z^\gamma) \quad \text{with} \quad \gamma < 2. \tag{4}$$

Recently, Ivrii and Sigal [IS] proved the analogue of the Scott conjecture for molecules. Our main result, announced in [FS1], is as follows.

Theorem: *$E(Z) = -c_0 Z^{7/3} + \frac{1}{8} Z^2 - c_1 Z^{5/3} + O(Z^{5/3-\varepsilon_0})$ with $\varepsilon_0 = \frac{1}{2835}$.*

It would be interesting to prove an analogous result for molecules by combining our ideas with those of Ivrii and Sigal. We would also like to know more accurate asymptotic formulas for $E(Z)$, containing additional correction terms beyond $Z^{5/3}$. Prediction of chemical phenomena from first principles requires a knowledge of $E(Z)$ and its analogue for molecules far beyond our current understanding.

We sketch the physical reasoning that leads to Schwinger's formula (3), and then give the strategy of the proof of the Scott conjecture. Next we give a crude outline of the proof

[1] In the introduction, we neglect electron spin to simplify notation. When we prove our main results, we will take spin into account.

of our theorem. Then we explain further the subset of our proof which appears in this paper. Our introduction concludes with a conjecture on the next term in the asymptotics of $E(Z)$.

The starting point in discussing atoms is an elementary observation on free particles in a box. For N free particles in a box $Q \subset \mathbb{R}^3$, the minimum possible kinetic energy $KE(N,Q)$ is equal to the lowest eigenvalue of $-\Delta$ acting on antisymmetric $\Psi(x_1,\dots,x_N) \in L^2(Q^N)$ with appropriate boundary conditions. One computes $KE(N,Q)$ trivially, by separation of variables. For large N, the answer is

$$KE(N,Q) \approx c_{TF}\rho^{5/3}|Q| \tag{5}$$

where $\rho = N/|Q|$ is the density of particles in the box, and c_{TF} is a universal constant.

This suggests a way to approximate the energy $\langle H_{NZ}\Psi,\Psi\rangle$ of a wave function $\Psi(x_1\dots x_N)$ in terms of the electron density

$$\rho(x_1) = N \int\limits_{\mathbb{R}^{3(N-1)}} |\Psi(x_1,x_2,\dots,x_N)|^2 dx_2\dots dx_N. \tag{6}$$

In fact, we set

$$\varepsilon_{TF}(\rho) = c_{TF}\int\limits_{\mathbb{R}^3}\rho^{5/3}(x)dx - \int\limits_{\mathbb{R}^3}\frac{Z}{|x|}\rho(x)dx + \frac{1}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\rho(x)\rho(y)}{|x-y|}dxdy. \tag{7}$$

Here, the first term on the right is an approximation to the kinetic energy motivated by (5), and the remaining terms on the right are simply the classical electric potential energy for a charge density ρ and a nucleus of charge Z. Thomas and Fermi independently proposed that the ground-state energy $E(Z)$ is approximately equal to the minimum of $\varepsilon_{TF}(\rho)$ over all possible densities $\rho(x)$. Moreover, they proposed the minimizing density ρ_{TF} for (7) as an approximation to the electron density for an atom in its ground state. This is an immense simplification, since the original problem deals with $\Psi(x_1\dots x_N)$ for $N \gg 1$, while Thomas-Fermi theory deals merely with a function on $\mathbb{R}^3$. An elementary computation with the Euler-Lagrange equation for (7) leads to an ordinary differential equation for ρ_{TF}, which may therefore be understood in great detail. In particular, Thomas-Fermi theory predicts that

$$E(Z) \approx -c_0 Z^{7/3}, \tag{8}$$

which is correct as far as it goes, but much too crude.

A more refined prediction for $E(Z)$ comes from the *Hartree-Fock approximation.*[2] The idea is that since the electron density is approximately ρ_{TF}, each electron behaves as if it were moving in a potential

$$V_{TF}(x) = -\frac{Z}{|x|} + \int\limits_{\mathbb{R}^3}\frac{\rho_{TF}(y)dy}{|x-y|}. \tag{9}$$

[2]This is not exactly the same as the usual Hartree-Fock approximation.

Therefore it is reasonable to approximate the ground-state of the true Hamiltonian H_{NZ} by that of the much simpler Hamiltonian

$$H_{hf} = \sum_{k=1}^{N} (-\Delta_{x_k} + V_{TF}(x_k)), \text{ acting on antisymmetric } \Psi(x_1 \dots x_N). \tag{10}$$

Unlike the original Hamiltonian, (10) can be diagonalized using separation of variables, and the state of lowest energy can be written explicitly in terms of the eigenfunctions of $-\Delta + V_{TF}$. So again, the problem is reduced from $3N$ to 3 variables. In fact, suppose E_k are the (negative) eigenvalues of $-\Delta + V_{TF}$, and let $\varphi_k(x)$ be the corresponding (normalized) eigenfunctions. Then the ground-state wave function for (10), which we call Ψ_{hf}, is an antisymmetrized product of the φ_k. As an approximation to the ground-state energy of an atom, it is natural to use

$$E_{hf}(Z) = \langle H_{NZ}\Psi_{hf}, \Psi_{hf}\rangle . \tag{11}$$

Note that we use the exact Hamiltonian H_{NZ} in (11), even though Ψ_{hf} arose from the simplified Hamiltonian (10). Elementary computation gives the formula

(12)
$$\begin{aligned} E_{hf}(Z) = \operatorname{sneg}(-\Delta + V_{TF}) &- \frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)}{|x-y|} dxdy - \frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\mathcal{S}(x,y)|^2}{|x-y|} dxdy \\ &+ \frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} [\rho_{hf}(x) - \rho_{TF}(x)][\rho_{hf}(y) - \rho_{TF}(y)] \frac{dxdy}{|x-y|}, \end{aligned}$$

with

$$\operatorname{sneg}(-\Delta + V_{TF}) = \sum_k E_k, \tag{13}$$

$$\rho_{hf}(x) = \sum_k |\varphi_k(x)|^2, \tag{14}$$

$$\mathcal{S}(x,y) = \sum_k \varphi_k(x)\overline{\varphi_k(y)}. \tag{15}$$

To get more explicit information from (12), we approximate $\operatorname{sneg}(-\Delta + V_{TF})$, ρ_{hf} and $\mathcal{S}$. The *semiclassical approximations* for these quantities are as follows.

$$\operatorname{sneg}(-\Delta + V_{TF}) \approx -\frac{1}{15\pi^2} \int\limits_{\mathbb{R}^3} |V_{TF}(x)|^{5/2} dx, \tag{16}$$

$$\rho_{hf}(x) \approx \frac{1}{6\pi^2} |V_{TF}(x)|^{3/2}, \tag{17}$$

(18)
$$\frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} |\mathcal{S}(x,y)|^2 \frac{dxdy}{|x-y|} \approx c_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x) dx, \text{ for a universal constant } c_D.$$

We omit the motivation for (16), (17), (18) and content outselves with the remark that they are closely related to Weyl's theorem on eigenvalues of the Laplacian. Formula (18) and its application to atoms are due to Dirac.

Putting (16), (17), (18) into (12), we obtain the semiclassical approximation for $E_{hf}(Z)$. From the first two terms on the right in (12), we recover the Thomas-Fermi energy $-c_0 Z^{7/3}$. The third term on the right of (12) takes the form $-c_1' Z^{5/3}$ for a universal constant c_1'. The final term in (12) vanishes in the semiclassical approximation, by virtue of (9), (17) and the Euler-Lagrange equation for ρ_{TF}. Altogether, we have

$$E_{hf}(Z) \approx -c_0 Z^{7/3} - c_1' Z^{5/3}. \tag{19}$$

The last term in (19) is called the Dirac correction. Comparing (19) with the correct formula (3), we see that the Z^2-term is missing from (19), and the $Z^{5/3}$ coefficient is wrong. The trouble is that (16) is only a crude approximation.

A refined form of (16) was proposed by Scott (see [L2]) and Schwinger [S]. For potentials V with a Coulomb singularity $V(x) \approx -Z|x|^{-1}$ at the origin, their formula is

$$\operatorname{sneg}(-\Delta + V) \approx -\frac{1}{15\pi^2} \int\limits_{V<0} |V|^{5/2} + \frac{1}{8} Z^2 + \frac{1}{48\pi^2} \int\limits_{V<0} |V|^{1/2} \Delta V. \tag{20}$$

Scott guessed the Z^2-term by working out the elementary example

$$V(x) = E_0 - Z|x|^{-1}. \tag{21}$$

Schwinger deduced the last term in (20) from the form of the heat kernel for $e^{-t(-\Delta+V)}$, which in turn he guessed from the known case of the harmonic oscillator. Using (20), (17), (18) to approximate the right-hand side of (12), we obtain Schwinger's formula (3) for the ground-state energy. This concludes our discussion of heuristic methods.

Next we explain some ideas from the rigorous discussion of atoms. There are two main issues: justifying the approximations (16), (17), (18), (20) in the calculation of the Hartree-Fock energy; and comparing the Hartree-Fock energy $E_{hf}(Z)$ with the true ground-state energy $E(Z)$. The second issue is deeper, since it forces us to understand an interacting N-particle system. In this introduction, we concentrate on comparing $E_{hf}(Z)$ with $E(Z)$. Note that

$$E_{hf}(Z) = \langle H_{NZ} \Psi_{hf}, \Psi_{hf} \rangle \geq \inf_{N,\Psi} \langle H_{NZ} \Psi, \Psi \rangle = E(Z), \tag{22}$$

so the problem is to prove a lower bound for $E(Z)$.

The main tool used previously to prove lower bounds for $E(Z)$ is a pointwise inequality of Lieb [L1] for the Coulomb potential. With $V_{\text{Coulomb}}(x_1 \dots x_N) = -\sum_{k=1}^{N} Z|x_k|^{-1} + \sum_{1 \leq j < k \leq N} |x_j - x_k|^{-1}$, Lieb's inequality is

$$V_{\text{Coulomb}}(x_1 \dots x_N) \geq \sum_{k=1}^{N} W(x_k) - E_0, \tag{23}$$

with $W(x)$ close to $V_{TF}(x)$, and E_0 close to $\frac{1}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|}$. We explain how to use (23), and then explain how to prove it. Assuming (23), we see at once that

$$H_{NZ} = \sum_{k=1}^{N}(-\Delta_{x_k}) + V_{\text{Coulomb}} \geq \sum_{k=1}^{N}(-\Delta_{x_k} + W(x_k)) - E_0,$$

and the right hand side may be diagonalized by separation of variables. Hence,

$$E(Z) \geq \text{sneg}(-\Delta + W) - E_0. \tag{24}$$

We expect the right-hand side of (24) to approximate

$$\text{sneg}(-\Delta + V_{TF}) - \frac{1}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)}{|x-y|}dxdy.$$

Comparing this expression with (12), and recalling the semiclassical approximations (17) and (18), we guess that the right-hand side of (24) is $E_{hf}(Z) + O(Z^{5/3})$. So if we can compute the right-hand sides of (12) and (24), then (22) and (24) will give rigorous upper and lower bounds for $E(Z)$, which we expect to differ by $O(Z^{5/3})$. This reduces the computation of $E(Z)$ from $3N$ dimensions to 3, provided we are willing to tolerate errors $O(Z^{5/3})$. The solution of the Scott conjecture is based on (23).

To prove Lieb's inequality (23), we can start with the elementary identity

$$|x - x'|^{-1} = \frac{1}{\pi}\iint\limits_{\substack{y\in\mathbb{R}^3\\ R>0}} \chi_{x,x'\in B(y,R)}\frac{dydR}{R^5} \quad \text{for} \quad x, x' \in \mathbb{R}^3. \tag{25}$$

Except for the value of the constant $\frac{1}{\pi}$, identity (25) is forced by the fact that both sides transform in the same way under translations, rotations and dilations. Summing (25) over all pairs of particles $x = x_j$, $x' = x_k$, we get

$$\sum_{j<k}|x_j - x_k|^{-1} = \frac{1}{\pi}\iint\limits_{\substack{y\in\mathbb{R}^3\\ R>0}} \frac{N_{yR}(N_{yR}-1)}{2}\frac{dydR}{R^5}, \tag{26}$$

with $N_{yR} = [\text{number of } x_j \in B(y,R)] = \sum_{j=1}^{N}\chi_{B(y,R)}(x_j)$. In general, a potential

$$V(x_1 \dots x_N) = \iint\limits_{\substack{y\in\mathbb{R}^3\\ R>0}} F(N_{yR}, y, R)dydR \tag{27}$$

has the form $\sum_{k=1}^{N} W(x_k)$ if $F = f(y,R) \cdot N_{yR}$. If instead $F = f(y,R) \cdot \frac{N_{yR}(N_{yR}-1)}{2}$ with $f \geq 0$, then (27) has the form $V = \sum_{j<k} K(x_j, x_k)$ for a non-negative symmetric two-body interaction $K(x,y)$. Finally, if F depends only on y and R in (27), then the potential $V(x_1 \ldots x_N)$ is merely a constant.

For an atom in its ground state, we guess that the number N_{yR} of electrons in $B(y,R)$ is approximately $\bar{N}_{yR} \equiv \int_{B(y,R)} \rho_{TF}$. So in (26) it is natural to complete the square and write

$$\frac{1}{2}N_{yR}(N_{yR}-1) = \frac{1}{2}(N_{yR} - \bar{N}_{yR})^2 + f(y,R)N_{yR} + g(y,R). \tag{28}$$

When we put (28) into (26), the term $f(y,R)N_{yR}$ will contribute $\sum_k W(x_k)$, and the term $g(y,R)$ will contribute a constant. The term $\frac{1}{2}(N_{yR} - \bar{N}_{yR})^2$ is hard to understand, but its contribution is non-negative. If $\bar{N}_{yR} \gg 1$, then we hope $(N_{yR} - \bar{N}_{yR})^2$ will be negligibly small compared to the other terms in (28), because $N_{yR} \approx \bar{N}_{yR}$ for statistical reasons. Hence we get a rigorous lower bound

$$\frac{1}{2}N_{yR}(N_{yR}-1) \geq f(y,R)N_{yR} + g(y,R), \tag{28a}$$

which is useful when $\bar{N}_{yR} > 1$ (say). When $\bar{N}_{yR} \leq 1$, we use instead the trivial lower bound $\frac{1}{2}N_{yR}(N_{yR}-1) \geq 0$. Therefore, (26) implies that

$$\sum_{j<k} |x_j - x_k|^{-1} \geq \iint_{\{\bar{N}_{yR}>1\}} f(y,R)N_{yR}\frac{dydR}{R^5} + \iint_{\{\bar{N}_{yR}>1\}} g(y,R)\frac{dydR}{R^5},$$

which has the form

$$\sum_{j<k} |x_j - x_k|^{-1} \geq \sum_k W(x_k) - E_0. \tag{29}$$

Adding $-\sum_k \frac{Z}{|x_k|}$ to both sides of (29), we obtain Lieb's inequality (23). This proof is different from that of [L1], but is closely related to it.

The above proof shows clearly that inequality (23) inevitably sacrifices an error $O(Z^{5/3})$ in estimating the ground-state energy. In fact, we discarded the term

$$\frac{1}{2\pi} \iint_{\{\bar{N}_{yR}>1\}} (N_{yR} - \bar{N}_{yR})^2 \frac{dydR}{R^5} \tag{30}$$

in the potential energy.

To keep (30) as small as possible, we tried to pick $\bar{N}_{yR}$ close to the expected number of electrons in $B(y,R)$ for an atom in its ground state. Nevertheless, the expected value of $(N_{yR} - \bar{N}_{yR})^2$ will be at least as large as the variance of the random variable N_{yR}. Hence by applying (23), we discard an expected potential energy at least as large as

$$\frac{1}{2\pi} \iint_{\{\bar{N}_{yR}>1\}} \text{Variance } (N_{yR}) \frac{dydR}{R^5}. \tag{31}$$

For a Hartree-Fock atom, a plausible semiclassical approximation to (31) has the order of magnitude $Z^{5/3}$. The main contribution to (31) comes from (y,R) with $|y| \sim Z^{-1/3}$, $R \sim Z^{-2/3}$, $\bar{N}_{yR} \sim 1$.

This shows that the use of (23) leads to an error $\sim Z^{5/3}$ in $E(Z)$. It shows also that computing $E(Z)$ modulo $o(Z^{5/3})$ is closely related to finding the variance of N_{yR} for an atom in its ground state, with $|y| \sim Z^{-1/3}$ and $R \sim Z^{-2/3}$.

Next we give a crude outline of our proof of our main theorem on the ground-state energy. There are four main steps:

(A) (Lower bound)

$$E(Z) \geq \text{sneg}(-\Delta + V_{TF}) - \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)}{|x-y|} dxdy - c_D \int_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx - CZ^{5/3-\varepsilon_0}$$

(B) (Density)

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} [\rho_{hf}(x) - \rho_{TF}(x)][\rho_{hf}(y) - \rho_{TF}(y)] \frac{dxdy}{|x-y|} < CZ^{5/3-\varepsilon_0}$$

(C) (Correlation Function)

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} |\mathbb{S}(x,y)|^2 \frac{dxdy}{|x-y|} > c_D \int_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx - CZ^{5/3-\varepsilon_0}$$

(D) (Eigenvalue Sum)

$$\text{sneg}(-\Delta+V_{TF}) = -\frac{1}{15\pi^2} \int_{\mathbb{R}^3} |V_{TF}(x)|^{5/2} dx + \frac{1}{8} Z^2 + \frac{1}{48\pi^2} \int_{\mathbb{R}^3} |V_{TF}(x)|^{1/2} \Delta V_{TF}(x) dx + O(Z^{5/3-\varepsilon_0}).$$

Here, (A) is our substitute for Lieb's pointwise inequality (23), while (B), (C) and (D) justify the semiclassical approximations as corrected by Scott and Schwinger.

From (A)$\cdots$(D) we can easily read off our main theorem on $E(Z)$. In fact, (12), (22) and (A) provide upper and lower bounds for $E(Z)$ that differ by

$$\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}[\rho_{hf}(x)-\rho_{TF}(x)][\rho_{hf}(y)-\rho_{TF}(y)]\frac{dxdy}{|x-y|}+$$

$$\left\{c_D\int_{\mathbb{R}^3}\rho_{TF}^{4/3}(x)dx-\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}|\mathcal{S}(x,y)|^2\frac{dxdy}{|x-y|}\right\}+CZ^{5/3-\varepsilon_0}.$$

This expression is less than $C'Z^{5/3-\varepsilon_0}$, by (B) and (C). Therefore,

$$E(Z)=$$

$$=\operatorname{sneg}(-\Delta+V_{TF})-\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\rho_{TF}(x)\rho_{TF}(y)\frac{dxdy}{|x-y|}-c_D\int_{\mathbb{R}^3}\rho_{TF}^{4/3}(x)dx+O(Z^{5/3-\varepsilon_0}),$$

so that (D) yields Schwinger's formula for $E(Z)$ with an error $O(Z^{5/3-\varepsilon_0})$. Thus, our main theorem is reduced to (A)$\cdots$(D).

We indicate some of the ideas in the proof of the lower bound (A). The first step is to prove a pointwise lower bound

$$V_{\text{Coulomb}}(x_1\ldots x_N)\geq\sum_{k=1}^{N}W(x_k)-E_0+\sum_{j<k}K(x_j,x_k),\tag{32}$$

with $K(x,x')$ a short-range non-negative two-body interaction. This follows by changing slightly the proof of (23). In fact, using (26), we can break up the Coulomb interaction as

$$V_{\text{Coulomb}}=V_{\text{Long-range}}+V_{\text{Short-range}},\ \text{with}\tag{33}$$

$$V_{\text{Long-range}}=\frac{1}{\pi}\iint_{\bar{N}_{yR}\geq Z^{\varepsilon_0}}\frac{N_{yR}(N_{yr}-1)}{2}\frac{dydR}{R^5}\ \text{and}\tag{34}$$

$$V_{\text{Short-range}}=\frac{1}{\pi}\iint_{\bar{N}_{yR}<Z^{\varepsilon_0}}\frac{N_{yR}(N_{yR}-1)}{2}\frac{dydR}{R^5}.\tag{35}$$

Applying (28a) to the integrand in (34), we get

$$V_{\text{Long-range}}\geq\sum_{k=1}^{N}W(x_k)-E_0.\tag{36}$$

On the other hand,

$$V_{\text{Short-range}} = \sum_{j<k} K(x_j, x_k), \text{ with} \tag{37}$$

$$K(x,x') = \frac{1}{\pi} \iint\limits_{\bar{N}_{yR} < Z^{\varepsilon_0}} \chi_{x,x' \in B(y,R)} \frac{dydR}{R^5}. \tag{38}$$

Moreover, (38) shows that $K(x,x')$ is short-range in the following sense. If the particles $x_1 \dots x_N$ are independent and distributed according to ρ_{TF}, then each x_j will interact with only $O(Z^{\varepsilon_0})$ of the x_k. Thus we have easily carried out the first step in the proof of (A). Later, we will give another proof of (32), closer in spirit to Lieb [L1].

The point of (32) is to bound H_{NZ} from below by a Hamiltonian $H_{\text{lower bound}}$ in which the interaction between particles may be treated as a small perturbation. In fact, (32) yields at once

$$H_{NZ} \geq \sum_{k=1}^{N} (-\Delta_{x_k} + W(x_k)) - E_0 + \sum_{j<k} K(x_j, x_k) \equiv H_{\text{lower bound}}. \tag{39}$$

Regarding the term $\sum\limits_{j<k} K(x_j, x_k)$ as a small perturbation in (39), we get the approximate formula

$$\text{sneg}(-\Delta + W) - E_0 + \left\langle \sum_{j<k} K(x_j, x_k) \Psi_0, \Psi_0 \right\rangle \tag{40}$$

for the lowest eigenvalue of $H_{\text{lower bound}}$, where Ψ_0 is the ground-state eigenfunction for $\sum\limits_k (-\Delta_{x_k} + W(x_k))$. Using a semiclassical approximation for the last term in (40), we obtain the heuristic formula

$$\begin{aligned}&(\text{lowest eigenvalue of } H_{\text{lower bound}}) \approx \\ &\qquad \text{sneg}(-\Delta + W) - E_0 + \frac{1}{2} \iint\limits_{\mathbb{R}^3 \times \mathbb{R}^3} K(x,y) \{\rho_{TF}(x) \rho_{TF}(y) - |\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\} dxdy,\end{aligned}$$

where $\mathcal{S}_\rho(y)$ is an elementary function (the correlation for an ideal gas).

We will prove the rigorous inequality

$$\begin{aligned}\langle H_{\text{lower bound}} \Psi, \Psi \rangle \geq{}& \text{sneg}(-\Delta + W) - E_0 + \\ & \frac{1}{2} \iint\limits_{\mathbb{R}^3 \times \mathbb{R}^3} K(x,y) \{\rho_{TF}(x) \rho_{TF}(y) - |\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\} dxdy - CZ^{5/3-\varepsilon_0}\end{aligned} \tag{41}$$

for antisymmetric $\Psi(x_1 \dots x_N)$ of norm 1.

From (39) and (41) follows immediately

$$E(Z) \geq \operatorname{sneg}(-\Delta + W) - E_0 + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} K(x,y)\{\rho_{TF}(x)\rho_{TF}(y) - |\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\} dxdy - CZ^{5/3-\varepsilon_0}$$

which is equivalent to (A). Thus, (A) is reduced to (41).

The idea in proving (41) is to study wave functions Ψ for which $\langle \sum_k (-\Delta_{x_k} + W(x_k))\Psi, \Psi \rangle$ is nearly as low as possible. Our results show that

$$\left\langle \sum_{k=1}^{N} (-\Delta_{x_k} + W(x_k))\Psi, \Psi \right\rangle \leq \operatorname{sneg}(-\Delta + W) + Z^{7/3-\varepsilon_1} \tag{42}$$

implies

$$\left\langle \sum_{j<k} K(x_j, x_k)\Psi, \Psi \right\rangle \geq \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} K(x,y)\{\rho_{TF}(x)\rho_{TF}(y) - |\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\} dxdy - CZ^{5/3-\varepsilon_0}. \tag{43}$$

To deduce (41), we first suppose that (42) holds. In that case,

$$\begin{aligned}\left\langle H_{\text{lower bound}}\Psi, \Psi \right\rangle &\geq \operatorname{sneg}(-\Delta + W) - E_0 + \left\langle \sum_{j<k} K(x_j, x_k)\Psi, \Psi \right\rangle \\ &\geq \operatorname{sneg}(-\Delta + W) - E_0 + \\ &+ \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} K(x,y)\{\rho_{TF}(x)\rho_{TF}(y) - |\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\} dxdy \\ &\qquad - CZ^{5/3-\varepsilon_0},\end{aligned}$$

by (43) and the definition of $H_{\text{lower bound}}$. So (41) holds whenever Ψ satisfies (42). On the other hand, if (42) fails, then trivially

$$\begin{aligned}\left\langle H_{\text{lower bound}}\Psi, \Psi \right\rangle &\geq \left\langle \sum_{k=1}^{N} (-\Delta_{x_k} + W(x_k))\Psi, \Psi \right\rangle - E_0 \\ &\geq \operatorname{sneg}(-\Delta + W) + Z^{7/3-\varepsilon_1} - E_0.\end{aligned}$$

This implies (41), since the integral in (41) has order of magnitude $Z^{\frac{5}{3}+\frac{2}{3}\varepsilon_0} \ll Z^{\frac{7}{3}-\varepsilon_1}$. Hence (41) holds in either case. So the main point in the proof of (A) is that (42) implies (43). Our discussion of (A) concludes with some explanation of this implication.

Any wave function Ψ that satisfies (42) ought to behave much like Ψ_0, the ground state of $\sum_{k=1}^{N}(-\Delta_{x_k}+W(x_k))$. Hence it is plausible that

$$\left\langle \sum_{j<k} K(x_j,x_k)\Psi,\Psi \right\rangle \approx \left\langle \sum_{j<k} K(x_j,x_k)\Psi_0,\Psi_0 \right\rangle,$$

which is close to (43). However, one has to be careful. It is quite simple to produce Ψ satisfying (42), for which $\langle \sum_{j<k} K(x_j,x_k)\Psi,\Psi\rangle$ is much larger than $\langle \sum_{j<k} K(x_j,x_k)\Psi_0,\Psi_0\rangle$. (We just modify Ψ_0 by adding many particles in a small ball.) So the sign of the inequality is essential in (43).

We prove that (42) implies (43) by first establishing an analogous result in which $-\Delta+W$ is replaced by $-\Delta$. Thus, the heart of the matter is a theorem on N free particles in a box, which we now state. Let $T=\mathbb{R}^3/L\mathbb{Z}^3$ be a flat torus, and let $\Psi(x_1\dots x_N)\in L^2(T^N)$ be antisymmetric with norm 1. Let $K(x,y)$ be a short-range Coulomb interaction on $T\times T$. That is, we suppose $0\le K(x,y)=K(y,x)\le |x-y|^{-1}\chi_{|x-y|<r_{\max}}$.

Assuming that Ψ has kinetic energy near the minimum possible, we will control $\langle \sum_{j<k} K(x_j,x_k)\Psi,\Psi\rangle$. Recall that the ground state Ψ_0 for the kinetic energy has

$$\|\nabla\Psi_0\|^2 \approx c_{TF}\rho^{5/3}L^3 \quad \text{with} \quad \rho=NL^{-3}= \text{ density, and}$$

$$\left\langle \sum_{j<k} K(x_j,x_k)\Psi_0,\Psi_0 \right\rangle \approx \frac{1}{2}\iint_{T\times T} K(x,y)\{\rho^2-|\mathcal{S}_\rho(x-y)|^2\}dxdy.$$

Theorem on free particles: *Let T, K, Ψ be as above. Assume that $\|\nabla\Psi\|^2\le(1+\delta)c_{TF}\rho^{5/3}L^3$, and that*

$$\delta<c_0(\rho r_{\max}^3+1)^{-m_0},\ N>C_0(\rho r_{\max}^3+1)^{m_0}$$

for positive universal constants c_0, C_0, m_0. Then

$$\left\langle \sum_{j<k} K(x_j,x_k)\Psi,\Psi \right\rangle \ge \frac{1}{2}\iint_{T\times T} K(x,y)\{\rho^2-|\mathcal{S}_\rho(x-y)|^2\}dxdy-(\delta+N^{-1})^{\varepsilon_0}\rho^{4/3}L^3$$

for a universal constant $\varepsilon_0>0$.

Our full result on free particles is slightly stronger than the above, but more complicated to state.

Let us summarize our discussion of (A). The standard idea for proving lower bounds for $E(Z)$ is to compare the actual Hamiltonian with a non-interacting one. Our idea is to compare the actual Hamiltonian with a weakly interacting one, and then control the weakly interacting Hamiltonian by using our theorem on free particles.

We illustrate what we know about weakly interacting systems by a simple example. Let $T = \mathbb{R}^3/L\mathbb{Z}^3$ as before, and define a Hamiltonian

$$H^{\tau NL} = \sum_{k=1}^{N}(-\Delta_{x_k}) + \tau \sum_{1\le j<k\le N} \chi_{|x_j - x_k|<1},$$

acting on antisymmetric $\Psi(x_1 \dots x_N) \in L^2(T^N)$. Here, τ is a real parameter. For τ real and $\rho > 0$, we pass to the thermodynamic limit by defining

$$E(\tau,\rho) = \lim_{\substack{N,L\to\infty \\ \frac{N}{L^3}\to\rho}} \left\{ \frac{\text{lowest eigenvalue of } H^{\tau NL}}{N} \right\}. \tag{44}$$

Thus, $E(\tau,\rho)$ is the energy per particle for a zero-temperature gas of interacting Fermions, and τ controls the strength of the interaction. It is easy to see that the limit (44) exists when $\tau \ge 0$, but not when $\tau < 0$. Our results show that $\frac{\partial}{\partial\tau}E(\tau,\rho)$ exists at $\tau = 0$, and is given by an obvious perturbation-theoretic formula. We would like to understand more fully how $E(\tau,\rho)$ behaves as $\tau \to 0$. This is probably closely related to atoms.

In our proof of (A), we used a very weak assumption (42). Simpler proofs and sharper theorems might follow if we knew how to exploit a stronger hypothesis.

Our introduction is nearly complete. In this paper we will prove (A) and (C), leaving (B) and (D) to be established in [FS2,...,7]. Our exposition includes many details, to lighten the task of checking the correctness of our results. Curiously, (C) follows as a consequence of our proof of (A). The proofs of (A) and (C) go over easily for molecules, while our discussion of (B) and (D) applies only to atoms, since it is based on ordinary differential equations. From [FS7] it is natural to conjecture a sharp formula for $\text{sneg}(-\Delta + V_{TF})$, which refines (D). The formula is as follows.

For $\ell \ge 0$ and $r \in (0,\infty)$, define $V_\ell(r) = \frac{\ell(\ell+1)}{r^2} + V_{TF}(r)$, and let $\ell_{\max}$ be the largest integer for which $V_\ell(r)$ is negative for some r. Define

$$n_\ell = \int_{\{V_\ell<0\}} |V_\ell(r)|^{-1/2} dr \quad \text{and} \quad \psi_\ell = \frac{1}{\pi}\int_{\{V_\ell<0\}} |V_\ell(r)|^{1/2} dr$$

for $1 \le \ell \le \ell_{\max}$. Finally, set $\beta(t) = -\frac{1}{12} + \min_{k\in\mathbb{Z}} |t-k|^2$. Then we conjecture that

(45)

$$\text{sneg}(-\Delta + V_{TF}) \approx -\frac{1}{15\pi^2}\int_{\mathbb{R}^3} |V_{TF}(x)|^{5/2}dx + \frac{Z^2}{8} + \frac{1}{48\pi^2}\int_{\mathbb{R}^3} |V_{TF}(x)|^{1/2}\Delta V_{TF}(x)dx$$
$$+ (\text{const}) \sum_{1\le\ell\le\ell_{\max}} \frac{(2\ell+1)}{n_\ell}\beta(\psi_\ell).$$

As explained in [F], the last term in (45) is related to classical theorems of analytic number theory.

From (45) we expect that

$$E(Z) \approx -c_0 Z^{7/3} + \frac{1}{8} Z^2 - c_1 Z^{5/3} + (\text{const}) \sum_{1 \leq \ell \leq \ell_{\max}} \frac{(2\ell+1)}{n_\ell} \beta(\psi_\ell).$$

Finally, we refer the reader to the last section of this paper for additional results on quantum states for an atom having nearly the lowest possible energy.

Free Particles in a Box

In this section, we study N-particle wave functions Ψ on a box in $\mathbb{R}^3$, with periodic boundary conditions. We shall compare Ψ with the state Ψ_0 of lowest possible kinetic energy. Our goal is to prove that if Ψ has kinetic energy near enough to the minimum, then Ψ behaves much like Ψ_0.

The precise setup is as follows. We fix $L > 0$ and define the flat torus $T = \mathbb{R}^3/L\mathbb{Z}^3$. Suppose we are given a function spin: $\{1 \dots N\} \to \{1 \dots q\}$ and a complex-valued function $\Psi(x_1 \dots x_N)$ on T^N, with L^2 norm 1. We assume that the wave function satisfies

(1) $$\Psi(x_{\sigma_1} \dots x_{\sigma_N}) = (\operatorname{sgn}\sigma)\Psi(x_1 \dots x_N) \text{ for permutations } \sigma \text{ that preserve spin.}$$

The kinetic energy of Ψ is defined as $\|\nabla\Psi\|^2_{L^2(T^N)}$. Given the map spin: $\{1 \dots N\} \to \{1 \dots q\}$, let Ψ_0 be a wave function of norm 1 and satisfying (1), with lowest possible kinetic energy. The properties of Ψ_0 are elementary and well-known. In particular, for N large, the minimum kinetic energy is asymptotic to

$$\|\nabla\Psi_0\|^2 \sim c_{TF} \sum_{1 \le s \le q} N_s^{5/3} L^{-2}, \quad \text{with}$$

(2) $$c_{TF} = \frac{(6\pi^2)^{5/3}}{10\pi^2}, \quad \text{and}$$

(3) $$N_s = \text{Number of } j \in \{1 \dots N\} \text{ with spin } s.$$

We assume that Ψ has low kinetic energy in the sense that

(4) $$\|\nabla\Psi\|^2 \le (1+\delta) c_{TF} \sum_{1 \le s \le q} N_s^{5/3} L^{-2}, \quad 0 < \delta < 1$$

If δ is small, then we shall prove that Ψ behaves much like Ψ_0. Specifically, we shall study the correlation functions

(5) $$\mathcal{S}_s(x_1, x_2, \Psi) = \sum_{\text{spin}(j)=s} \int_{T^{N-1}} \Psi(y_1 \dots y_{j-1} x_1 y_{j+1} \dots y_N) \bar{\Psi}(y_1 \dots y_{j-1} x_2 y_{j+1} \dots y_N) dy_1 \dots dy_{j-1} dy_{j+1} \dots dy_N$$

and the potential energy $\langle V\Psi, \Psi\rangle$ for potentials $V(x_1 \dots x_N) = \sum_{1 \le j < k \le N} K(x_j, x_k)$ defined in terms of suitable 2-body interactions $K(x, y) \ge 0$.

Our goal is to show that if N is large and (4) holds with small δ, then $\mathcal{S}_s(x_1, x_2, \Psi)$ is close to $\mathcal{S}_s(x_1, x_2, \Psi_0)$ and $\langle V\Psi, \Psi\rangle \ge \langle V\Psi_0, \Psi_0\rangle$ modulo a small error. We noted before that $\langle V\Psi, \Psi\rangle$ need not be close to $\langle V\Psi_0, \Psi_0\rangle$.

In this section c, C, C' etc. denote constants that depend only on q. Similarly, c_ε, C_ε, C'_ε etc. denote constants depending only on ε, q.

We assume that all N_s in (3) exceed a large universal constant, and that the ratios $N_s/N_{s'}$ are bounded above and below by universal constants.

Naturally, we shall be expanding in Fourier series on the flat torus T. Hence, we introduce the lattice $\Lambda = \frac{2\pi}{L}\mathbb{Z}^3 \subset \mathbb{R}^3$. We begin with a few preliminary lemmas on lattice points.

Lemma 1: *For $RL > C$, the number of points in $\Lambda \cap \overline{B(0,R)}$ is equal to $\frac{1}{6\pi^2}R^3L^3 \cdot (1 + \mathit{Error})$, with $|\mathit{Error}| \le CR^{-1}L^{-1}$.*

Proof: Associate to each $\xi \in \Lambda$ a cube of side $\frac{2\pi}{L}$ centered at ξ. Call this cube Q_ξ. The number of ξ with $Q_\xi \subset \overline{B(0,R)}$ is equal to $\mathrm{vol}\left(\bigcup_{Q_\xi \subset \overline{B(0,R)}} Q_\xi\right) \Big/ \left(\frac{2\pi}{L}\right)^3$ since the Q_ξ are pairwise disjoint.

Since $\bigcup_{Q_\xi \subset \overline{B(0,R)}} Q_\xi$ contains $B\left(0, R - \frac{100}{L}\right)$, it follows that

$$[\text{Number of } \xi \in \Lambda \cap \overline{B(0,R)}] \ge \mathrm{vol}\left(\bigcup_{Q_\xi \subset \overline{B(0,R)}} Q_\xi\right) \Big/ \left(\frac{2\pi}{L}\right)^3$$

$$\ge \frac{4\pi}{3}(R - 100L^{-1})^3 \Big/ \left(\frac{2\pi}{L}\right)^3 \ge \left(\frac{4\pi}{3}\right)(2\pi)^{-3}R^3L^3 \cdot (1 - CR^{-1}L^{-1})$$

$$= \frac{1}{6\pi^2}R^3L^3 \cdot (1 - CR^{-1}L^{-1}).$$

Similarly, the number of ξ with $Q_\xi \cap \overline{B(0,R)} \ne 0$ is less than or equal to $\frac{4\pi}{3}(R+100L^{-1})^3/\left(\frac{2\pi}{L}\right)^3$, so

$$[\text{Number of } \xi \in \Lambda \cap \overline{B(0,R)}] \le \frac{1}{6\pi^2}R^3L^3 \cdot (1 + CR^{-1}L^{-1}).$$

□

Lemma 2: *For $RL \ge C$ and $\rho_0 = \frac{1}{6\pi^2}R^3$, we have*

$$\sum_{\xi \in \Lambda \cap \overline{B(0,R)}} |\xi|^2 = c_{TF}\rho_0^{5/3}L^3 \cdot (1 + \mathit{Error}),$$

with $|\mathit{Error}| \le CR^{-1}L^{-1}$.

Proof: We use the cubes Q_ξ from the proof of Lemma 1. Let S denote the set of $\xi \in \Lambda$ for which $Q_\xi \subset B(0,R)$. If $\xi \in S$, then the function $\eta \mapsto |\eta|^2$ has gradient at most $2R$ on

Q_ξ, so

$$\left| |\xi|^2 - \frac{1}{|Q_\xi|} \int_{\eta \in Q_\xi} |\eta|^2 d\eta \right| \leq 2R(\operatorname{diam} Q_\xi) \leq CRL^{-1}.$$

Summing over $\xi \in S$, we obtain

$$\text{(6)} \qquad \left| \sum_{\xi \in S} |\xi|^2 - \frac{L^3}{(2\pi)^3} \int_{\eta \in \bigcup_S Q_\xi} |\eta|^2 \right| \leq CRL^{-1} \cdot (\text{Number of } \xi \in S)$$
$$\leq CRL^{-1} \cdot R^3 L^3$$
$$= CR^4 L^2, \text{ by Lemma 1.}$$

Now $\bigcup_S Q_\xi \subset B(0,R)$, and $B(0,R) \setminus \bigcup_S Q_\xi \subset B(0,R) \setminus B(0, R - 100L^{-1})$. Therefore,

$$\text{(7)} \qquad \frac{L^3}{(2\pi)^3} \int_{\eta \in B(0,R) \setminus \bigcup_S Q_\xi} |\eta|^2 d\eta \leq \frac{L^3}{(2\pi)^3} \int_{\eta \in B(0,R) \setminus B(0,R-100L^{-1})} |\eta|^2 d\eta$$
$$\leq CL^3 \cdot R^2 \mathrm{vol}(B(0,R) \setminus B(0, R-100L^{-1})) \leq C' L^3 R^2 \cdot R^2 L^{-1}$$
$$= C' R^4 L^2.$$

Similarly, $\xi \in \Lambda \cap \overline{B(0,R)} \setminus S$ implies that $Q_\xi \subset B\left(0, R + \frac{100}{L}\right) \setminus B\left(0, R - \frac{100}{L}\right)$. Hence,

$$\left(\frac{2\pi}{L}\right)^3 \cdot [\text{Number of } \xi \in \Lambda \cap \overline{B(0,R)} \setminus S] \leq \mathrm{vol}\left(B\left(0, R + \frac{100}{L}\right) \setminus B\left(0, R - \frac{100}{L}\right)\right)$$
$$\leq CR^2 L^{-1}, \text{ i.e. } [\text{Number of } \xi \in \Lambda \cap \overline{B(0,R)} \setminus S]$$
$$\leq CR^2 L^2.$$

Therefore,

$$\text{(8)} \qquad \sum_{\xi \in \Lambda \cap \overline{B(0,R)} \setminus S} |\xi|^2 \leq R^2 \cdot [\text{Number of } \xi \in \Lambda \cap \overline{B(0,R)} \setminus S]$$
$$\leq CR^4 L^2.$$

Combining (6), (7), (8) and noting that $S \subset \Lambda \cap \overline{B(0,R)}$, we obtain

$$\text{(9)} \qquad \left| \sum_{\xi \in \Lambda \cap \overline{B(0,R)}} |\xi|^2 - \frac{L^3}{(2\pi)^3} \int_{B(0,R)} |\eta|^2 d\eta \right| \leq CR^4 L^2$$

The integral in (9) is equal to $\int_0^R r^2 \cdot 4\pi r^2 dr = \frac{4\pi}{5} R^5$, so that

$$(10) \qquad \left| \sum_{\xi \in \Lambda \cap \overline{B(0,R)}} |\xi|^2 - \left(\frac{4\pi}{5}\right)(2\pi)^{-3} R^5 L^3 \right| \leq C R^4 L^2.$$

Since

$$\begin{aligned} c_{TF} \rho_0^{5/3} &= \frac{(6\pi^2)}{10\pi^2}^{5/3} \cdot \left(\frac{1}{6\pi^2} R^3\right)^{5/3} = \frac{1}{10\pi^2} R^5 \\ &= \left(\frac{4\pi}{5}\right)(2\pi)^{-3} R^5 \text{ by (2) and the definition of } \rho_0, \end{aligned}$$

equation (10) is equivalent to the conclusion of Lemma 2. □

Lemma 3: *For $RL > C_1^2$ and $\rho_0 = \frac{1}{6\pi^2} R^3$, let $A \subset \Lambda$ be a set of lattice points containing at least $\rho_0 L^3 \cdot (1 - C_1 R^{-1} L^{-1})$ points. Define $H(A)$ to be the number of points of $\Lambda \cap \overline{B(0,R)}$ that do not belong to A. Then*

$$\sum_{\xi \in A} |\xi|^2 \geq c_{TF} \rho_0^{5/3} L^3 \cdot \left(1 - \frac{C'}{RL}\right) + \frac{c(H(A))^2}{RL^3}.$$

Proof: First we establish the weaker inequality

$$(11) \qquad \sum_{\xi \in A} |\xi|^2 \geq c_{TF} \rho_0^{5/3} L^3 \cdot \left(1 - \frac{C'}{RL}\right).$$

Suppose A contains N points, $N \geq \rho_0 L^3 \cdot (1 - C_1 R^{-1} L^{-1})$. It is possible to pick A to minimize $\sum_{\xi \in A} |\xi|^2$ among all N-element subsets of Λ. In fact, pick any $A_0 \subset \Lambda$ with N elements. If $A \subset \Lambda$ contains an element $\tilde{\xi}$ with $|\tilde{\xi}|^2 \geq 2 \sum_{\xi \in A_0} |\xi|^2$, then $\sum_{\xi \in A} |\xi|^2 > \sum_{\xi \in A_0} |\xi|^2$. Hence it is enough to minimize $\sum_{\xi \in A} |\xi|^2$ among N-element subsets of $B\left(0, 2\left[\sum_{\xi \in A_0} |\xi|^2\right]^{1/2}\right) \cap \Lambda$. There are only finitely many such subsets, so the minimum is attained.

Thus, suppose $A \subset \Lambda$, with A containing N points and $\sum_{\xi \in A} |\xi|^2$ as small as possible. If $\xi_1 \in A$ and $\xi_2 \in \Lambda \setminus A$, then $|\xi_1| \leq |\xi_2|$, for otherwise we would have

$$\sum_{\xi \in A'} |\xi|^2 < \sum_{\xi \in A} |\xi|^2 \quad \text{with} \quad A' = (A \cup \{\xi_2\}) \setminus \{\xi_1\}.$$

With $R_1 = \max\{|\xi| : \xi \in A\}$ and $R_2 = \min\{|\xi| : \xi \in \Lambda \setminus A\}$, we have therefore $R_1 \le R_2$. Hence, $\Lambda \cap B(0,R_1) \subset A \subset \Lambda \cap \overline{B(0,R_1)}$, where $B(0,R_1)$ denotes an open ball. So

$$\sum_{\xi \in \Lambda \cap \overline{B(0,R_1)}} |\xi|^2 \ge \sum_{\xi \in A} |\xi|^2 \ge \sum_{\xi \in \Lambda \cap B(0,R_1)} |\xi|^2, \tag{12}$$

and

$$[\text{Number of points in } \Lambda \cap \overline{B(0,R_1)}] \ge N \ge [\text{Number of points in } \Lambda \cap B(0,R_1)] \tag{13}$$

Since $N \ge \rho_0 L^3 \cdot (1 - C_1 R^{-1} L^{-1}) \ge \frac{1}{2}\rho_0 L^3 (\text{because } RL > C_1^2) = \frac{1}{12\pi^2} R^3 L^3 \ge \frac{C_1^6}{12\pi^2}$, we must have $R_1 L >$ (Large Constant), otherwise the upper bound for N in (13) would be false. Therefore, (13) and Lemma 1 yield

$$\left| N - \frac{1}{6\pi^2} R_1^3 L^3 \right| \le C R_1^2 L^2.$$

Combining this with $N \ge \rho_0 L^3 \cdot (1 - C_1 R^{-1} L^{-1})$, we see that

$$\frac{1}{6\pi^2} R_1^3 L^3 (1 + C R_1^{-1} L^{-1}) \ge N \ge \frac{1}{6\pi^2} R^3 L^3 (1 - C R^{-1} L^{-1})$$

by definition of ρ_0. This implies $R_1 \ge R \cdot (1 - C' R^{-1} L^{-1})$. Therefore, (12) and lemma 2 yield

$$\sum_{\xi \in A} |\xi|^2 \ge c_{TF} \rho_0^{5/3} L^3 \cdot (1 - C'' R^{-1} L^{-1}),$$

which is the desired estimate.

Having proven (11), we now turn to the sharper estimate asserted by Lemma 3. Suppose first that

$$H(A) > C_2 R^2 L^2 \tag{14}$$

for a large constant C_2 to be picked in a moment. Then fix $R_1 < R$ so that

$$\frac{L^3}{(2\pi)^3} \mathrm{vol}\{B(0,R) \setminus B(0,R_1)\} = \frac{H(A)}{2}. \tag{15}$$

Note that we can find such an R_1, since by Lemma 1 and the definition of $H(A)$ we have

$$H(A) \le [\text{Number of points in } \Lambda \cap \overline{B(0,R)}] < \frac{3}{2} \frac{L^3}{(2\pi)^3} \mathrm{vol}\, B(0,R).$$

From (15) and Lemma 1, we learn that the number of points in $\Lambda \cap \{\overline{B(0,R)} \setminus \overline{B(0,R_1)}\}$ is at most

$$\frac{L^3}{(2\pi)^3} \mathrm{vol}\{B(0,R) \setminus B(0,R_1)\} + C R^2 L^2 = \frac{1}{2} H(A) + C R^2 L^2.$$

The set $[\Lambda \cap \overline{B(0,R)}] \setminus A$ contains $H(A)$ points, at most $\frac{1}{2}H(A) + CR^2L^2$ of which belong to $\overline{B(0,R)} \setminus \overline{B(0,R_1)}$. Therefore, $[\Lambda \cap \overline{B(0,R_1)}] \setminus A$ contains at least $\frac{1}{2}H(A) - CR^2L^2$ points.

We can also derive a lower bound for the number of points in $A \setminus \overline{B(0,R)}$. To see this, recall that A contains at least $\rho_0 L^3 \cdot (1 - C_1 R^{-1} L^{-1})$ points. The number of these points that lie in $\overline{B(0,R)}$ is equal to [Number of points in $\Lambda \cap \overline{B(0,R)}] - H(A)$, which is at most $\rho_0 L^3 \cdot (1 + CR^{-1}L^{-1}) - H(A)$, by Lemma 1 and the definition of ρ_0. Hence, $A \setminus \overline{B(0,R)}$ contains at least

$$\{\rho_0 L^3 \cdot (1 - C_1 R^{-1} L^{-1})\} - \{\rho_0 L^3 \cdot (1 + CR^{-1}L^{-1}) - H(A)\} \\ = H(A) - C' R^2 L^2 \quad \text{points.}$$

If we pick C_2 large enough in (14), then our lower bounds for the number of points in $\Lambda \cap \overline{B(0,R_1)} \setminus A$ and in $A \setminus \overline{B(0,R)}$ show that these sets both contain at least $\frac{1}{4}H(A)$ elements.

Hence we can define a new subset $\widetilde{A} \subset \Lambda$ by removing from A at least $\frac{1}{4}H(A)$ points lying outside $\overline{B(0,R)}$, and replacing them by an equal number of points of $\Lambda \cap \overline{B(0,R_1)} \setminus A$. Evidently, A and $\widetilde{A}$ contain the same number of points, so (11) applied to $\widetilde{A}$ yields

$$\sum_{\xi \in \widetilde{A}} |\xi|^2 \geq c_{TF} \rho_0^{5/3} L^3 \cdot \left(1 - \frac{C'}{RL}\right). \tag{16}$$

Every time we remove a point of $A \setminus \overline{B(0,R)}$ and replace it by a point of $\Lambda \cap \overline{B(0,R_1)} \setminus A$, the sum $\sum_{\xi \in A} |\xi|^2$ decreases by at least $(R^2 - R_1^2) \geq R \cdot (R - R_1)$. Therefore,

$$\sum_{\xi \in A} |\xi|^2 \geq \sum_{\xi \in \widetilde{A}} |\xi|^2 + cH(A) \cdot R(R - R_1). \tag{17}$$

For $0 \leq R_1 < R$ we have $\mathrm{vol}(B(0,R) \setminus B(0,R_1)) \sim R^2 \cdot (R - R_1)$, so the definition (15) of R_1 yields

$$L^3 R^2 (R - R_1) \geq cH(A), \quad \text{i.e.}$$

$R(R - R_1) \geq c\frac{H(A)}{RL^3}$. Putting this into (17), we find that

$$\sum_{\xi \in A} |\xi|^2 \geq \sum_{\xi \in \widetilde{A}} |\xi|^2 + \frac{c(H(A))^2}{RL^3},$$

which, together with (16), implies

$$\sum_{\xi \in A} |\xi|^2 \geq c_{TF} \rho_0^{5/3} L^3 \cdot \left(1 - \frac{C'}{RL}\right) + \frac{c(H(A))^2}{RL^3}.$$

This is the conclusion of the Lemma. However, to prove it, we assumed that $H(A) > C_2R^2L^2$.

It remains to prove the lemma assuming that $H(A) \le C_2R^2L^2$. In this case, $\frac{(H(A))^2}{RL^3} \le C_3R^3L = \frac{C_3R^5L^3}{R^2L^2} = \frac{C_4\rho_0^{5/3}L^3}{R^2L^2}$. Thus, the conclusion of the lemma follows if we can show that $\sum_{\xi\in A}|\xi|^2 \ge c_{TF}\rho_0^{5/3}L^3\cdot\left(1-\frac{C''}{LR}+\frac{C_4}{L^2R^2}\right)$. Since $LR > 1$, this inequality with a large enough C'' follows at once from (11). The proof of the Lemma is complete. □

In addition to Fourier-expanding on the whole flat torus T, we shall also take Fourier expansions on subcubes $Q \subset T$. Unfortunately, the basic exponentials $e^{i\xi\cdot x}\chi_Q(x)$ behave badly as functions on T, and we will have to make them smooth across the boundary ∂Q. The following lemma constructs an orthonormal family of smooth functions supported in Q. We will use these functions as a substitute for the exponentials on Q.

Lemma 4: *Fix $\varepsilon > 0$. Suppose we are given $\rho > 0$ and a cube $Q \subset \mathbb{R}^3$ centered at 0. Assume $\rho|Q| > C_\varepsilon$ but $\operatorname{diam} Q < \frac{1}{10}L$. Then we can find smooth orthonormal functions $\varphi_1(x), \varphi_2(x), \ldots, \varphi_{\underline{N}}(x)$ supported in Q, with the following properties:*

(A) $|\underline{N} - \rho|Q|| \le C_\varepsilon(\rho|Q|)^{\frac{8}{9}+3\varepsilon}$

(B) *Set $\widehat{\varphi}_\alpha(\xi) = \int_{\mathbb{R}^3} e^{-i\xi\cdot x}\varphi_\alpha(x)dx$. Then*

$$\|\widehat{\varphi}_\alpha\|_{L^\infty} \le C|Q|^{1/2},$$

and

$$\sum_{\xi\in\Lambda\setminus B(0,r_F)} \frac{|\widehat{\varphi}_\alpha(\xi)|^2}{L^3} \le C_{m\varepsilon}\underline{N}^{-m} \quad (\text{any } m > 0),$$

where r_F is the Fermi radius, given by

$$\rho = \frac{1}{6\pi^2}r_F^3. \tag{18}$$

(C) *For $x, y \in \frac{3}{4}Q$ (= the middle 3/4 of Q), we have*

$$\left|\sum_{1\le\alpha\le\underline{N}} \varphi_\alpha(x)\overline{\varphi_\alpha(y)} - \mathcal{S}_\rho(x-y)\right| \le C_\varepsilon\rho\cdot\left(\underline{N}^{-\frac{1}{9}+3\varepsilon} + \frac{|x-y|}{\operatorname{diam} Q}\right),$$

with

$$\mathcal{S}_\rho(\mathfrak{z}) = \int_{B(0,r_F)} e^{i\eta\cdot\mathfrak{z}}\frac{d\eta}{(2\pi)^3} \quad \text{and} \quad r_F \quad \text{given by (18).} \tag{19}$$

Proof: Say $Q = [-D, D]^3$. Define a function $\theta(t)$ of one variable, with the following properties.

$\theta(t) = 1$ if $|t| \leq D \cdot \left(1 - (\rho|Q|)^{\varepsilon - \frac{1}{9}}\right) \equiv D_1$.

$1 > \theta(t) > 0$ if $D \cdot \left(1 - (\rho|Q|)^{\varepsilon - \frac{1}{9}}\right) < |t| < D$.

$\theta(t) = 0$ if $|t| \geq D$.

$\left|\left(\frac{d}{dt}\right)^\alpha \theta(t)\right| \leq C_\alpha \left[D \cdot (\rho|Q|)^{\varepsilon - \frac{1}{9}}\right]^{-\alpha}$ for $\alpha \geq 0$, all t.

$\theta(t)$ is an even function of t.

Then define $\phi_\#(t) = \int_0^t \theta^2(s)ds$ and define $\Phi: \mathbb{R}^3 \to \mathbb{R}^3$ by $\Phi(x_1, x_2, x_3) = (\phi_\#(x_1), \phi_\#(x_2), \phi_\#(x_3))$. The restriction of Φ to the open cube Q^{interior} is a diffeomorphism of Q^{interior} to the cube $(-D_\#, +D_\#)^3$, with $D_\# = \int_0^\infty \theta^2(t)dt$. For $\eta \in \frac{2\pi}{2D_\#}\mathbb{Z}^3 \cap B(0, r_F \cdot \left(1 - (\rho|Q|)^{\varepsilon - \frac{1}{9}})\right)$, we define

$$\varphi_\eta(x) = \frac{(\det \Phi'(x))^{1/2}}{(2D_\#)^{3/2}} \exp(i\eta \cdot \Phi(x)).$$

These are smooth functions supported in Q, since the Jacobian factor $(\det \Phi'(x))^{1/2}$ is equal to $\theta(x_1)\theta(x_2)\theta(x_3)$. To see that they are orthonormal, we make the change of variable $y = \Phi(x)$ on Q^{interior}, so that

$$\int_{\mathbb{R}^3} \varphi_\eta(x)\overline{\varphi_{\eta'}(x)}dx = \int_Q \varphi_\eta(x)\overline{\varphi_{\eta'}(x)}dx = (2D_\#)^{-3} \int_Q \det \Phi'(x) \cdot \exp(i[\eta - \eta'] \cdot \Phi(x))dx$$

$$= (2D_\#)^{-3} \int_{[-D_\#, +D_\#]^3} \exp(i[\eta - \eta'] \cdot y)dy = \left\{ \begin{matrix} 1 \text{ if } & \eta = \eta' \\ 0 & \text{otherwise} \end{matrix} \right\}.$$

According to Lemma 1, the number $\underset{\sim}{N}$ of φ_η is equal to

$$\text{(20)} \qquad \frac{1}{6\pi^2}\left[r_F \cdot \left(1 - (\rho|Q|)^{\varepsilon - \frac{1}{9}}\right)\right]^3 \cdot (2D_\#)^3 + \text{Error},$$

with $|\text{Error}| \leq Cr_F^2 D_\#^2 \leq C' r_F^2 D^2 = C''(\rho|Q|)^{2/3}$. By definition of $D_\#$ and $\theta(t)$ we have

$$|D_\# - D| \leq C\,(\rho|Q|)^{\varepsilon - \frac{1}{9}}\,D.$$

Putting this into (20) and recalling (18), we obtain

$$\underset{\sim}{N} = \rho|Q| + \text{Error}, \text{ with } |\text{Error}| \leq C\,(\rho|Q|)^{\varepsilon + \frac{8}{9}}.$$

This proves part (A) of the lemma.

To prove part (B) of the lemma, we first estimate $\|\widehat{\varphi}_\eta\|_{L^\infty}$. Since $0 \le \det \Phi' \le 1$ and $D_\# \sim D$, we have

$$\|\widehat{\varphi}_\eta\|_{L^\infty} \le \|\varphi_\eta\|_{L^1} \le \int\limits_Q (2D_\#)^{-3/2} dx = (2D)^3 \cdot (2D_\#)^{-3/2} \le CD^{3/2} \le C(\operatorname{vol} Q)^{1/2},$$

as asserted in part (B). The second assertion of part (B) concerns $\widehat{\varphi}_\eta(\xi)$ for $|\xi| > r_F$. To handle $\widehat{\varphi}_\eta(\xi)$, we recall an old stationary phase argument. Suppose we are given functions $g(t)$, $a(t)$ of one variable, satisfying

$$\left|\left(\frac{d}{dt}\right)^m a\right| \le C_m(\tau B)^{-m}$$

$$\left|\left(\frac{d}{dt}\right)^{m+1} g\right| \le C_m B^{-m},$$

$$\left|\frac{dg}{dt}\right| \ge \tau, \quad \text{with} \quad 0 < \tau < 1.$$

Suppose also that a is supported in an interval I. Under these hypotheses, we investigate the integral

$$X = \int\limits_I a(t) e^{i\lambda g(t)} dt \quad \text{for large} \quad \lambda.$$

Integration by parts gives

$$X = \pm \frac{i}{\lambda} \int\limits_I \left\{ \frac{d}{dt} \left[\frac{a(t)}{g'(t)} \right] \right\} e^{i\lambda g(t)} dt. \tag{20 bis}$$

We estimate the derivatives of $\frac{d}{dt}\left[\frac{a(t)}{g'(t)}\right]$. The derivative $\left(\frac{d}{dt}\right)^m \frac{1}{g'(t)}$ is a sum of terms of the form

$$\frac{1}{[g'(t)]^{1+k}} \prod_{\nu=1}^{k} \left(\frac{d}{dt}\right)^{m_\nu} g'(t) \quad \text{with} \quad m_\nu \ge 1 \quad \text{and} \quad m_1 + \cdots + m_k = m. \tag{21}$$

In particular, $0 \le k \le m$. Our estimates on $g'(t)$ and its derivatives show that the term (21) is dominated by

$$\frac{C_m}{\tau^{1+k}} \prod_{\nu=1}^{k} B^{-m_\nu} \le \frac{C_m}{\tau} \cdot (\tau B)^{-m}.$$

Therefore,

$$\left|\left(\frac{d}{dt}\right)^m \frac{1}{g'(t)}\right| \le \frac{C_m}{\tau} (\tau B)^{-m}.$$

Combining this with our assumptions on $a(t)$, we find that

$$\left|\left(\frac{d}{dt}\right)^m \left[\frac{a(t)}{g'(t)}\right]\right| \leq \frac{C'_m}{\tau} \cdot (\tau B)^{-m}.$$

In particular,

$$\left|\left(\frac{d}{dt}\right)^m \left\{\frac{d}{dt}\left[\frac{a(t)}{g'(t)}\right]\right\}\right| \leq \frac{C'_m}{\tau^2 B} \cdot (\tau B)^{-m}.$$

Hence, equation (20 bis) gives

$$X = \frac{\pm i}{\tau^2 \lambda B} \int_I \tilde{a}(t) e^{i\lambda g(t)} dt, \quad \text{with} \quad \tilde{a}(t) = \tau^2 B \frac{d}{dt}\left[\frac{a(t)}{g'(t)}\right]$$

satisfying

$$\left|\left(\frac{d}{dt}\right)^m \tilde{a}(t)\right| \leq C'_m \cdot (\tau B)^{-m},$$

and with $\tilde{a}$ supported in I. Thus, $\tilde{a}$ satisfies the same assumptions we imposed on a. Repeating this trick M times, we may write

$$X = (\tau^2 \lambda B)^{-M} \int_I a_M(t) e^{i\lambda g(t)} dt,$$

with a_M supported on I, and

$$\left|\left(\frac{d}{dt}\right)^m a_M\right| \leq C_{mM} (\tau B)^{-m}.$$

In particular,

$$|X| \leq (\tau^2 \lambda B)^{-M} \int_I |a_M(t)| dt \leq C_M |I| \cdot (\tau^2 \lambda B)^{-M}, \tag{22}$$

with M as large as we please.

This is our basic stationary phase inequality. To apply it, note that

$$\widehat{\varphi}_\eta(\xi) = (2D_\#)^{-3/2} \int_{\mathbb{R}^3} (\det \Phi'(x))^{1/2} \exp(i[-\xi \cdot x + \eta \cdot \Phi(x)]) dx. \tag{23}$$

Suppose $|\xi| > r_F$ and $|\eta| \leq r_F \cdot \left(1 - (\rho|Q|)^{\varepsilon - \frac{1}{9}}\right)$. Set $\tau = (\rho|Q|)^{\varepsilon - \frac{1}{9}}$, $B = (\rho|Q|)^{\varepsilon - \frac{1}{9}} D$, $\lambda = |\xi|$,

$$g(x) = \frac{\xi}{|\xi|} \cdot x - \frac{\eta}{|\xi|} \cdot \Phi \quad \text{for} \quad x \in \mathbb{R}^3, \; a(x) = (\det \Phi'(x))^{1/2} = \theta(x_1)\theta(x_2)\theta(x_3) \tag{24}$$

for $x = (x_1, x_2, x_3) \in \mathbb{R}^3$. Then we see that

$$|\partial_x^\alpha a(x)| \leq C_\alpha B^{-\alpha} \leq C_\alpha (\tau B)^{-\alpha}, \tag{25}$$

by the defining properties of θ.

Also, $\Phi'(x)$ is a diagonal matrix with entries $\theta^2(x_i)$, at $x = (x_1, x_2, x_3)$. Therefore, $|\partial_x^\alpha(\nabla\Phi)| \leq C_\alpha B^{-\alpha}$, again by the defining properties of θ. Since $|\eta| \leq |\xi|$, equation (24) therefore implies

$$|\partial_x^\alpha \nabla g(x)| \leq C_\alpha B^{-\alpha} \quad \text{for} \quad x \in \mathbb{R}^3,\ \alpha \quad \text{any multi-index.} \tag{26}$$

We pick an orthonormal basis e_1, e_2, e_3 of $\mathbb{R}^3$ with $e_1 = \frac{\xi}{|\xi|}$, and we let (y_1, y_2, y_3) be the coordinates of a given point x with respect to e_1, e_2, e_3. In terms of these coordinates,

$$\frac{\partial g}{\partial y_1} \geq 1 - \frac{|\eta|}{|\xi|}, \quad \text{since } |\nabla\Phi| \leq 1 \tag{27}$$

as one sees at once in the original coordinate system. Our assumptions on $|\xi|$ and $|\eta|$ yield $1 - \frac{|\eta|}{|\xi|} \geq \tau$, so (25), (26), (27) imply

$$|\partial_{y_1}^m a| \leq C_m (\tau B)^{-m},\ |\partial_{y_1}^m (\partial_{y_1} g)| \leq C_m B^{-m},\ \partial_{y_1} g \geq \tau \tag{28}$$

for any $m \geq 0$ and any (y_1, y_2, y_3). For fixed (y_2, y_3), estimates (28) are the hypotheses of the stationary phase inequality (22). Note also that a is supported in $\{|y_1| \leq CD\}$. Therefore, by (22) with $|I| \sim D$, we have

$$\left| \int_{-\infty}^{\infty} a(y_1, y_2, y_3) \exp(-i\lambda g(y_1, y_2, y_3)) dy_1 \right| \leq \frac{C_M D}{(\tau^2 \lambda B)^M},\ M \text{ as large as we please.} \tag{29}$$

The left-hand side here is zero for $|(y_2, y_3)| \geq CD$, in view of the fact that $a = (\det \Phi')^{1/2}$ is supported in Q.

Hence, integrating (29) over $(y_1, y_2) \in \mathbb{R}^3$, we obtain

$$\left| \int_{\mathbb{R}^3} (\det \Phi')^{1/2} \exp(-i\xi \cdot x + i\eta \cdot \Phi(x)) dx \right| \leq \frac{C_M D^3}{(\tau^2 \lambda B)^M}.$$

Putting this into (23) and recalling the definitions of τ, λ, B, we obtain for $|\xi| \geq r_F$, $|\eta| \leq r_F \cdot \left(1 - (\rho|Q|)^{\varepsilon - \frac{1}{9}}\right)$ the estimate

$$|\widehat{\varphi}_\eta(\xi)| \leq C_M D^{3/2} \left\{ (\rho|Q|)^{2\varepsilon - \frac{2}{9}} |\xi| (\rho|Q|)^{\varepsilon - \frac{1}{9}} D \right\}^{-M},$$

i.e.

$$|\widehat{\varphi}_\eta(\xi)| \le C_M D^{\frac{3}{2}} \left\{ (\rho|Q|)^{3\varepsilon-\frac{1}{3}} |\xi| D \right\}^{-M} \tag{30}$$

Since $r_F \sim \rho^{1/3}$ and $D \sim |Q|^{\frac{1}{3}}$, $\rho|Q| \sim \underset{\sim}{\mathrm{N}}$, we have

$$\begin{aligned}(\rho|Q|)^{3\varepsilon-\frac{1}{3}}|\xi|D &= r_F^{-1}|\xi| \cdot (r_F D)(\rho|Q|)^{3\varepsilon-\frac{1}{3}} \\ &\sim r_F^{-1}|\xi|(\rho|Q|)^{1/3} \cdot (\rho|Q|)^{3\varepsilon-\frac{1}{3}} \sim \underset{\sim}{\mathrm{N}}^{3\varepsilon}|\xi| r_F^{-1},\end{aligned}$$

so that (30) may be rewritten as

$$|\widehat{\varphi}_\eta(\xi)| \le C_M |Q|^{1/2} (\underset{\sim}{\mathrm{N}}^{3\varepsilon}|\xi| r_F^{-1})^{-M}, \text{ with } M \text{ as large as we please.} \tag{31}$$

Estimate (31) holds for $|\xi| \ge r_F$, $|\eta| \le r_F \cdot \left(1 - (\rho|Q|)^{\varepsilon - \frac{1}{9}}\right)$.

From (31) we can complete the proof of conclusion (B). Again we introduce cubes Q_ξ of side $\frac{2\pi}{L}$ centered at $\xi \in \Lambda$. Thus the Q_ξ are pairwise disjoint. If $|\xi| \ge r_F \sim \rho^{1/3}$ and $\zeta \in Q_\xi$, then $|\zeta| \ge r_F - \operatorname{diam} Q_\xi \ge c\rho^{1/3} - 100L^{-1}$. Note that $L^{-1} \ll \rho^{1/3}$ since $1 \ll \rho|Q| \sim \rho D^3 \le \rho L^3$. Thus $|\xi| \ge r_F$ and $\zeta \in Q_\xi$ imply $|\zeta| > c r_F$. Also,

$$\int_{Q_\xi} \left(\frac{r_F}{|\zeta|}\right)^M d\zeta \ge c_M \left(\frac{r_F}{|\xi|}\right)^M L^{-3} \quad \text{for} \quad |\xi| \ge r_F.$$

Therefore, (31) implies

$$\begin{aligned}\sum_{\xi \in \Lambda \smallsetminus B(0,r_F)} L^{-3} |\widehat{\varphi}_\eta(\xi)|^2 &\le C_M |Q| \underset{\sim}{\mathrm{N}}^{-3\varepsilon M} \sum_{\xi \in \Lambda \smallsetminus B(0,r_F)} \left(\frac{r_F}{|\xi|}\right)^M L^{-3} \\ &\le C'_M |Q| \underset{\sim}{\mathrm{N}}^{-3\varepsilon M} \sum_{\xi \in \Lambda \smallsetminus B(0,r_F)} \int_{Q_\xi} \left(\frac{r_F}{|\zeta|}\right)^M d\zeta \\ &\le C''_M |Q| \underset{\sim}{\mathrm{N}}^{-3\varepsilon M} \int_{\mathbb{R}^3 \smallsetminus B(0,cr_F)} \left(\frac{r_F}{|\zeta|}\right)^M d\zeta \\ &\le C'''_M |Q| \underset{\sim}{\mathrm{N}}^{-3\varepsilon M} r_F^3 \quad \text{for} \quad M > 3.\end{aligned} \tag{32}$$

Since $r_F^3|Q| \sim \rho|Q| \sim \underset{\sim}{\mathrm{N}}$, (32) may be rewritten as

$$\sum_{\xi \in \Lambda \smallsetminus B(0,r_F)} |\widehat{\varphi}_\eta(\xi)|^2 L^{-3} \le C_M \underset{\sim}{\mathrm{N}}^{1-3\varepsilon M}.$$

For M large enough, depending on m and ε, this implies

$$\sum_{\xi \in \Lambda \smallsetminus B(0,r_F)} \frac{|\widehat{\varphi}_\eta(\xi)|^2}{L^3} \leq C_{\varepsilon m} \underline{\mathrm{N}}^{-m},$$

completing the proof of conclusion (B).

Turning to conclusion (C), we take $x, y \in \frac{3}{4}Q$. Then Φ is the identity map near x and near y, so that

$$\varphi_\eta(x) = (2D_\#)^{-3/2} e^{i\eta \cdot x} \quad \text{and} \quad \varphi_\eta(y) = (2D_\#)^{-3/2} e^{i\eta \cdot y}.$$

Hence

$$\sum_\eta \varphi_\eta(x)\overline{\varphi_\eta(y)} = (2D_\#)^{-3} \sum_{\substack{\eta \in \frac{2\pi}{(2D_\#)}\mathbb{Z}^3 \\ |\eta| < r_F \cdot \left(1 - (\rho|Q|)^{\varepsilon - \frac{1}{9}}\right)}} \exp(i\eta \cdot [x-y]) \tag{33}$$

Set $\tilde{r}_F = r_F \cdot \left(1 - (\rho|Q|)^{\varepsilon - \frac{1}{9}}\right)$, and introduce a cube Q_η centered at $\eta \in \frac{2\pi}{(2D_\#)}\mathbb{Z}^3$, with side $\frac{2\pi}{(2D_\#)}$. We have

$$\begin{aligned} |\exp(i\eta \cdot [x-y]) - \frac{(2D_\#)^3}{(2\pi)^3} \int_{Q_\eta} \exp(i\zeta \cdot [x-y]) d\zeta| &\leq C|x-y| \operatorname{diam} Q_\eta \\ &\sim \frac{C|x-y|}{\operatorname{diam} Q}, \end{aligned}$$

since $|\nabla_\zeta \exp(i\zeta \cdot [x-y])| \leq |x-y|$.

Summing over $\eta \in \frac{2\pi}{(2D_\#)}\mathbb{Z}^3$ with $|\eta| < \tilde{r}_F$, and defining E = union of all the Q_η with $\eta \in \frac{2\pi}{(2D_\#)}\mathbb{Z}^3$ and $|\eta| < \tilde{r}_F$, we obtain

$$\begin{aligned} &|(2D_\#)^{-3} \sum_{\substack{\eta \in \frac{2\pi}{2D_\#}\mathbb{Z}^3 \\ |\eta| < \tilde{r}_F}} \exp(i\eta \cdot [x-y]) - \int_E \exp(i\zeta \cdot [x-y]) \frac{d\zeta}{(2\pi)^3}| \leq \\ &\frac{C|x-y|}{\operatorname{diam} Q} D_\#^{-3} \cdot [\text{Number of } \eta \in \frac{2\pi}{2D_\#}\mathbb{Z}^3 \text{ with } |\eta| < \tilde{r}_F]. \end{aligned} \tag{34}$$

The right-hand side of (34) has the order of magnitude $\frac{C|x-y|}{\operatorname{diam} Q} D_\#^{-3} \cdot [D_\#^3 r_F^3]$, by Lemma 1 and the fact that $D_\#^3 r_F^3 \sim D^3 \rho \sim |Q|\rho \gg 1$. Therefore, (33) and (34) yield

$$\begin{aligned} \left| \sum_\eta \varphi_\eta(x)\overline{\varphi_\eta(y)} - \int_E \exp(i\eta \cdot [x-y]) \frac{d\zeta}{(2\pi)^3} \right| &\leq \frac{C|x-y|}{\operatorname{diam} Q} r_F^3 \\ &\leq C'\rho \frac{|x-y|}{\operatorname{diam} Q} \end{aligned} \tag{35}$$

By definition of the set E, we have

$$B(0,\tilde{r}_F-100D^{-1})\subset E\subset B(0,\tilde{r}_F+100D^{-1}),$$

so that

$$|\chi_E-\chi_{B(0,\tilde{r}_F)}|\le\chi_{B(0,\tilde{r}_F+100D^{-1})\setminus B(0,\tilde{r}_F-100D^{-1})}.$$

Consequently,

$$(36)\qquad \left|\int_E \exp(i\zeta\cdot[x-y])\frac{d\zeta}{(2\pi)^3}-\int_{B(0,\tilde{r}_F)}\exp(i\zeta\cdot[x-y])\frac{d\zeta}{(2\pi)^3}\right|$$
$$\le \int_{B(0,\tilde{r}_F+100D^{-1})\setminus B(0,\tilde{r}_F-100D^{-1})}|\exp(i\zeta\cdot[x-y])|\frac{d\zeta}{(2\pi)^3}$$
$$\le Cr_F^2D^{-1}.$$

(Recall that $\tilde{r}_F\sim r_F\gg D^{-1}$ since $r_F^3D^3\sim\rho|Q|\gg 1$.) The right-hand side of (36) may be rewritten as

$$\frac{C'\rho}{r_FD}\sim\frac{C'\rho}{(\rho|Q|)^{1/3}}\sim\frac{C'\rho}{\underline{\mathrm{N}}^{1/3}}.$$

Hence, (35) and (36) yield

$$(37)\qquad \left|\sum_\eta\varphi_\eta(x)\overline{\varphi_\eta(y)}-\int_{B(0,\tilde{r}_F)}\exp(i\zeta\cdot[x-y])\frac{d\zeta}{(2\pi)^3}\right|\le C\rho\left(\frac{|x-y|}{\operatorname{diam}Q}+\underline{\mathrm{N}}^{-\frac{1}{3}}\right).$$

Also,

$$\left|\int_{B(0,\tilde{r}_F)}\exp(i\zeta\cdot[x-y])\frac{d\zeta}{(2\pi)^3}-\int_{B(0,r_F)}\exp(i\zeta\cdot[x-y])\frac{d\zeta}{(2\pi)^3}\right|$$
$$\le\operatorname{vol}\{B(0,r_F)\setminus B(0,\tilde{r}_F)\}\le Cr_F^2\cdot(r_F-\tilde{r}_F)$$
$$\sim C\rho\cdot(\rho|Q|)^{\varepsilon-\frac{1}{9}}\sim C\rho\underline{\mathrm{N}}^{\varepsilon-\frac{1}{9}}.$$

Combining this with (37), we obtain

$$\left|\sum_\eta\varphi_\eta(x)\overline{\varphi_\eta(y)}-\int_{B(0,r_F)}\exp(i\zeta\cdot[x-y])\frac{d\zeta}{(2\pi)^3}\right|\le C\rho\left(\frac{|x-y|}{\operatorname{diam}Q}+\underline{\mathrm{N}}^{\varepsilon-\frac{1}{9}}\right).$$

This proves conclusion (C), completing the proof of Lemma 4. □

For each spin s ($1\le s\le q$), define the density $\rho_s=\frac{N_s}{L^3}$ of particles with spin s, and define the Fermi radius r_F^s by $\rho_s=\frac{1}{6\pi^2}(r_F^s)^3$ as in (18). Let Q be a cube in $\mathbb{R}^3$, centered at 0, with $\operatorname{diam}Q<\frac{1}{10}L$ but $\rho_s|Q|>C_\varepsilon$ (as in Lemma 4) for each s. Lemma 4 constructs a finite orthonormal family $\varphi_{1,s}(x)$, $\varphi_{2,s}(x), \dots, \varphi_{\underline{\mathrm{N}}_s,s}(x)$ of smooth functions supported in Q. According to Lemma 4, we have

$$(38) \qquad |\underline{\mathrm{N}}_s - \rho_s|Q|\,| \le C_\varepsilon(\rho_s|Q|)^{\frac{8}{9}+3\varepsilon}$$

$$(39) \qquad |\widehat{\varphi}_{\alpha,s}(\xi)| \le C|Q|^{1/2} \quad \text{for all} \quad \xi,\ 1 \le \alpha \le \underline{\mathrm{N}}_s$$

$$(40) \qquad \sum_{\xi \in \Lambda \setminus B(0,r_F^s)} \frac{|\widehat{\varphi}_{\alpha,s}(\xi)|^2}{L^3} \le C_{m\varepsilon}\underline{\mathrm{N}}_s{}^{-m} \quad (\text{any } m>0) \text{ for } \quad 1 \le \alpha \le \underline{\mathrm{N}}_s.$$

$$(41) \qquad \left|\sum_{1\le\alpha\le\underline{\mathrm{N}}_s} \varphi_{\alpha,s}\overline{\varphi_{\alpha,s}(y)} - \mathcal{S}_{\rho_s}(x-y)\right| \le C_\varepsilon \rho_s \cdot \left(\underline{\mathrm{N}}_s^{-\frac{1}{9}+3\varepsilon} + \frac{|x-y|}{\operatorname{diam} Q}\right)$$

$$\text{for } x, y \in \frac{3}{4}Q, \text{ with } \mathcal{S}_\rho(\mathfrak{z}) \text{ defined by (19).}$$

Here $\widehat{\varphi}(\xi) = \int_{\mathbb{R}^3} e^{-i\xi\cdot x}\varphi(x)dx$.

For each s, we complete $\varphi_{1,s}\dots\varphi_{\underline{\mathrm{N}}_s,s}$ to an orthonormal basis $(\varphi_{\alpha,s})_{1\le\alpha<\infty}$ of $L^2(Q)$. We regard Q as a subset of T, and we regard the $\varphi_{\alpha,s}$ as functions on T, vanishing outside Q. Let $(\varphi_{\alpha,s})_{-\infty<\alpha\le 0}$ be an orthonormal basis for the L^2 functions supported in $T \setminus Q$, for each fixed s. Thus, for each s, $(\varphi_{\alpha,s})_{-\infty<\alpha<\infty}$ is an orthonormal basis for $L^2(T)$. For each $\mathfrak{z} \in T$ we form the translates $\varphi^{\mathfrak{z}}_{\alpha,s}(x) = \varphi_{\alpha,s}(x-\mathfrak{z})$. Thus for fixed $\mathfrak{z}$ and s, the $(\varphi^{\mathfrak{z}}_{\alpha,s})_{-\infty<\alpha<\infty}$ form an orthonormal basis of $L^2(T)$, with $\varphi^{\mathfrak{z}}_{\alpha,s}$ supported in $Q+\mathfrak{z}$ when $\alpha \ge 1$, and supported in $T \setminus (Q+\mathfrak{z})$ when $\alpha \le 0$.

For each $\mathfrak{z} \in T$, we make a Fourier expansion of the wave function Ψ as follows.

$$(42) \qquad \Psi(x_1\dots x_N) = \sum_{\alpha_1\dots\alpha_N} C^{\mathfrak{z}}_{\alpha_1\dots\alpha_N} \prod_{s=1}^{q}\left(\prod_{\text{spin}(j)=s} \varphi^{\mathfrak{z}}_{\alpha_j,s}(x_j)\right).$$

Note that

$$(43) \qquad \sum_{\alpha_1\dots\alpha_N} |C^{\mathfrak{z}}_{\alpha_1\dots\alpha_N}|^2 = 1,$$

and that the $C^{\mathfrak{z}}_{\alpha_1\dots\alpha_N}$ are antisymmetric under spin-preserving permutations of the indices. In particular, $C^{\mathfrak{z}}_{\alpha_1\dots\alpha_N} \ne 0$ implies that the α_j for $\text{spin}(j)=s$ are all distinct.

We also make a standard Fourier expansion of Ψ:

$$(44) \qquad \Psi(x_1\dots x_N) = \sum_{\xi_1\dots\xi_N\in\Lambda} A_{\xi_1\dots\xi_N} \frac{e^{i\xi_1\cdot x_1}}{L^{3/2}} \cdots \frac{e^{i\xi_N\cdot x_N}}{L^{3/2}}.$$

We have

$$(45) \qquad \sum_{\xi_1\dots\xi_N\in\Lambda} |A_{\xi_1\dots\xi_N}|^2 = 1,$$

and $A_{\xi_1 \ldots \xi_N}$ is antisymmetric under spin-preserving permutations of indices. In particular, $A_{\xi_1 \ldots \xi_N} \neq 0$ implies that the ξ_j for $\text{spin}(j) = s$ are all distinct.

We will show that assumption (4) on the kinetic energy has consequences for the coefficients $C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N}$. In fact, let $\mathcal{B}$ denote the set of $(\alpha_1 \ldots \alpha_N)$ with the property that for each s and each α $(1 \leq \alpha \leq \underline{\text{N}}_s)$, there is an index j with $\text{spin}(j) = s$ and $\alpha_j = \alpha$. We shall see that for most $\mathfrak{z} \in T$, the quantity

$$\sum_{(\alpha_1 \ldots \alpha_N) \notin \mathcal{B}} |C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N}|^2 \quad \text{is small compared to 1.}$$

To prove this, we introduce the numbers $\mu_s(\mathfrak{z}, \alpha)$, defined by setting

$$\text{(46)} \qquad 1 - \mu_s(\mathfrak{z}, \alpha) = \sum_{\text{spin}(j)=s} \int_{T^{N-1}} \left| \int_T \overline{\varphi^{\mathfrak{z}}_{\alpha,s}(x_j)} \Psi(x_1 \ldots x_N) dx_j \right|^2 dx_1 \ldots dx_{j-1} dx_{j+1} \ldots dx_N.$$

The $\mu_s(\mathfrak{z}, \alpha)$ are closely related to the $C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N}$. In fact, (42) gives

$$\int_T \overline{\varphi^{\mathfrak{z}}_{\alpha,s_0}(x_j)} \Psi(x_1 \ldots x_N) dx_j = \sum_{\alpha_1 \ldots \alpha_N} \chi_{\alpha_j = \alpha} C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N} \prod_{s=1}^{q} \Bigg(\prod_{\substack{\text{spin}(i)=s \\ i \neq j}} \varphi^{\mathfrak{z}}_{\alpha_i,s}(x_i) \Bigg)$$

as functions of $(x_1 \ldots x_{j-1} x_{j+1} \ldots x_N)$, provided $\text{spin}(j) = s_0$. This implies that

$$\int_{T^{N-1}} \left| \int_T \overline{\varphi^{\mathfrak{z}}_{\alpha,s_0}(x_j)} \Psi(x_1 \ldots x_N) dx_j \right|^2 dx_1 \ldots dx_{j-1} dx_{j+1} \ldots dx_N$$
$$= \sum_{\alpha_1 \ldots \alpha_N} \chi_{\alpha_j = \alpha} |C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N}|^2$$

for $\text{spin}(j) = s_0$. Summing over all j of spin s_0, we conclude that

$$1 - \mu_{s_0}(\mathfrak{z}, \alpha) = \sum_{\alpha_1 \ldots \alpha_N} |C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N}|^2 \cdot \Bigg(\sum_{\text{spin}(j)=s_0} \chi_{\alpha_j = \alpha} \Bigg).$$

This and (43) yield

$$\text{(47)} \qquad \mu_{s_0}(\mathfrak{z}, \alpha) = \sum_{\alpha_1 \ldots \alpha_N} |C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N}|^2 \cdot \Bigg\{ 1 - \sum_{\text{spin}(j)=s_0} \chi_{\alpha_j = \alpha} \Bigg\}.$$

Since the α_j with $\text{spin}(j) = s_0$ are all distinct for $C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N} \neq 0$, the quantity in braces is equal to 0 if $\alpha_j = \alpha$ for some j with spin s_0, and 1 otherwise. Hence, with

$$\text{(48)} \qquad \mathcal{B}_{\alpha,s} = \{(\alpha_1 \ldots \alpha_N) | \alpha_j = \alpha \text{ for some } j \text{ with spin } s\ \},$$

equation (47) becomes

(49)
$$\mu_s(\mathfrak{z},\alpha) = \sum_{(\alpha_1\ldots\alpha_N)\notin\mathcal{B}_{\alpha,s}} |C^{\mathfrak{z}}_{\alpha_1\ldots\alpha_N}|^2.$$

For $1 \le s \le q$ and $1 \le \alpha \le \underline{\mathrm{N}}_s$, we will show that $\mu_s(\mathfrak{z},\alpha)$ is very small for most $\mathfrak{z} \in T$. Equation (49) will then imply that $\sum\limits_{(\alpha_1\ldots\alpha_N)\notin\mathcal{B}} |C^{\mathfrak{z}}_{\alpha_1\ldots\alpha_N}|^2$ is very small, since

(50)
$$\mathcal{B} = \bigcap_{1\le s\le q}\Big(\bigcap_{1\le\alpha\le\underline{\mathrm{N}}_s} \mathcal{B}_{\alpha,s}\Big).$$

To estimate $\mu_s(\mathfrak{z},\alpha)$ for most $\mathfrak{z}$, we merely compute $Av_{\mathfrak{z}\in T}\mu_s(\mathfrak{z},\alpha)$ using (44). We have

$$\varphi^{\mathfrak{z}}_{\alpha,s}(x_j) = \varphi_{\alpha,s}(x_j - \mathfrak{z}) = L^{-3}\sum_{\xi\in\Lambda} \widehat{\varphi}_{\alpha,s}(\xi)e^{-i\xi\cdot\mathfrak{z}}e^{i\xi\cdot x_j},$$

so (44) implies

$$\int_T \overline{\varphi^{\mathfrak{z}}_{\alpha,s}(x_j)}\Psi(x_1\ldots x_N)dx_j = \sum_{\xi_1\ldots\xi_N\in\Lambda} \overline{\widehat{\varphi}_{\alpha,s}(\xi_j)}A_{\xi_1\ldots\xi_N}\frac{e^{+i\xi_j\cdot\mathfrak{z}}}{L^{3/2}}\prod_{\ell\ne j}\frac{e^{+i\xi_\ell\cdot x_\ell}}{L^{3/2}},$$

which in turn gives

$$\int_{\mathfrak{z}\in T}\int_{T^{N-1}}\left|\int_T \overline{\varphi^{\mathfrak{z}}_{\alpha,s}(x_j)}\Psi(x_1\ldots x_N)dx_j\right|^2 dx_1\ldots dx_{j-1}dx_{j+1}\ldots dx_N d\mathfrak{z}$$
$$= \sum_{\xi_1\ldots\xi_N\in\Lambda} |\widehat{\varphi}_{\alpha,s}(\xi_j)|^2|A_{\xi_1\ldots\xi_N}|^2.$$

For fixed s, we sum this identity over all j of spin s, and then divide by L^3. We obtain

$$Av_{\mathfrak{z}\in T}[1-\mu_s(\mathfrak{z},\alpha)] = \sum_{\xi_1\ldots\xi_N\in\Lambda} |A_{\xi_1\ldots\xi_N}|^2\cdot\Big(\sum_{\mathrm{spin}(j)=s}\frac{|\widehat{\varphi}_{\alpha,s}(\xi_j)|^2}{L^3}\Big).$$

In view of (45), this is equivalent to

(51)
$$Av_{\mathfrak{z}\in T}\mu_s(\mathfrak{z},\alpha) = \sum_{\xi_1\ldots\xi_N\in\Lambda} |A_{\xi_1\ldots\xi_N}|^2\cdot\Big(1 - \sum_{\mathrm{spin}(j)=s}\frac{|\widehat{\varphi}_{\alpha,s}(\xi_j)|^2}{L^3}\Big).$$

Suppose $A_{\xi_1\ldots\xi_N} \ne 0$. Then the ξ_j with $\mathrm{spin}(j) = s$ are all distinct, so that

(52)
$$\sum_{\mathrm{spin}(j)=s}\frac{|\widehat{\varphi}_{\alpha,s}(\xi_j)|^2}{L^3} = \sum_{\xi\in\mathcal{A}_s(\xi_1\ldots\xi_N)}\frac{|\widehat{\varphi}_{\alpha,s}(\xi)|^2}{L^3},$$

with

$$(53)\qquad \mathcal{A}_s(\xi_1\dots\xi_N)=\{\xi_j \bigm| \operatorname{spin}(j)=s\}.$$

Also, $1=\|\varphi_{\alpha,s}\|^2_{L^2(T)}=\sum_{\xi\in\Lambda}\frac{|\widehat{\varphi}_{\alpha,s}(\xi)|^2}{L^3}$. Combining this with (52), we obtain for $A_{\xi_1\dots\xi_N}\neq 0$ that

$$(54)\qquad \Big(1-\sum_{\operatorname{spin}(j)=s}\frac{|\widehat{\varphi}_{\alpha,s}(\xi_j)|^2}{L^3}\Big)=\sum_{\xi\in\Lambda\smallsetminus\mathcal{A}_s(\xi_1\dots\xi_N)}\frac{|\widehat{\varphi}_{\alpha,s}(\xi)|^2}{L^3}$$
$$\leq\Big[\sum_{\xi\in\Lambda\smallsetminus B(0,r_F^s)}\frac{|\widehat{\varphi}_{\alpha,s}(\xi)|^2}{L^3}\Big]+\sum_{\xi\in\Lambda\cap B(0,r_F^s)\smallsetminus\mathcal{A}_s(\xi_1\dots\xi_N)}\frac{|\widehat{\varphi}_{\alpha,s}(\xi)|^2}{L^3}$$
$$\leq\Big[\sum_{\xi\in\Lambda\smallsetminus B(0,r_F^s)}\frac{|\widehat{\varphi}_{\alpha,s}(\xi)|^2}{L^3}\Big]+\frac{\|\widehat{\varphi}_{\alpha,s}\|^2_{L^\infty}}{L^3}H_s(\xi_1\dots\xi_N),$$

with $H_s(\xi_1\dots\xi_N)$ equal to the number of points of $\Lambda\cap B(0,r_F^s)$ not belonging to $\mathcal{A}_s(\xi_1\dots\xi_N)$. That is, $H_s(\xi_1\dots\xi_N)$ is the number of points of $\Lambda\cap B(0,r_F^s)$ which do not arise as ξ_j with j of spin s.

Putting (39) and (40) into the right-hand side of (54), we learn that

$$\Big(1-\sum_{\operatorname{spin}(j)=s}\frac{|\widehat{\varphi}_{\alpha,s}(\xi_j)|^2}{L^3}\Big)\leq C_{m\varepsilon}\underline{N}_s^{-m}+\frac{C|Q|}{L^3}H_s(\xi_1\dots\xi_N),$$

provided that $A_{\xi_1\dots\xi_N}\neq 0$ and $1\leq\alpha\leq\underline{N}_s$. Putting this into (51) and using (45), we obtain

$$(55)\qquad Av_{\mathfrak{z}\in T}\mu_s(\mathfrak{z},\alpha)\leq C_{m\varepsilon}\underline{N}_s^{-m}+\frac{C|Q|}{L^3}\sum_{\xi_1\dots\xi_N\in\Lambda}|A_{\xi_1\dots\xi_N}|^2H_s(\xi_1\dots\xi_N)$$
$$\text{for}\quad 1\leq\alpha\leq\underline{N}_s.$$

The second term on the right can be estimated in terms of the kinetic energy by using Lemma 4. In fact, (4) and (44) give

$$(56)\qquad (1+\delta)c_{TF}\sum_{s=1}^{q}N_s^{5/3}L^{-2}\geq\|\nabla\Psi\|^2=\sum_{\xi_1\dots\xi_N\in\Lambda}|A_{\xi_1\dots\xi_N}|^2\Big(\sum_{j=1}^{N}|\xi_j|^2\Big).$$

Suppose $A_{\xi_1\dots\xi_N}\neq 0$. Then for each s, the ξ_j with $\operatorname{spin}(j)=s$ are all distinct, and there are N_s of them altogether. With $\mathcal{A}_s(\xi_1\dots\xi_N)$ as the subset of Λ (see (53)), and with ρ_s as the density, we apply Lemma 3 to conclude that

$$\sum_{\xi\in\mathcal{A}_s(\xi_1\dots,\xi_N)}|\xi_j|^2\geq c_{TF}N_s^{5/3}L^{-2}-CN_s^{4/3}L^{-2}+\frac{c}{\rho_s^{1/3}L^3}(H_s(\xi_1\dots\xi_N))^2,$$

with $H_s(\xi_1 \dots \xi_N)$ as in (55). Summing on s, we obtain

$$\sum_{j=1}^{N} |\xi_j|^2 \geq \sum_{s=1}^{q} (c_{TF} N_s^{5/3} L^{-2} - C N_s^{4/3} L^{-2}) + \sum_{s=1}^{q} \frac{c}{\rho_s^{1/3} L^3} (H_s(\xi_1 \dots \xi_N))^2.$$

Substituting this into (56) and recalling (45), we learn that

$$(1+\delta) c_{TF} \sum_{s=1}^{q} N_s^{5/3} L^{-2} \geq \sum_{s=1}^{q} (c_{TF} N_s^{5/3} L^{-2} - C N_s^{4/3} L^{-2}) + \sum_{s=1}^{q} \frac{c}{\rho_s^{1/3} L^3} \sum_{\xi_1 \dots \xi_N} |A_{\xi_1 \dots \xi_N}|^2 H_s^2(\xi_1 \dots \xi_N)$$

which is equivalent to

$$(57) \qquad \sum_s \frac{c}{\rho_s^{1/3} L^3} \sum_{\xi_1 \dots \xi_N} |A_{\xi_1 \dots \xi_N}|^2 (H_s(\xi_1 \dots \xi_N))^2 \leq C\delta \sum_s N_s^{5/3} L^{-2} + C \sum_s N_s^{4/3} L^{-2}.$$

Since $\rho_s^{1/3} L^3 = \left(\frac{N_s}{L^3}\right)^{1/3} L^3 = N_s^{1/3} L^2$, and since $N_1 + \cdots + N_s = N$, estimate (57) implies

$$(58) \qquad \sum_{\xi_1 \dots \xi_N} |A_{\xi_1 \dots \xi_N}|^2 (H_s(\xi_1 \dots \xi_N))^2 \leq C\delta N^2 + C N^{5/3} \quad \text{for} \quad 1 \leq s \leq q$$

To apply (58) to (55), we use Cauchy-Schwartz:

$$\sum_{\xi_1 \dots \xi_N} |A_{\xi_1 \dots \xi_N}|^2 H_s(\xi_1 \dots \xi_N) \leq \left(\sum_{\xi_1 \dots \xi_N} |A_{\xi_1 \dots \xi_N}|^2 \right)^{1/2} \left(\sum_{\xi_1 \dots \xi_N} |A_{\xi_1 \dots \xi_N}|^2 H^2(\xi_1 \dots \xi_N) \right)^{1/2} \leq CN(\delta + N^{-1/3})^{1/2} \qquad \text{by (45), (58).}$$

Putting this inequality into (55), we get

$$(59) \qquad Av_{\mathfrak{z} \in T} \mu_s(\mathfrak{z}, \alpha) \leq C_{m\varepsilon} \underline{\mathrm{N}}_s^{-m} + \frac{C|Q|}{L^3} \cdot N(\delta + N^{-1/3})^{1/2} \quad \text{for } 1 \leq s \leq q,\ 1 \leq \alpha \leq \underline{\mathrm{N}}_s.$$

We are assuming the N_s all have the same order of magnitude, so $\frac{N}{L^3} \sim \frac{N_s}{L^3} \sim \rho_s$. Hence $N \frac{|Q|}{L^3} \sim \rho_s |Q| \sim \underline{\mathrm{N}}_s$ by (38). Thus, (59) may be rewritten as

$$(60) \qquad Av_{\mathfrak{z} \in T} \mu_s(\mathfrak{z}, \alpha) \leq C_{m\varepsilon} \underline{\mathrm{N}}_s^{-m} + C\underline{\mathrm{N}}_s \cdot (\delta + N^{-1/3})^{1/2} \text{ for } 1 \leq s \leq q,\ 1 \leq \alpha \leq \underline{\mathrm{N}}_s.$$

Estimates (49), (50), (60) give us the desired control over $\sum_{(\alpha_1 \ldots \alpha_N) \notin \mathcal{B}} |C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N}|^2$ for most $\mathfrak{z} \in T$.

We can also use $\mu_s(\mathfrak{z}, \alpha)$ to control the number of electrons in the cube $Q + \mathfrak{z}$. Define

$$\mathcal{N}_{s\mathfrak{z}}(x_1 \ldots x_N) = \sum_{\text{spin}(j)=s} \chi_{Q+\mathfrak{z}}(x_j) = \text{number of particles of spin } s \text{ in } Q + \mathfrak{z}.$$

Lemma 5: *We have the estimates*

$$Av_{\mathfrak{z} \in T} \langle (\underline{N}_s - \mathcal{N}_{s\mathfrak{z}})_+ \Psi, \Psi \rangle \leq C_{m\varepsilon} \underline{N}_s^{-m} + C\underline{N}_s^2 (\delta + N^{-1/3})^{1/2}$$
$$Av_{\mathfrak{z} \in T} \langle (\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s)_+ \Psi, \Psi \rangle \leq C\underline{N}_s^2 (\delta + N^{-1/3})^{1/2} + C_\varepsilon \underline{N}_s^{\frac{8}{9}+3\varepsilon}$$

Proof: Define

$$\mathcal{N}_s^{\text{hi}}(\alpha_1 \ldots \alpha_N) = [\text{Number of } j \text{ with spin}(j) = s \text{ and } \alpha_j > \underline{N}_s]$$
$$\mathcal{N}_s^{\text{med}}(\alpha_1 \ldots \alpha_N) = [\text{Number of } j \text{ with spin}(j) = s \text{ and } 1 \leq \alpha_j \leq \underline{N}_s]$$
$$\mathcal{N}_s^{\text{low}}(\alpha_1 \ldots \alpha_N) = [\text{Number of } j \text{ with spin}(j) = s \text{ and } -\infty < \alpha_j \leq 0].$$

Recall that $\varphi^{\mathfrak{z}}_{\alpha,s}(.)$ is supported in $Q + \mathfrak{z}$ for $\alpha \geq 1$, and in the complement of $Q + \mathfrak{z}$ for $-\infty < \alpha \leq 0$. Therefore,

(60 bis) $$\mathcal{N}_{s\mathfrak{z}}(x_1 \ldots x_N) = \mathcal{N}_s^{\text{hi}}(\alpha_1 \ldots \alpha_N) + \mathcal{N}_s^{\text{med}}(\alpha_1 \ldots \alpha_N) \qquad \text{for}$$

$$(x_1 \ldots x_N) \in \text{supp} \prod_{s=1}^{q} \left(\prod_{\text{spin}(j)=s} \varphi^{\mathfrak{z}}_{\alpha_j s}(x_j) \right).$$

This observation and (42) imply

$$(\underline{N}_s - \mathcal{N}_{s\mathfrak{z}}(x_1 \ldots x_N))_+ \cdot \Psi(x_1 \ldots x_N) =$$
$$\sum_{\alpha_1 \ldots \alpha_N} (\underline{N}_s - \mathcal{N}_s^{\text{hi}}(\alpha_1 \ldots \alpha_N) - \mathcal{N}_s^{\text{med}}(\alpha_1 \ldots \alpha_N))_+ C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N} \prod_{1 \leq s \leq q} \left(\prod_{\text{spin}(j)=s} \varphi^{\mathfrak{z}}_{\alpha_j s}(x_j) \right).$$

Combining this with (42), we get

(61) $$\langle (\underline{N}_s - \mathcal{N}_{s\mathfrak{z}})_+ \Psi, \Psi \rangle = \sum_{\alpha_1 \ldots \alpha_N} (\underline{N}_s - \mathcal{N}_s^{\text{hi}}(\alpha_1 \ldots \alpha_N) - \mathcal{N}_s^{\text{med}}(\alpha_1 \ldots \alpha_N))_+ |C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N}|^2.$$

On the other hand, (48) and (49) show that

$$\mu_s(\mathfrak{z}, \alpha) = \sum_{\alpha_1 \ldots \alpha_N} \chi_{\,\alpha \text{ is not one of the } \alpha_j \text{ with spin}(j)=s} |C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N}|^2,$$

and therefore

$$(62)\qquad \sum_{1\le\alpha\le \underline{N}_s} \mu_s(\mathfrak{z},\alpha) = \sum_{\alpha_1\ldots\alpha_N} |C^{\mathfrak{z}}_{\alpha_1\ldots\alpha_N}|^2\cdot \text{[Number of } \alpha\in\{1\cdots\underline{N}_s\} \text{ not among the } \alpha_j \text{ with spin}(j)=s]$$

$$= \sum_{\alpha_1\ldots\alpha_N} (\underline{N}_s - \mathcal{N}_s^{\mathrm{med}}(\alpha_1\ldots\alpha_N))\cdot|C^{\mathfrak{z}}_{\alpha_1\ldots\alpha_N}|^2.$$

Since $\mathcal{N}_s^{\mathrm{hi}}(\alpha_1\ldots\alpha_N)\ge 0$ and $\underline{N}_s \ge \mathcal{N}_s^{\mathrm{med}}(\alpha_1\ldots\alpha_N)\ge 0$, for $C_{\alpha_1\ldots\alpha_N}\neq 0$, we have

$$(\underline{N}_s - \mathcal{N}_s^{\mathrm{hi}}(\alpha_1\ldots\alpha_N) - \mathcal{N}_s^{\mathrm{med}}(\alpha_1\ldots\alpha_N))_+ \le (\underline{N}_s - \mathcal{N}_s^{\mathrm{med}}(\alpha_1\ldots\alpha_N))_+ = (\underline{N}_s - \mathcal{N}_s^{\mathrm{med}}(\alpha_1\ldots\alpha_N)).$$

Hence, comparing (61) with (62), we learn that

$$\langle(\underline{N}_s - \mathcal{N}_{s\mathfrak{z}})_+\Psi,\Psi\rangle \le \sum_{1\le\alpha\le\underline{N}_s} \mu_s(\mathfrak{z},\alpha).$$

Therefore, (60) shows that

$$(63)\qquad Av_{\mathfrak{z}\in T}\langle(\underline{N}_s - \mathcal{N}_{s\mathfrak{z}})_+\Psi,\Psi\rangle \le C_{m\varepsilon}\underline{N}_s^{-m} + C\underline{N}_s^2\cdot(\delta+N^{-1/3})^{1/2},$$

which is the first conclusion of Lemma 5.

The second conclusion of Lemma 5 is an easy consequence of the first. In fact, we have

$$Av_{\mathfrak{z}\in T}\langle\mathcal{N}_{s\mathfrak{z}}\Psi,\Psi\rangle =$$
$$L^{-3}\int_{\mathfrak{z}\in T}\int_{T^N}\sum_{\mathrm{spin}(j)=s}\chi_{Q+\mathfrak{z}}(x_j)|\Psi(x_1\ldots x_N)|^2dx_1\ldots dx_N d\mathfrak{z} =$$
$$\sum_{\mathrm{spin}(j)=s}\int_{T^N}\left\{L^{-3}\int_{\mathfrak{z}\in T}\chi_{Q+\mathfrak{z}}(x_j)d\mathfrak{z}\right\}|\Psi(x_1\ldots x_N)|^2dx_1\ldots dx_N =$$
$$\frac{|Q|}{L^3}\sum_{\mathrm{spin}(j)=s}\int_{T^N}|\Psi(x_1\ldots x_N)|^2dx_1\ldots dx_N = \frac{|Q|}{L^3}N_s = \rho_s|Q|,$$

and so

$$(64)\qquad Av_{\mathfrak{z}\in T}\langle(\underline{N}_s - \mathcal{N}_{s\mathfrak{z}})\Psi,\Psi\rangle = \underline{N}_s - \rho_s|Q|.$$

Since

$$(\underline{N}_s - \mathcal{N}_{s\mathfrak{z}}) = (\underline{N}_s - \mathcal{N}_{s\mathfrak{z}})_+ - (\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s)_+,$$

we have

$$Av_{\mathfrak{z}\in T}\langle(\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s)_+\Psi,\Psi\rangle = Av_{\mathfrak{z}\in T}\langle(\underline{N}_s - \mathcal{N}_{s\mathfrak{z}})_+\Psi,\Psi\rangle$$
$$-Av_{\mathfrak{z}\in T}\langle(\underline{N}_s - \mathcal{N}_{s\mathfrak{z}})\Psi,\Psi\rangle \le C_{m\varepsilon}\underline{N}_s^{-m} + C\underline{N}_s^2\cdot(\delta+N^{-1/3})^{1/2} + |\underline{N}_s - \rho_s|Q|| \text{ by (63), (64).}$$

Applying (38), we obtain

$$Av_{\mathfrak{z}\in T}\langle(\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s)_+\Psi,\Psi\rangle \le C_{m\varepsilon}\underline{N}_s^{-m} + C\underline{N}_s^2\cdot(\delta+N^{-1/3})^{1/2} + C_\varepsilon\underline{N}_s^{\frac{8}{9}+3\varepsilon},$$

which is equivalent to the second conclusion of Lemma 5. □

The following result gives additional control over $\mathcal{N}_{s\mathfrak{z}}$.

Lemma 6: $Av_{\mathfrak{z}\in T}\langle \mathcal{N}_{s\mathfrak{z}}^{5/3}(diam\, Q)^{-2}\Psi,\Psi\rangle \le C\rho^{5/3}|Q|$, *with* $\rho = \frac{N}{L^3}$.

Proof: Let $Q' = Q + \mathfrak{z}$ for fixed $\mathfrak{z}$, and let $\Phi(x_1 \dots x_n)$ be an antisymmetric function on $(Q')^n$, not necessarily of norm 1. Then

$$\int_{Q'^n} \sum_{j=1}^{n} |\nabla_{x_j}\Phi(x_1\dots x_n)|^2 dx_1\dots dx_n \ge cn^{5/3}(\mathrm{diam}\, Q)^{-2}\chi_{n\ge 2} \cdot \int_{Q'^n} |\Phi(x_1\dots x_n)|^2 dx_1\dots dx_n, \tag{65}$$

as follows from expanding Φ in terms of the eigenfunctions of the Laplacian on Q, with Neumann boundary conditions.

Next, suppose Q' and s are fixed, and the set of $j \in \{1\dots N\}$ of spin s is partitioned into J_{in} and J_{out}. Let J_{other} denote the set of j with spin different from s. For fixed $(x_j)_{j\in J_{\text{out}}\cup J_{\text{other}}}$, we regard $\Psi(x_1\dots x_N)$ as a function of $(x_j)_{j\in J_{\text{in}}}$. Apply (65), and then integrate over the set of all $(x_j)_{j\in J_{\text{out}}\cup J_{\text{other}}}$ with $x_j \notin Q'$ for $j \in J_{\text{out}}$. The result is as follows.

(66)
$$\int_{T^N} \prod_{j\in J_{\text{in}}} \chi_{Q'}(x_j)\cdot \prod_{j\in J_{\text{out}}} \chi_{Q'^c}(x_j)\cdot \sum_{k\in J_{\text{in}}} |\nabla_{x_k}\Psi(x_1\dots x_N)|^2 dx_1\dots dx_N$$
$$\ge c\int_{T^N} n^{5/3}(\mathrm{diam}\, Q)^{-2}\chi_{n\ge 2}\prod_{j\in J_{\text{in}}}\chi_{Q'}(x_j)\prod_{j\in J_{\text{out}}}\chi_{Q'^c}(x_j)|\Psi(x_1\dots x_N)|^2 dx_1\dots dx_N,$$

where Q'^c = complement of Q', and n is the number of j in J_{in}. (If $n = 0$, then (65) does not apply, but (66) obviously holds anyway, since both sides are zero.)

In the support of the integrand on the right of (66), $n = \mathcal{N}_{s\mathfrak{z}}(x_1\dots x_N)$. Hence, (66) may be rewritten as

$$\sum_{\text{spin}(k)=s}\int_{T^N}\left(\prod_{j\in J_{\text{in}}}\chi_{Q'}(x_j)\right)\cdot\left(\prod_{j\in J_{\text{out}}}\chi_{Q'^c}(x_j)\right) \cdot \chi_{k\in J_{\text{in}}}|\nabla_{x_k}\Psi(x_1\dots x_N)|^2 dx_1\dots dx_N$$
$$\ge c\int_{T^N}\left(\prod_{j\in J_{\text{in}}}\chi_{Q'}(x_j)\right)\cdot\left(\prod_{j\in J_{\text{out}}}\chi_{Q'^c}(x_j)\right)\cdot \mathcal{N}_{s\mathfrak{z}}^{5/3}(x_1\dots x_N) \cdot \chi_{\mathcal{N}_{s\mathfrak{z}}(x_1\dots x_N)\ge 2}(\mathrm{diam}\, Q)^{-2}\cdot|\Psi(x_1\dots x_N)|^2 dx_1\dots dx_N$$

Summing this estimate over all possible partitions of $\{j \mid \operatorname{spin}(j) = s\}$ into $J_{\text{in}} \cup J_{\text{out}}$, we obtain

$$\sum_{\operatorname{spin}(k)=s} \int_{T^N} \chi_{Q+\mathfrak{z}}(x_k) \cdot |\nabla_{x_k}\Psi(x_1 \dots x_N)|^2 dx_1 \dots dx_N \geq c(\operatorname{diam} Q)^{-2} \langle \mathcal{N}_{s\mathfrak{z}}^{5/3} \chi_{\mathcal{N}_{s\mathfrak{z}} \geq 2} \Psi, \Psi \rangle$$

Integrating over $\mathfrak{z} \in T$, we then get

$$\begin{aligned} &Av_{\mathfrak{z} \in T} \langle c\mathcal{N}_{s\mathfrak{z}}^{5/3} \chi_{\mathcal{N}_{s\mathfrak{z}} \geq 2} (\operatorname{diam} Q)^{-2} \Psi, \Psi \rangle \leq \\ &\quad L^{-3} \sum_{\operatorname{spin}(k)=s} \int_{\mathfrak{z} \in T} \int_{T^N} \chi_{Q+\mathfrak{z}}(x_k) |\nabla_{x_k}\Psi(x_1 \dots x_N)|^2 dx_1 \dots dx_N d\mathfrak{z} \\ &\quad = \sum_{\operatorname{spin}(k)=s} \int_{T^N} \left\{ L^{-3} \int_{\mathfrak{z} \in T} \chi_{Q+\mathfrak{z}}(x_k) d\mathfrak{z} \right\} \cdot |\nabla_{x_k}\Psi(x_1 \dots x_N)|^2 dx_1 \dots dx_N \\ &\quad = \frac{|Q|}{L^3} \sum_{\operatorname{spin}(k)=s} \int_{T^N} |\nabla_{x_k}\Psi(x_1 \dots x_N)|^2 dx_1 \dots dx_N \leq \frac{|Q|}{L^3} \|\nabla\Psi\|^2. \end{aligned}$$

A crude application of the basic kinetic energy assumption (4) yields $\|\nabla\Psi\|^2 \leq C\rho^{5/3}L^3$, so that (67) implies

$$Av_{\mathfrak{z} \in T} \left\langle c\mathcal{N}_{s\mathfrak{z}}^{5/3} \chi_{\mathcal{N}_{s\mathfrak{z}} \geq 2} (\operatorname{diam} Q)^{-2} \Psi, \Psi \right\rangle \leq C\rho^{5/3}|Q|. \tag{68}$$

Trivially, we have also

$$\begin{aligned} Av_{\mathfrak{z} \in T} \left\langle c\mathcal{N}_{s\mathfrak{z}}^{5/3} \chi_{\mathcal{N}_{s\mathfrak{z}} \leq 1} (\operatorname{diam} Q)^{-2} \Psi, \Psi \right\rangle &\leq (\operatorname{diam} Q)^{-2} \\ &= c\rho^{5/3}|Q| \cdot (\rho^{-5/3}|Q|^{-5/3}) \leq C\rho^{5/3}|Q|, \text{ since } \rho|Q| \geq 1. \end{aligned} \tag{69}$$

Adding (68) and (69), we obtain the conclusion of Lemma 6. □

For each $\mathfrak{z} \in T$, we decompose the wave function Ψ as follows.

$$\Psi = \Phi^{\mathfrak{z}}_{\text{main}} + \Phi^{\mathfrak{z}}_{\text{error}}, \quad \text{with} \tag{70}$$

$$\Phi^{\mathfrak{z}}_{\text{main}} = \sum_{(\alpha_1 \dots \alpha_N) \in \mathcal{B}} C^{\mathfrak{z}}_{\alpha_1 \dots \alpha_N} \prod_{s=1}^{q} \left(\prod_{\operatorname{spin}(j)=s} \varphi^{\mathfrak{z}}_{\alpha_j s}(x_j) \right) \tag{71}$$

$$\Phi^{\mathfrak{z}}_{\text{error}} = \sum_{(\alpha_1 \dots \alpha_N) \notin \mathcal{B}} C^{\mathfrak{z}}_{\alpha_1 \dots \alpha_N} \prod_{s=1}^{q} \left(\prod_{\operatorname{spin}(j)=s} \varphi^{\mathfrak{z}}_{\alpha_j s}(x_j) \right). \tag{72}$$

Here, $\mathcal{B}$ is given by (48), (50); and $C^{\mathfrak{z}}_{\alpha_1\ldots\alpha_N}$ is given by (42). From (49), (50), (60) we see that $\Phi^{\mathfrak{z}}_{\text{error}}$ has small norm for most $\mathfrak{z} \in T$. More precisely, we have

$$\begin{aligned}\|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 &= \sum_{(\alpha_1\ldots\alpha_N)\notin\mathcal{B}} |C^{\mathfrak{z}}_{\alpha_1\ldots\alpha_N}|^2 \\ &\leq \sum_{s=1}^{q} \sum_{1\leq\alpha\leq\underline{N}_s} \left(\sum_{(\alpha_1\ldots\alpha_N)\notin\mathcal{B}_{\alpha,s}} |C^{\mathfrak{z}}_{\alpha_1\ldots\alpha_N}|^2 \right) \text{ (by (50))} \\ &= \sum_{s=1}^{q} \sum_{1\leq\alpha\leq\underline{N}_s} \mu_s(\mathfrak{z},\alpha) \text{ (by (49))},\end{aligned}$$

and therefore

$$Av_{\mathfrak{z}\in T}(\|\Phi^{\mathfrak{z}}_{\text{error}}\|^2) \leq C_{m\varepsilon}\underline{N}^{-m} + C\underline{N}^2 \cdot (\delta + N^{-1/3})^{1/2} \text{ (by (60))}. \tag{73}$$

Here, $\underline{N} = \rho|Q| \sim \underline{N}_1 + \cdots + \underline{N}_s$.

For additional control over $\Phi^{\mathfrak{z}}_{\text{error}}$ and $\Phi^{\mathfrak{z}}_{\text{main}}$, we recall the definitions of $\mathcal{N}^{\text{hi}}_s$, $\mathcal{N}^{\text{med}}_s$, $\mathcal{N}^{\text{low}}_s$ in the proof of Lemma 5. Equation (60 bis) shows that

$$\begin{aligned}\mathcal{N}^{5/3}_{s\mathfrak{z}}\Phi^{\mathfrak{z}}_{\text{error}} &= \sum_{(\alpha_1\ldots\alpha_N)\notin\mathcal{B}} [\mathcal{N}^{\text{hi}}_s(\alpha\ldots\alpha_N) \\ &\qquad + \mathcal{N}^{\text{med}}_s(\alpha_1\ldots\alpha_N)]^{5/3} C^{\mathfrak{z}}_{\alpha_1\ldots\alpha_N} \prod_{s=1}^{q}\left(\prod_{\text{spin } j=s} \varphi^{\mathfrak{z}}_{\alpha_j s}(x_j)\right) \\ \mathcal{N}^{5/3}_{s\mathfrak{z}}\Phi^{\mathfrak{z}}_{\text{main}} &= \sum_{(\alpha_1\ldots\alpha_N)\in\mathcal{B}} [\mathcal{N}^{\text{hi}}_s(\alpha_1\ldots\alpha_N) \\ &\qquad + \mathcal{N}^{\text{med}}_s(\alpha_1\ldots\alpha_N)]^{5/3} C^{\mathfrak{z}}_{\alpha_1\ldots\alpha_N} \prod_{s=1}^{q}\left(\prod_{\text{spin } j=s} \varphi^{\mathfrak{z}}_{\alpha_j s}(x_j)\right) \\ \mathcal{N}^{5/3}_{s\mathfrak{z}}\Psi &= \sum_{\alpha_1\ldots\alpha_N} [\mathcal{N}^{\text{hi}}_s(\alpha_1\ldots\alpha_N) \\ &\qquad + \mathcal{N}^{\text{med}}_s(\alpha_1\ldots\alpha_N)]^{5/3} C^{\mathfrak{z}}_{\alpha_1\ldots\alpha_N} \prod_{s=1}^{q}\left(\prod_{\text{spin } j=s} \varphi^{\mathfrak{z}}_{\alpha_j s}(x_j)\right).\end{aligned}$$

Combining these equations with (42), (71), (72), we obtain

$$\begin{aligned}&\langle \mathcal{N}^{5/3}_{s\mathfrak{z}}\Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}}\rangle + \langle \mathcal{N}^{5/3}_{s\mathfrak{z}}\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}}\rangle \\ &\qquad = \langle \mathcal{N}^{5/3}_{s\mathfrak{z}}\Psi, \Psi\rangle.\end{aligned}$$

Hence, by lemma 6, we get

$$Av_{\mathfrak{z}\in T}\langle \mathcal{N}_{s\mathfrak{z}}^{5/3}\Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}}\rangle \le C\underline{N}^{5/3} \quad \text{and} \tag{74}$$

$$Av_{\mathfrak{z}\in T}\langle \mathcal{N}_{s\mathfrak{z}}^{5/3}\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}}\rangle \le C\underline{N}^{5/3}. \tag{75}$$

Similarly,

$$\langle (\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s)_+\Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}}\rangle + \langle (\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s)_+\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}}\rangle = \langle (\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s)_+\Psi, \Psi\rangle,$$

so that Lemma 5 yields

$$Av_{\mathfrak{z}\in T}\langle (\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s)_+\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}}\rangle \le C\underline{N}^2(\delta + N^{-1/3})^{1/2} + C_\varepsilon \underline{N}^{\frac{8}{9}+3\varepsilon}. \tag{76}$$

From (42), (71), (72) we see that

$$\|\Phi^{\mathfrak{z}}_{\text{main}}\|^2 + \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 = \|\Psi\|^2 = 1 \quad \text{for each } \mathfrak{z}\in T. \tag{77}$$

Finally, $\Phi^{\mathfrak{z}}_{\text{main}}(x_1 \dots x_N)$ and $\Phi^{\mathfrak{z}}_{\text{error}}(x_1 \dots x_N)$ are antisymmetric under spin-preserving permutations of $(x_1 \dots x_N)$.

Equations (73)–(77) are our basic estimates for $\Phi^{\mathfrak{z}}_{\text{main}}$, $\Phi^{\mathfrak{z}}_{\text{error}}$.

The next step is to introduce the antisymmetrized product $\Phi^{\mathfrak{z}}_{\text{basic}}$ of the $\varphi^{\mathfrak{z}}_{\alpha,s}$ $(1 \le s \le q,\ 1 \le \alpha \le \underline{N}_s)$, and then express $\Phi^{\mathfrak{z}}_{\text{main}}$ as an antisymmetrized product of $\Phi^{\mathfrak{z}}_{\text{basic}}$ with an auxiliary wave function $\Phi^{\mathfrak{z}}_{\text{extra}}$. Fix once and for all a subset $J \subset \{1 \dots N\}$ with the property that $\underline{N}_s$ of the indices in J have spin s $(1 \le s \le q)$. (We can find a J, since the total number of indices $1 \dots N$ with spin s is $N_s = \rho_s L^3 \gg \rho_s|Q| \sim \underline{N}_s$.) We write J^c for the complement of J in $\{1 \dots N\}$. Also, we fix once and for all a sequence $(\widetilde{\beta}_j)_{j\in J}$ with the property that given$1 \le s \le q$ and $1 \le \alpha \le \underline{N}_s$, there is one and only one $j \in J$ with $\text{spin}(j) = s$ and $\widetilde{\beta}_j = \alpha$. Write x_J for $(x_j)_{j\in J}$ and x_{J^c} for $(x_j)_{j\in J^c}$. The many-particle wave function $\Phi^{\mathfrak{z}}_{\text{basic}}$ is defined by

$$\Phi^{\mathfrak{z}}_{\text{basic}}(x_J) = \prod_{s=1}^{q}(\underline{N}_s!)^{-1/2}\sum_\sigma (\operatorname{sgn}\sigma)\prod_{s=1}^{q}\left(\prod_{\substack{j\in J\\ \text{spin}(j)=s}} \varphi^{\mathfrak{z}}_{\widetilde{\beta}_{\sigma j},s}(x_j)\right), \tag{78}$$

where σ runs over all spin-preserving permutations of J. Note that$\Phi^{\mathfrak{z}}_{\text{basic}}(x_J)$ has norm 1 and is antisymmetric under spin-preserving permutations of the $(x_j)_{j\in J}$.

Next suppose $\Phi_1(x_J)$ and $\Phi_2(x_{J^c})$ are antisymmetric under spin-preserving permutations. Then their antisymmetrized product is defined as

$$(\Phi_1 \wedge \Phi_2)(x_1 \dots x_N) = c(J)\cdot \sum_\sigma (\operatorname{sgn}\sigma)\Phi_1((x_{\sigma j})_{j\in J})\Phi_2((x_{\sigma j})_{j\in J^c}) \tag{79}$$

with σ running over spin-preserving permutations of $\{1 \dots N\}$ and

$$c(J) = \prod_{s=1}^{q}\{\underline{N}_s!(N_s - \underline{N}_s)!N_s!\}^{-1/2}. \tag{80}$$

Thus, $\Phi_1 \wedge \Phi_2$ is antisymmetric under spin-preserving permutations.

Lemma 7: *For each* $\mathfrak{z} \in T$, *we can find a wave function* $\Phi^{\mathfrak{z}}_{\text{extra}}(x_{J^c})$, *antisymmetric under spin-preserving permutations, and satisfying the equation*

$$\Phi^{\mathfrak{z}}_{\text{main}} = \Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}. \tag{81}$$

We can express $\Phi^{\mathfrak{z}}_{\text{extra}}$ *as a series*

$$\Phi^{\mathfrak{z}}_{\text{extra}}(x_{J^c}) = \sum_{(\beta_j)_{j \in J^c}} F((\beta_j)_{j \in J^c}) \cdot \prod_{s=1}^{q} \left(\prod_{\substack{j \in J^c \\ \text{spin}\, j = s}} \varphi^{\mathfrak{z}}_{\beta_j, s}(x_j) \right) \tag{82}$$

with coefficients $F((\beta_j)_{j \in J^c})$ *satisfying*

$$F((\beta_j)_{j \in J^c}) = 0 \tag{83}$$

if for any $j \in J^c$ *with spin*$(j) = s$ *we have* $1 \le \beta_j \le \underline{N}_s$.

Proof: By definition of $\Phi^{\mathfrak{z}}_{\text{basic}}$, we can write

$$\Phi^{\mathfrak{z}}_{\text{basic}}(x_J) = \sum_{(\beta_j)_{j \in J}} E((\beta_j)_{j \in J}) \prod_{s=1}^{q} \left(\prod_{\substack{j \in J \\ \text{spin}(j) = s}} \varphi^{\mathfrak{z}}_{\beta_j, s}(x_j) \right) \tag{84}$$

with coefficients $E((\beta_j)_{j \in J})$ satisfying:

$$E((\beta_j)_{j \in J}) = 0 \quad \text{unless there is a spin-preserving permutation } \tau \text{ of } J \text{ for which } \beta_j = \widetilde{\beta}_{\tau j} \text{ (all } j \in J). \tag{85}$$

In particular, $E((\widetilde{\beta}_j)_{j \in J})$ is a non-zero constant.

We take $\Phi^{\mathfrak{z}}_{\text{extra}}$ given by (82), with coefficients $F((\beta_j)_{j \in J})$ antisymmetric under spin-preserving permutations. Then from (82) and (84) we compute the antisymmetrized product $\Phi^{\mathfrak{z}}_{basic} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}$, namely

$$\begin{aligned} &\left(\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}\right)(x_1 \dots x_N) = \\ &c(J) \sum_{\beta_1 \dots \beta_N} \sum_{\sigma} (\operatorname{sgn} \sigma) E((\beta_j)_{j \in J}) F((\beta_j)_{j \in J^c}) \prod_{s=1}^{q} \left(\prod_{\text{spin}\, j = s} \varphi^{\mathfrak{z}}_{\beta_j s}(x_{\sigma j}) \right) \end{aligned} \tag{86}$$

with σ running over spin-preserving permutations of $\{1 \dots N\}$.

Let us expand $\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}$ in a Fourier series

$$\left(\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}\right)(x_1 \dots x_N) = \sum_{\alpha_1 \dots \alpha_N} G(\alpha_1 \dots \alpha_N) \prod_{s=1}^{q} \left(\sum_{\text{spin}\, j = s} \varphi^{\mathfrak{z}}_{\alpha_j, s}(x_j) \right) \tag{87}$$

We will compute $G(\alpha_1 \ldots \alpha_N)$ in case the α_j ($j \in \{1 \ldots N\}$ of fixed spin) are all distinct, and $\alpha_j = \widetilde{\beta}_j$ for all $j \in J$. Immediately from (86), (87) we get

$$(88) \qquad G(\alpha_1 \ldots \alpha_N) = c(J) \sum_{\beta_1 \ldots \beta_N} \sum_{\sigma} (\operatorname{sgn} \sigma) E((\beta_j)_{j \in J}) F((\beta_j)_{j \in J^c}) \cdot \int_{T^N} \prod_{s=1}^{q} \left(\prod_{\text{spin } j = s} \varphi^{\mathfrak{z}}_{\beta_j, s}(x_{\sigma j}) \right) \cdot \prod_{s'=1}^{q} \left(\prod_{\text{spin } j' = s'} \overline{\varphi^{\mathfrak{z}}_{\alpha_{j'}, s'}(x_{j'})} \right) dx_1 \ldots dx_N$$

We use the orthonormality of the $\varphi^{\mathfrak{z}}_{\alpha,s}$ for fixed $\mathfrak{z}$, s. The integral in (88) is zero unless $\beta_j = \alpha_{\sigma j}$ for all j, in which case the integral is 1. Therefore, (88) may be rewritten as

$$(89) \qquad G(\alpha_1 \ldots \alpha_N) = c(J) \sum_{\sigma} (\operatorname{sgn} \sigma) E((\alpha_{\sigma j})_{j \in J}) F((\alpha_{\sigma j})_{j \in J^c}),$$

with σ running over spin-preserving permutations of $\{1 \ldots N\}$.

For a non-zero term in (89) we must have $\alpha_{\sigma j} = \widetilde{\beta}_{\tau j}$ for all $j \in J$, with τ a spin-preserving permutation of J. For all $j \in J$ we have $\alpha_j = \widetilde{\beta}_j$, and therefore a non-zero term in (89) has $\alpha_{\sigma j} = \alpha_{\tau j}$ for $j \in J$.

Since α_j for $j \in \{1 \ldots N\}$ of fixed spin are all distinct, this shows that $\sigma j = \tau j$ for $j \in J$. In other words the only σ that give rise to non-zero terms in (89) are those that carry J into itself, and hence also carry J^c into itself. For such σ we have

$$(\operatorname{sgn} \sigma) E((\alpha_{\sigma j})_{j \in J}) \cdot F((\alpha_{\sigma j})_{j \in J^c}) = E((\alpha_j)_{j \in J}) \cdot F((\alpha_j)_{j \in J^c})$$

by the antisymmetry properties of $E(\,\cdot\,), F(\,\cdot\,)$. Therefore, (89) implies

$$(90) \qquad G(\alpha_1 \ldots \alpha_N) = c'(J) E((\alpha_j)_{j \in J}) F((\alpha_j)_{j \in J^c}),$$

with $c'(J) = c(J) \cdot$ (Number of possible spin-preserving σ which preserve J, J^c). Since $(\alpha_j)_{j \in J} = (\widetilde{\beta}_j)_{j \in J}$ and $E((\widetilde{\beta}_j)_{j \in J})$ is a non-zero constant, (90) shows that

$$(91) \qquad G(\alpha_1 \ldots \alpha_N) = c''(J) \cdot F((\alpha_j)_{j \in J^c}) \quad \text{provided the } \alpha_j \text{ of fixed spin are all distinct and } \alpha_j = \widetilde{\beta}_j \text{ for } j \in J.$$

Equation (91) shows that we may pick the $F((\alpha_j)_{j \in J^c})$ to satisfy the antisymmetry under spin-preserving permutations, and

$$(92) \qquad G(\alpha_1 \ldots \alpha_N) = C^{\mathfrak{z}}_{\alpha_1 \ldots \alpha_N} \quad \text{whenever the } \alpha_j \text{ of fixed spin are all distinct, and } \alpha_j = \widetilde{\beta}_j \text{ for } j \in J.$$

This specifies uniquely $F((\alpha_j)_{j\in J^c})$ when none of the α_j $(j \in J^c, \mathrm{spin}\, j = s)$ satisfies $1 \le \alpha_j \le \underset{\sim}{N}_s$. We may simply set

$$F((\alpha_j)_{j\in J^c}) = 0 \quad \text{otherwise.}$$

Thus, (82), (83) hold, and Φ^{3}_{extra} has the required antisymmetry.

Moreover, (71), (87), (92) imply

$$(93) \qquad \left(\Phi^{3}_{\text{main}} - \Phi^{3}_{\text{basic}} \wedge \Phi^{3}_{\text{extra}}\right)(x_1 \dots x_N) = \sum_{\alpha_1\dots\alpha_N} H_{\alpha_1\dots\alpha_N} \prod_{s=1}^{q} \left(\prod_{\mathrm{spin}(j)=s} \varphi^{3}_{\alpha_j,s}(x_j) \right)$$

with

$$(94) \qquad H_{\alpha_1\dots\alpha_N} = 0 \quad \text{whenever} \quad \alpha_j = \widetilde{\beta}_j \quad \text{for} \quad j \in J.$$

Recall that $\mathcal{B}$ consists of all $(\alpha_1 \dots \alpha_N)$ for which we can solve $\alpha_j = \alpha$ with $\mathrm{spin}(j) = s$, whenever $1 \le s \le q$ and $1 \le \alpha \le \underset{\sim}{N}_s$. Also, recall that the $\widetilde{\beta}_j$ with $j \in J$ of spin s are precisely $1, \dots, \underset{\sim}{N}_s$. So, given any $(\alpha_1 \dots \alpha_N) \in \mathcal{B}$, we can find a spin-preserving permutation σ of $\{1 \dots N\}$ so that $\alpha_{\sigma j} = \widetilde{\beta}_j$ for $j \in J$. Equation (94) then shows that $H_{\alpha_{\sigma 1}\dots\alpha_{\sigma N}} = 0$. The antisymmetry properties of $(H_{\alpha_1\dots\alpha_N})$ that follow from (93) then imply $H_{\alpha_1\dots\alpha_N} = 0$. Thus, we have shown that

$$(95) \qquad H_{\alpha_1\dots\alpha_N} = 0 \quad \text{for all} \quad (\alpha_1 \dots \alpha_N) \in \mathcal{B}.$$

From (85), (86) we see that $\left(\Phi^{3}_{\text{basic}} \wedge \Phi^{3}_{\text{extra}}\right)(x_1 \dots x_N)$ is a linear combination of terms

$$\prod_{s=1}^{q} \left(\prod_{\mathrm{spin}\, j=s} \varphi^{3}_{\alpha_j,s}(x_j) \right) \quad \text{with} \quad (\alpha_1 \dots \alpha_N) \in \mathcal{B}.$$

By definition (71), the same can be said of Φ^{3}_{main}, hence also of $(\Phi^{3}_{\text{main}} - \Phi^{3}_{\text{basic}} \wedge \Phi^{3}_{\text{extra}})$. So (93) shows that

$$H_{\alpha_1\dots\alpha_N} = 0 \quad \text{for all} \quad (\alpha_1 \dots \alpha_N) \notin \mathcal{B}.$$

This and (95) show that all the $H_{\alpha_1\dots\alpha_N} = 0$, so $\Phi^{3}_{\text{main}} - \Phi^{3}_{\text{basic}} \wedge \Phi^{3}_{\text{extra}} = 0$ by (93).

Thus, (81), (82), (83) all hold. The proof of Lemma 7 is complete. $\square$

Next, we note an important orthogonality relation between Φ^{3}_{basic} and Φ^{3}_{extra}.

Definition: Suppose $\Phi_1((x_j)_{j\in J})$ and $\Phi_2((x_j)_{j\in J^c})$ are antisymmetric under spin-preserving permutations, and that Φ_1 is continuous. If $j_1 \in J$, then we write $\Phi_1(x_{j_1}; (x_j)_{j\in J\smallsetminus\{j_1\}})$ for $\Phi_1((x_j)_{j\in J})$. Similarly, if $j_2 \in J^c$ then we write $\Phi_2(x_{j_2}; (x_j)_{j\in J^c\smallsetminus\{j_2\}})$ for $\Phi_2((x_j)_{j\in J^c})$. The wave functions Φ_1 and Φ_2 are called *strongly orthogonal* if for every $j_1 \in J$ and $j_2 \in J^c$ with $\text{spin}(j_1) = \text{spin}(j_2)$, the following holds: Given $(x_j)_{j\in J^c\smallsetminus\{j_2\}}$ outside a set of measure zero, we have

$$\int_T \Phi_1(x; (x_j)_{j\in J\smallsetminus\{j_1\}})\overline{\Phi_2(x; (x_j)_{j\in J^c\smallsetminus\{j_2\}})}dx = 0 \quad (96)$$

$$\text{for all} \quad (x_j)_{j\in J\smallsetminus\{j_1\}}.$$

In particular, $\Phi^{\mathfrak{z}}_{\text{basic}}$ and $\Phi^{\mathfrak{z}}_{\text{extra}}$ are strongly orthogonal. To see this, note that for $(x_j)_{j\in J\smallsetminus\{j_1\}}$ fixed, the function $x_{j_1} \mapsto \Phi^{\mathfrak{z}}_{\text{basic}}$ belongs to the span of the $\varphi^{\mathfrak{z}}_{\alpha s}$ with $s = \text{spin}(j_1)$ and $1 \le \alpha \le \underset{\sim}{N}_s$. On the other hand, for fixed $(x_j)_{j\in J^c\smallsetminus\{j_2\}}$, the function $x_{j_2} \mapsto \Phi^{\mathfrak{z}}_{\text{extra}}$ belongs to the span of the $\varphi^{\mathfrak{z}}_{\alpha s}$ with $s = \text{spin}(j_2)$ and $\alpha \notin \{1 \dots \underset{\sim}{N}_s\}$, by virtue of (82) and (83). Hence, (96) follows from the orthogonality of the $\varphi^{\mathfrak{z}}_{\alpha s}$ for fixed $\mathfrak{z}$, s.

We set down some general results on antisymmetrized products of strongly orthogonal wave functions, and then return later to the particular case of $\Phi^{\mathfrak{z}}_{\text{basic}}$ and $\Phi^{\mathfrak{z}}_{\text{extra}}$.

Strong orthogonality simplifies calculations for $\Phi_1 \wedge \Phi_2$, because of the following result.

Lemma 8: *Suppose $\Phi_1((x_j)_{j\in J})$ and $\Phi_2((x_j)_{j\in J^c})$ are strongly orthogonal. Let σ be a spin-preserving permutation of $\{1 \dots N\}$, and suppose $\sigma j_0 = j_1$, with one of j_0, j_1 belonging to J and the other to J^c. Let $F(x_1 \dots x_N)$ be a function on T^N that does not depend on x_{j_1}. Then*

$$\int_{T^N} F(x_1 \dots x_N)\Phi_1((x_j)_{j\in J})\Phi_2((x_j)_{j\in J^c})\bar{\Phi}_1((x_{\sigma j})_{j\in J})\bar{\Phi}_2((x_{\sigma j})_{j\in J^c})dx_1 \dots dx_N = 0.$$

Proof: Say $j_0 \in J$ and $j_1 \in J^c$. Then our integral may be written as

$$\int_{T^{N-1}} F(x_1 \dots x_N)\Phi_1((x_j)_{j\in J})\bar{\Phi}_2((x_{\sigma j})_{j\in J^c})\left[\int_T \Phi_2((x_j)_{j\in J^c})\bar{\Phi}_1((x_{\sigma j})_{j\in J})dx_{j_1}\right]\prod_{i\neq j_1} dx_i,$$

and the inner integral is zero, by strong orthogonality.

Similarly, if $j_0 \in J^c$ and $j_1 \in J$, then our integral may be written as

$$\int_{T^{N-1}} F(x_1 \dots x_N)\Phi_2((x_j)_{j\in J^c})\bar{\Phi}_1((x_{\sigma j})_{j\in J})\left[\int_T \Phi_1((x_j)_{j\in J})\bar{\Phi}_2((x_{\sigma j})_{j\in J^c})dx_{j_1}\right]\prod_{i\neq j_1} dx_i.$$

Again, the inner integral is zero, by strong orthogonality. □

As our first application of Lemma 8, we compute the norm of $\Phi_1 \wedge \Phi_2$.

Lemma 9: *If $\Phi_1((x_j)_{j\in J})$ and $\Phi_2((x_j)_{j\in J^c})$ are strongly orthogonal and antisymmetric under spin-preserving permutations, then $\|\Phi_1 \wedge \Phi_2\| = \|\Phi_1\| \cdot \|\Phi_2\|$.*

Proof: By definition of $\Phi_1 \wedge \Phi_2$ we have

$$\|\Phi_1 \wedge \Phi_2\|^2 = [c(J)]^2 \sum_{\sigma,\pi} (\operatorname{sgn}\sigma)(\operatorname{sgn}\pi) \int_{T^N} \Phi_1((x_{\sigma j})_{j\in J})\Phi_2((x_{\sigma j})_{j\in J^c})\bar{\Phi}_1((x_{\pi j})_{j\in J}) \cdot \bar{\Phi}_2((x_{\pi j})_{j\in J^c}) dx_1 \ldots x_N,$$

where σ, π run over spin-preserving permutations of $\{1 \ldots N\}$.

Set $\tilde{x}_j = x_{\sigma j}$ and $\tau = \sigma^{-1}\pi$, so that $x_{\pi j} = x_{\sigma\tau j} = \tilde{x}_{\tau j}$. Thus,

$$\|\Phi_1 \wedge \Phi_2\|^2 = [c(J)]^2 \sum_{\sigma\tau} (\operatorname{sgn}\tau) \int_{T^N} \Phi_1((\tilde{x}_j)_{j\in J})\Phi_2((\tilde{x}_j)_{j\in J^c})\bar{\Phi}_1((\tilde{x}_{\tau j})_{j\in J}) \bar{\Phi}_2((\tilde{x}_{\tau j})_{j\in J^c}) dx_1 \ldots dx_N. \tag{97}$$

If τ does not preserve the decomposition of $\{1 \ldots N\}$ into J and J^c, then the integral on the right in (97) is equal to zero, by Lemma 8. If τ does preserve that decomposition, then the antisymmetry properties of Φ_1 and Φ_2 show that the integral in (97) is equal to $(\operatorname{sgn}\tau)\|\Phi_1\|^2\|\Phi_2\|^2$. So (97) implies

$$\|\Phi_1 \wedge \Phi_2\|^2 = [c(J)]^2 \cdot (\text{Number of spin-preserving permutations } \sigma \text{ of } \{1 \ldots N\}) \cdot (\text{Number of spin-preserving permutations } \tau \text{ of } \{1 \ldots N\} \text{ that preserve } J,\ J^c) \cdot \|\Phi_1\|^2\|\Phi_2\|^2.$$

The right-hand side is simply $\|\Phi_1\|^2\|\Phi_2\|^2$, by virtue of our choice of $c(J)$ in (80). □

Next we apply Lemma 8 to calculate $\langle V(\Phi_1 \wedge \Phi_2), (\Phi_1 \wedge \Phi_2)\rangle$ for potentials $V = \sum_{j<k} K(x_j, x_k)$.

Lemma 10: *Suppose $K(x, y)$ is defined on $T \times T$ and satisfies $K(x, y) = K(y, x)$. Let $\Phi_1((x_j)_{j\in J})$ and $\Phi_2((x_j)_{j\in J^c})$ be strongly orthogonal and antisymmetric under spin-preserving permutations. Then*

$$\left\langle \sum_{1\le j<k\le N} K(x_j, x_k)(\Phi_1 \wedge \Phi_2), (\Phi_1 \wedge \Phi_2) \right\rangle =$$

$$\int_{T^N} \sum_{1\le \mu<\nu\le N} K(x_\mu, x_\nu)|\Phi_1((x_j)_{j\in J})|^2|\Phi_2((x_j)_{j\in J^c})|^2 dx_1 \ldots dx_N$$

$$- \sum_{\substack{\mu\in J, \nu\in J^c \\ \operatorname{spin}(\mu)=\operatorname{spin}(\nu)}} \int_{T^N} K(x_\mu, x_\nu)\Phi_1((x_j)_{j\in J})\Phi_2((x_j)_{j\in J^c})\bar{\Phi}_1((x_{\tau_{\mu\nu} j})_{j\in J}) \bar{\Phi}_2((x_{\tau_{\mu\nu} j})_{j\in J^c}) dx_1 \ldots dx_N,$$

where $\tau_{\mu\nu}$ denotes the transposition that interchanges μ and ν, and fixes all other indices.

Proof: By definition of $\Phi_1 \wedge \Phi_2$ we have

$$\left\langle \sum_{j\neq k} K(x_j, x_k)(\Phi_1 \wedge \Phi_2), (\Phi_1 \wedge \Phi_2) \right\rangle =$$

$$[c(J)]^2 \sum_{\substack{\sigma,\pi \\ j\neq k}} (\operatorname{sgn}\sigma)(\operatorname{sgn}\pi) \int_{T^N} K(x_j, x_k)\Phi_1((x_{\sigma\ell})_{\ell\in J})\Phi_2((x_{\sigma\ell})_{\ell\in J^c})\bar{\Phi}_1((x_{\pi\ell})_{\ell\in J})$$
$$\bar{\Phi}_2((x_{\pi\ell})_{\ell\in J^c})dx_1 \ldots dx_N,$$

where σ, π run over spin-preserving permutations of $\{1 \ldots N\}$. Let $\tilde{x}_\ell = x_{\sigma\ell}$ and $\tau = \sigma^{-1}\pi$, so that $x_{\pi\ell} = x_{\sigma(\tau\ell)} = \tilde{x}_{\tau\ell}$. Also, set $a = \sigma^{-1}j$ and $b = \sigma^{-1}k$, so that $x_j = x_{\sigma a} = \tilde{x}_a$ and $x_k = x_{\sigma b} = \tilde{x}_b$. Thus

$$\left\langle \sum_{j\neq k} K(x_j, x_k)(\Phi_1 \wedge \Phi_2), (\Phi_1, \wedge\Phi_2) \right\rangle = \tag{98}$$

$$[c(J)]^2 \sum_{\substack{\sigma,\tau \\ a\neq b}} (\operatorname{sgn}\tau) \int_{T^N} K(\tilde{x}_a, \tilde{x}_b)\Phi_1((\tilde{x}_\ell)_{\ell\in J})\Phi_2((\tilde{x}_\ell)_{\ell\in J^c})\bar{\Phi}_1((\tilde{x}_{\tau\ell})_{\ell\in J})$$
$$\bar{\Phi}_2((\tilde{x}_{\tau\ell})_{\ell\in J^c})d\tilde{x}_1 \ldots d\tilde{x}_N$$

Suppose a, b, σ, τ are given, and assume the integral on the right in (98) is not zero. Assume also that τ does *not* preserve J, J^c. Thus there is an $i \in J$ with $\tau i \in J^c$. Lemma 8 shows that $\tau i = a$ or b. Say $\tau i = a$, and set $s = \operatorname{spin}(i) = \operatorname{spin}(a)$. We know that τ restricts to a permutation of $I_s = \{1 \leq \ell \leq N \mid \operatorname{spin}(\ell) = s\}$, and that $\tau|_{I_s}$ does not respect the decomposition of I_s into $I_s \cap J$ and $I_s \cap J^c$. Hence there is some $j \in I_s \cap J^c$ for which $\tau j \in I_s \cap J$. Lemma 8 shows that $\tau j = a$ or b. Evidently $j \neq i$, since $j \in J^c$ while $i \in J$. Hence $\tau j \neq \tau i = a$, so $\tau j = b$. We conclude that j, i, a, b all have the same spin; that $\tau i = a$ and $\tau j = b$; that $i \in J$, $a \in J^c$, $j \in J^c$, $b \in J$. This assumes that $\tau i = a$ instead of b above. If instead, $\tau i = b$, then the same argument would produce $j \in J^c$ so that i, j, a, b all have the same spin; $\tau i = b$ and $\tau j = a$; $i \in J$, $b \in J^c$, $j \in J^c$, $a \in J$. In either case, we know that $\tau\ell \in J$ if and only if $\ell \in J$, provided $\tau\ell \neq a$ or b. (This follows from Lemma 8.) So there are only three cases in which the integral in (98) is non-zero, namely:

(A) τ preserves J and J^c, $a \neq b$;

(B) For some $i \in J$ and $j \in J^c$ we have $\tau i = a \in J^c$ and $\tau j = b \in J$. For all $\ell \neq i, j$ we have $\tau\ell \in J$ if and only if $\ell \in J$. Finally, i, j, a, b all have the same spin.

(C) For some $i \in J$ and $j \in J^c$ we have $\tau i = b \in J^c$ and $\tau j = a \in J$. For all $\ell \neq i, j$ we have $\tau\ell \in J$ if and only if $\ell \in J$. Finally, i, j, a, b all have the same spin.

The total contributions of the terms in case (B) and those in case (C) to the right-hand side of (98) are equal, since they may be made identical by interchanging the dummy indices a and b. Thus, (98) implies

(99)
$$\left\langle \frac{1}{2}\sum_{j\neq k} K(x_j,x_k)(\Phi_1\wedge\Phi_2),(\Phi_1\wedge\Phi_2)\right\rangle =$$
$$[c(J)]^2\cdot\frac{1}{2}\sum_{\sigma,\tau,a,b \text{ in Case (A)}}(\operatorname{sgn}\tau)\int_{T^N} K(\tilde{x}_a,\tilde{x}_b)\Phi_1((\tilde{x}_\ell)_{\ell\in J})\Phi_2((\tilde{x}_\ell)_{\ell\in J^c})$$
$$\bar{\Phi}_1((\tilde{x}_{\tau\ell})_{\ell\in J})\bar{\Phi}_2((\tilde{x}_{\tau\ell})_{\ell\in J^c})d\tilde{x}_1\dots d\tilde{x}_N$$
$$+[c(J)]^2\sum_{\sigma,\tau,a,b \text{ in Case (B)}}(\operatorname{sgn}\tau)\int_{T^N} K(\tilde{x}_a,\tilde{x}_b)\Phi_1((\tilde{x}_\ell)_{\ell\in J})\Phi_2((\tilde{x}_\ell)_{\ell\in J^c})$$
$$\bar{\Phi}_1((\tilde{x}_{\tau\ell})_{\ell\in J})\bar{\Phi}_2((\tilde{x}_{\tau\ell})_{\ell\in J^c})d\tilde{x}_1\dots d\tilde{x}_N$$
$$\equiv \text{Term 1} + \text{Term 2}.$$

In Case (B) we can write τ in the form $\tau=\widetilde{\tau}\tau_{ij}$, where $\widetilde{\tau}$ preserves spin and J, J^c; and τ_{ij} denotes the transposition of i and j as in the statement of Lemma 10.

Hence we can rewrite the integral in Case (B) in (99) by setting $x_\ell=\tilde{x}_{\widetilde{\tau}\ell}$ for $1\leq\ell\leq N$. Note that $\tilde{x}_a=\tilde{x}_{\tau i}=\tilde{x}_{\widetilde{\tau}\tau_{ij}i}=\tilde{x}_{\widetilde{\tau}j}=x_j$, while $\tilde{x}_b=\tilde{x}_{\tau j}=\tilde{x}_{\widetilde{\tau}\tau_{ij}j}=\tilde{x}_{\widetilde{\tau}i}=x_i$. Also, note that $\tilde{x}_\ell=x_{\widetilde{\tau}^{-1}\ell}$, and that $\tilde{x}_{\tau\ell}=\tilde{x}_{\widetilde{\tau}\tau_{ij}\ell}=x_{\tau_{ij}\ell}$. Therefore, the integral in Case (B) in (99) is equal to

$$\int_{T^N} K(x_j,x_i)\Phi_1((x_{\widetilde{\tau}^{-1}\ell})_{\ell\in J})\Phi_2((x_{\widetilde{\tau}^{-1}\ell})_{\ell\in J^c})\bar{\Phi}_1((x_{\tau_{ij}\ell})_{\ell\in J})\bar{\Phi}_2((x_{\tau_{ij}\ell})_{\ell\in J^c})dx_1\dots dx_N.$$

This in turn is equal to

$$(\operatorname{sgn}\widetilde{\tau})\int_{T^N} K(x_i,x_j)\Phi_1((x_\ell)_{\ell\in J})\Phi_2((x_\ell)_{\ell\in J^c})\bar{\Phi}_1((x_{\tau_{ij}\ell})_{\ell\in J})\bar{\Phi}_2((x_{\tau_{ij}\ell})_{\ell\in J^c})dx_1\dots dx_N,$$

since $\widetilde{\tau}$ preserves spin and J, J^c as well. Consequently, the second term on the right-hand side of (99) is equal to

(100)
$$\text{Term 2} = -[c(J)]^2\sum_{\substack{\sigma\\ \widetilde{\tau}}}\sum_{\substack{i\in J\\ j\in J^c\\ \text{spin}(i)=\text{spin}(j)}}\int_{T^N} K(x_i,x_j)\Phi_1((x_\ell)_{\ell\in J})\Phi_2((x_\ell)_{\ell\in J^c})$$
$$\bar{\Phi}_1((x_{\tau_{ij}\ell})_{\ell\in J})\bar{\Phi}_2((x_{\tau_{ij}\ell})_{\ell\in J^c})dx_1\dots dx_N.$$

The minus sign here arises from the product $(\operatorname{sgn}\tau)(\operatorname{sgn}\widetilde{\tau})$, since $\tau=\widetilde{\tau}\tau_{ij}$. The σ run over spin-preserving permutations of $\{1\dots N\}$, and the $\widetilde{\tau}$ run over spin-preserving permutations that also preserve J, J^c.

In view of the antisymmetry properties of Φ_1 and Φ_2, the integral in Case (A) in (99) is equal to

$$(\operatorname{sgn}\tau)\int_{T^N} K(x_a,x_b)|\Phi_1((x_\ell)_{\ell\in J})|^2\cdot|\Phi_2((x_\ell)_{\ell\in J^c})|^2 dx_1\dots dx_N.$$

Hence the first term on the right-hand side of (99) equals

$$\text{(101)}\quad \text{Term } 1=\frac{1}{2}[c(J)]^2\sum_{\sigma,\tau}\sum_{a\neq b}\int_{T^N} K(x_a,x_b)|\Phi_1((x_\ell)_{\ell\in J})|^2\cdot|\Phi_2((x_\ell)_{\ell\in J^c})|^2 dx_1\dots dx_N.$$

Here, σ runs over spin-preserving permutations of $\{1\dots N\}$, while τ runs over spin-preserving permutations that also preserve J, J^c.

In (100), the summand is independent of σ, $\widetilde{\tau}$; and the number of possible σ, $\widetilde{\tau}$ is $[c(J)]^{-2}$. Similarly, in (101), the summand is independent of σ, τ; and the number of possible σ, τ is $[c(J)]^{-2}$. Therefore, putting (100) and (101) into (99), we get

$$\left\langle \frac{1}{2}\sum_{j\neq k}\int_{T^N} K(x_j,x_k)(\Phi_1\wedge\Phi_2),(\Phi_1\wedge\Phi_2)\right\rangle =$$

$$\frac{1}{2}\sum_{a\neq b}\int_{T^N} K(x_a,x_b)|\Phi_1((x_\ell)_{\ell\in J})|^2\cdot|\Phi_2((x_\ell)_{\ell\in J^c})|^2 dx_1\dots dx_N$$

$$-\sum_{\substack{i\in J, j\in J^c\\ \text{spin}(i)=\text{spin}(j)}}\int_{T^N} K(x_i,x_j)\Phi_1((x_\ell)_{\ell\in J})\Phi_2((x_\ell)_{\ell\in J^c})\bar{\Phi}_1((x_{\tau_{ij}\ell})_{\ell\in J})\bar{\Phi}_2((x_{\tau_{ij}\ell})_{\ell\in J^c})$$

$$dx_1\dots dx_N.$$

This is the conclusion of Lemma 10. □

Corollary: *Under the assumptions of Lemma 10, we have*

$$\left\langle \sum_{1\leq j<k\leq N} K(x_j,x_k)(\Phi_1\wedge\Phi_2),(\Phi_1\wedge\Phi_2)\right\rangle \geq$$

$$\|\Phi_2\|^2\cdot\left\langle \frac{1}{2}\sum_{\substack{j,k\in J\\ j\neq k}} K(x_j,x_k)\Phi_1,\Phi_1\right\rangle,\ \textit{provided } K(x,y)\geq 0 \textit{ on } T\times T.$$

Proof: We keep the notation of Lemma 10, and note that

$$\left| \int_{T^N} K(x_\mu, x_\nu)\Phi_1((x_j)_{j\in J})\Phi_2((x_j)_{j\in J^c}) \bar{\Phi}_1((x_{\tau_{\mu\nu}j})_{j\in J})\bar{\Phi}_2((x_{\tau_{\mu\nu}j})_{j\in J^c})dx_1\dots dx_N \right| \tag{102}$$
$$\le \frac{1}{2}\int_{T^N} K(x_\mu, x_\nu)|\Phi_1((x_j)_{j\in J})|^2|\Phi_2((x_j)_{j\in J^c})|^2 dx_1\dots dx_N$$
$$+\frac{1}{2}\int_{T^N} K(x_\mu, x_\nu)|\Phi_1((x_{\tau_{\mu\nu}j})_{j\in J})|^2|\Phi_2((x_{\tau_{\mu\nu}j})_{j\in J^c})|^2 dx_1\dots dx_N.$$

We rewrite the second term by putting $\tilde{x}_j = x_{\tau_{\mu\nu}j}$. In particular,

$$K(x_\mu, x_\nu) = K(\tilde{x}_\nu, \tilde{x}_\mu) = K(\tilde{x}_\mu, \tilde{x}_\nu).$$

So the second term on the right in (102) equals

$$\frac{1}{2}\int_{T^N} K(\tilde{x}_\mu, \tilde{x}_\nu)|\Phi_1((\tilde{x}_j)_{j\in J})|^2|\Phi_2((\tilde{x}_j)_{j\in J^c})|^2 d\tilde{x}_1\dots d\tilde{x}_N,$$

which is obviously equal to the first term on the right in (102). Thus, (102) can be rewritten as

$$\left| \int_{T^N} K(x_\mu, x_\nu)\Phi_1((x_j)_{j\in J})\Phi_2((x_j)_{j\in J^c})\bar{\Phi}_1((x_{\tau_{\mu\nu}j})_{j\in J})\bar{\Phi}_2((x_{\tau_{\mu\nu}j})_{j\in J^c})dx_1\dots dx_N \right|$$
$$\le \int_{T^N} K(x_\mu, x_\nu)|\Phi_1((x_j)_{j\in J})|^2|\Phi_2((x_j)_{j\in J^c})|^2 dx_1\dots dx_N.$$

Putting this into the conclusion of Lemma 10, we get

$$\left\langle \sum_{1\le j<k\le N} K(x_j, x_k)(\Phi_1\wedge\Phi_2), (\Phi_1\wedge\Phi_2) \right\rangle \ge \tag{103}$$
$$\int_{T^N} \frac{1}{2}\sum_{\mu\ne\nu} K(x_\mu, x_\nu)|\Phi_1((x_j)_{j\in J})|^2|\Phi_2((x_j)_{j\in J^c})|^2 dx_1\dots dx_N$$
$$- \sum_{\substack{\mu\in J,\nu\in J^c\\ \mathrm{spin}(\mu)=\mathrm{spin}(\nu)}} \int_{T^N} K(x_\mu, x_\nu)|\Phi_1((x_j)_{j\in J})|^2|\Phi_2((x_j)_{j\in J^c})|^2 dx_1\dots dx_N$$
$$= \frac{1}{2}\sum_{\mu\ne\nu}\int_{T^N} K(x_\mu, x_\nu)|\Phi_1((x_j)_{j\in J})|^2|\Phi_2((x_j)_{j\in J^c})|^2 dx_1\dots dx_N$$

$$- \frac{1}{2} \sum_{\substack{\mu \in J, \nu \in J^c \\ \text{spin}(\mu)=\text{spin}(\nu)}} \int_{T^N} K(x_\mu, x_\nu) |\Phi_1((x_j)_{j\in J})|^2 |\Phi_2((x_j)_{j\in J^c})|^2 dx_1 \dots dx_N$$

$$- \frac{1}{2} \sum_{\substack{\mu \in J^c, \nu \in J \\ \text{spin}(\mu)=\text{spin}(\nu)}} \int_{T^N} K(x_\mu, x_\nu) |\Phi_1((x_j)_{j\in J})|^2 |\Phi_2((x_j)_{j\in J^c})|^2 dx_1 \dots dx_N$$

$$= \frac{1}{2} \sum_{(\mu,\nu)\in Y} \int_{T^N} K(x_\mu, x_\nu) |\Phi_1((x_j)_{j\in J})|^2 |\Phi_2((x_j)_{j\in J^c})|^2 dx_1 \dots dx_N,$$

where

$$Y = \{(\mu,\nu) \mid \mu \neq \nu\} \smallsetminus \{(\mu,\nu) \mid \mu \in J, \nu \in J^c, \text{spin}(\mu) = \text{spin}(\nu)\} \smallsetminus \{(\mu,\nu) \mid \mu \in J^c, \nu \in J, \text{spin}(\mu) = \text{spin}(\nu)\}.$$

Since $\{(\mu,\nu) \mid \mu \neq \nu \text{ and } \mu,\nu \in J\} \subset Y$, it follows from (103) that

(104)
$$\left\langle \sum_{1\le j<k\le N} K(x_j,x_k)(\Phi_1 \wedge \Phi_2), (\Phi_1 \wedge \Phi_2) \right\rangle \geq \frac{1}{2} \sum_{\substack{\mu,\nu \in J \\ \mu\neq\nu}} \int_{T^N} K(x_\mu, x_\nu) |\Phi_1((x_j)_{j\in J})|^2 |\Phi_2((x_j)_{j\in J^c})|^2 dx_1 \dots dx_N.$$

The right-hand side here is obviously equal to

$$\left\langle \frac{1}{2} \sum_{\substack{\mu\neq\nu \\ \mu,\nu\in J}} K(x_\mu,x_\nu)\Phi_1, \Phi_1 \right\rangle \cdot \|\Phi_2\|^2,$$

so (104) implies the assertion of the Corollary. □

Next, we study the correlation functions $\mathcal{S}_s(x, y, \Phi_1 \wedge \Phi_2)$ for an antisymmetrized product. Recall that the correlation functions are defined by (5) for wave functions $\Phi(x_1 \dots x_N)$. Analogous formulas define the correlation functions for $\Phi_1((x_j)_{j\in J})$ and $\Phi_2((x_j)_{j\in J^c})$. (See equations (105), (106) below.)

Lemma 11: *Suppose $\Phi_1((x_j)_{j\in J})$ and $\Phi_2((x_j)_{j\in J^c})$ are strongly orthogonal and antisymmetric under spin-preserving permutations. Then the correlation functions of Φ_1, Φ_2 and $\Phi_1 \wedge \Phi_2$ are related by*

$$\mathcal{S}_s(x,y,\Phi_1 \wedge \Phi_2) = \|\Phi_2\|^2 \mathcal{S}_s(x,y,\Phi_1) + \|\Phi_1\|^2 \mathcal{S}_s(x,y,\Phi_2)$$

Proof: Suppose first that Φ_1 and Φ_2 are smooth. Then $\Phi_1 \wedge \Phi_2$ is also smooth, and we can express the correlation functions by the formulas

(105) $$\mathcal{S}_s(x,y,\Phi_1) = \sum_{\substack{j\in J \\ \text{spin}(j)=s}} \int \Phi_1((x_\ell)_{\ell\in J}) \bar{\Phi}_1((y_\ell)_{\ell\in J}) \delta(x_j - x)\delta(y_j - y) \cdot$$

$$\prod_{\substack{\ell\in J\\ \ell\neq j}}\delta(x_\ell-y_\ell)\cdot\prod_{\ell\in J}dx_\ell dy_\ell$$

(106) $$\mathcal{S}_s(x,y,\Phi_2)=\sum_{\substack{j\in J^c\\ \text{spin}(j)=s}}\int\Phi_2((x_\ell)_{\ell\in J^c})\bar{\Phi}_2((y_\ell)_{\ell\in J^c})\delta(x_j-x)\delta(y_j-y)\cdot$$
$$\prod_{\substack{\ell\in J^c\\ \ell\neq j}}\delta(x_\ell-y_\ell)\cdot\prod_{\ell\in J^c}dx_\ell dy_\ell$$

(107)
$$\mathcal{S}_s(x,y,\Phi_1\wedge\Phi_2)=$$
$$[c(J)]^2\sum_{\substack{\text{spin}(j)=s\\ \sigma,\pi}}(\operatorname{sgn}\sigma)(\operatorname{sgn}\pi)\int\Phi_1((x_{\sigma\ell})_{\ell\in J})\Phi_2((x_{\sigma\ell})_{\ell\in J^c})\bar{\Phi}_1((y_{\pi\ell})_{\ell\in J})\bar{\Phi}_2((y_{\pi\ell})_{\ell\in J^c})\cdot$$
$$\delta(x_j-x)\delta(y_j-y)\cdot\prod_{\ell\neq j}\delta(x_\ell-y_\ell)\prod_{\ell=1}^{N}dx_\ell dy_\ell$$

Of course, (107) is the analogue of (105), (106) where we put in the definition of $\Phi_1\wedge\Phi_2$. In (107), j runs from 1 to N, and σ, π run over spin-preserving permutations of $\{1\dots N\}$.

To simplify (107) we write $x_{\sigma\ell}=\tilde{x}_\ell$, $y_{\sigma\ell}=\tilde{y}_\ell$, $\sigma^{-1}\pi=\tau$, and $\sigma^{-1}j=\mu$. Note that $y_{\pi\ell}=y_{\sigma\tau\ell}=\tilde{y}_{\tau\ell}$, $x_j=x_{\sigma\mu}=\tilde{x}_\mu$, $y_j=y_{\sigma\mu}=\tilde{y}_\mu$. Thus, (107) is equivalent to

(108)
$$\mathcal{S}_s(x,y,\Phi_1\wedge\Phi_2)=$$
$$[c(J)]^2\sum_{\substack{\sigma,\tau\\ \text{spin}(\mu)=s}}(\operatorname{sgn}\tau)\int\Phi_1((\tilde{x}_\ell)_{\ell\in J})\Phi_2((\tilde{x}_\ell)_{\ell\in J^c})\bar{\Phi}_1((\tilde{y}_{\tau\ell})_{\ell\in J})\bar{\Phi}_2((\tilde{y}_{\tau\ell})_{\ell\in J^c})\cdot$$
$$\delta(\tilde{x}_\mu-x)\delta(\tilde{y}_\mu-y)\prod_{\ell\neq\mu}\delta(\tilde{x}_\ell-\tilde{y}_\ell)\prod_{\ell=1}^{N}d\tilde{x}_\ell d\tilde{y}_\ell$$
$$\equiv\sum_{\substack{\sigma,\tau\\ \text{spin}(\mu)=s}}[c(J)]^2(\operatorname{sgn}\tau)\cdot\text{Term}(\sigma,\tau,\mu).$$

Fix (σ,τ,μ) in (108) with $\text{Term}(\sigma,\tau,\mu)\neq 0$. If we could find $\nu\in J$ with $\tau\nu\in J^c$ and $\tau\nu\neq\mu$, then by writing

$$\text{Term}(\sigma,\tau,\mu)=$$
$$\int\Phi_1((\tilde{x}_\ell)_{\ell\in J})\bar{\Phi}_2((\tilde{y}_{\tau\ell})_{\ell\in J^c})\left[\int\Phi_2((\tilde{x}_\ell)_{\ell\in J^c})\bar{\Phi}_1((\tilde{y}_{\tau\ell})_{\ell\in J})\delta(\tilde{x}_{\tau\nu}-\tilde{y}_{\tau\nu})d\tilde{x}_{\tau\nu}d\tilde{y}_{\tau\nu}\right]$$

$$\cdot\, \delta(\tilde{x}_\mu - x)\delta(\tilde{y}_\mu - y) \cdot \prod_{\ell\neq\mu,\tau\nu} \delta(\tilde{x}_\ell - \tilde{y}_\ell) \cdot \prod_{\ell\neq\tau\nu} d\tilde{x}_\ell d\tilde{y}_\ell$$

and applying strong orthogonality to the integral in brackets, we could show that $\text{Term}(\sigma,\tau,\mu) = 0$, contradicting our assumption. Hence $\nu \in J$ implies $\tau\nu \in J$ unless $\tau\nu = \mu$.

Similarly, if we could find $\nu \in J^c$ with $\tau\nu \in J$ and $\tau\nu \neq \mu$, then by writing

$$\text{Term}(\sigma,\tau,\mu) =$$
$$\int \Phi_2((\tilde{x}_\ell)_{\ell\in J^c})\bar{\Phi}_1((\tilde{y}_{\tau\ell})_{\ell\in J})\left[\int \Phi_1((\tilde{x}_\ell)_{\ell\in J})\bar{\Phi}_2((\tilde{y}_{\tau\ell})_{\ell\in J^c})\delta(\tilde{x}_{\tau\nu} - \tilde{y}_{\tau\nu})d\tilde{x}_{\tau\nu}d\tilde{y}_{\tau\nu}\right]$$
$$\cdot\, \delta(\tilde{x}_\mu - x)\delta(\tilde{y}_\mu - y) \prod_{\ell\neq\mu,\tau\nu} \delta(\tilde{x}_\ell - \tilde{y}_\ell) \cdot \prod_{\ell\neq\tau\nu} d\tilde{x}_\ell d\tilde{y}_\ell$$

and applying strong orthogonality to the integral in brackets, we could again show that $\text{Term}(\sigma,\tau,\mu) = 0$, contradicting our assumption. Hence, $\nu \in J^c$ implies $\tau\nu \in J^c$ unless $\tau\nu = \mu$.

Now we know that $\nu \in J$ if and only if $\tau\nu \in J$, unless $\tau\nu = \mu$. It follows that $\nu \in J$ if and only if $\tau\nu \in J$ for all $\nu \in \{1,\dots N\}$. Thus, in (108) we may restrict the sum to those (σ,τ,μ) with τ preserving J and J^c. The antisymmetry properties of Φ_1 and Φ_2 then show that (108) is equivalent to

(109)
$$\mathcal{S}_s(x,y,\Phi_1\wedge\Phi_2) =$$
$$[c(J)]^2 \sum_{\substack{\sigma,\tau \\ \text{spin}(\mu)=s}} \int \Phi_1((x_\ell)_{\ell\in J})\Phi_2((x_\ell)_{\ell\in J^c})\bar{\Phi}_1((y_\ell)_{\ell\in J})\bar{\Phi}_2((y_\ell)_{\ell\in J^c})\cdot$$
$$\delta(x_\mu - x)\delta(y_\mu - y)\prod_{\ell\neq\mu}\delta(x_\ell - y_\ell)\cdot\prod_{\ell=1}^{N} dx_\ell dy_\ell.$$

The sum runs over σ spin-preserving, and over spin-preserving τ that also preserve J and J^c. The summands here are independent of σ, τ; and the number of possible (σ,τ) is $[c(J)]^{-2}$ by (80). So (109) simplifies to

(110)
$$\mathcal{S}_s(x,y,\Phi_1\wedge\Phi_2) =$$
$$\sum_{\text{spin}(\mu)=s} \int \Phi_1((x_\ell)_{\ell\in J})\bar{\Phi}_1((y_\ell)_{\ell\in J})\Phi_2((x_\ell)_{\ell\in J^c})\bar{\Phi}_2((y_\ell)_{\ell\in J^c})\cdot$$
$$\delta(x_\mu - x)\delta(y_\mu - y)\cdot\prod_{\ell\neq\mu}\delta(x_\ell - y_\ell)\cdot\prod_{\ell=1}^{N} dx_\ell dy_\ell$$
$$\equiv \sum_{\text{spin}(\mu)=s} \text{Term}_*(\mu).$$

Comparing (110) with (105) and (106), we see that

$$\sum_{\substack{\mathrm{spin}(\mu)=s\\ \mu\in J}} \mathrm{Term}_*(\mu) = \|\Phi_2\|^2 \mathcal{S}_s(x,y,\Phi_1)$$

and

$$\sum_{\substack{\mathrm{spin}(\mu)=s\\ \mu\in J^c}} \mathrm{Term}_*(\mu) = \|\Phi_1\|^2 \mathcal{S}_s(x,y,\Phi_2).$$

Therefore, (110) implies

$$\mathcal{S}_s(x,y,\Phi_1\wedge\Phi_2) = \|\Phi_2\|^2\mathcal{S}_s(x,y,\Phi_1) + \|\Phi_1\|^2\mathcal{S}_s(x,y,\Phi_2),$$

which is the conclusion of Lemma 11.

In the above argument, we assumed Φ_1 and Φ_2 are smooth. This assumption was used only to introduce δ-functions into our formulas. Our equations still make sense, even if Φ_1, Φ_2 are non-smooth. In fact, we erase every $\delta(x_\ell - y_\ell)$ from our integrals, replace each y_ℓ by x_ℓ, and drop the integration over y_ℓ. Similarly for $\delta(x_j - x)$ or $\delta(\tilde{x}_\mu - x)$. Thus each of our equations is equivalent to a messier equation containing no δ-functions. Details may be left to the reader. □

We prepare to apply Lemmas 7, 9, 10, 11 to the study of $\Phi^{\mathfrak{z}}_{\mathrm{main}}$. To do so, we first extend our observtion on the strong orthogonality of $\Phi^{\mathfrak{z}}_{\mathrm{basic}}$ and $\Phi^{\mathfrak{z}}_{\mathrm{extra}}$. Define

$$\mathcal{N}^{\mathrm{extra}}_{s\mathfrak{z}}((x_j)_{j\in J^c}) = \sum_{\substack{j\in J^c\\ \mathrm{spin}(j)=s}} \chi_{Q+\mathfrak{z}}(x_j) = \text{number of particles } x_j\ (j\in J^c) \text{ of spin } s \text{ in } Q+\mathfrak{z}.$$

Given a family $(n_s)_{1\le s\le q}$ of non-negative integers n_s, we define

$$\Phi^{\mathfrak{z},(n_s)}_{\mathrm{extra}}((x_j)_{j\in J^c}) = \left(\prod_{s=1}^{q} \chi_{\mathcal{N}^{\mathrm{extra}}_{s\mathfrak{z}}=n_s}\right)\cdot \Phi^{\mathfrak{z}}_{\mathrm{extra}}((x_j)_{j\in J^c})$$

Thus, $\Phi^{\mathfrak{z},(n_s)}_{\mathrm{extra}}$ is antisymmetric under spin-preserving permutations, and $\Phi^{\mathfrak{z}}_{\mathrm{extra}}$ is the sum of $\Phi^{\mathfrak{z},(n_s)}_{\mathrm{extra}}$ over all possible families (n_s).

Lemma 12: *The wave functions $\Phi^{\mathfrak{z}}_{\mathrm{basic}}$ and $\Phi^{\mathfrak{z},(n_s)}_{\mathrm{extra}}$ are strongly orthogonal, and their antisymmetrized product $\Phi^{\mathfrak{z}}_{\mathrm{basic}}\wedge\Phi^{\mathfrak{z},(n_s)}_{\mathrm{extra}}$ is supported in $\{(x_1\dots x_N)\in T^N \mid \mathcal{N}_{s\mathfrak{z}}(x_1\dots x_N) = n_s + \underline{N}_s\}$.*

Proof: We use the same idea as in the proof of Lemma 5. The function $\Phi^{\mathfrak{z}}_{\mathrm{extra}}((x_j)_{j\in J^c})$ may be Fourier-expanded as follows:

$$\Phi^{\mathfrak{z}}_{\mathrm{extra}}((x_j)_{j\in J^c}) = \sum_{(\alpha_j)_{j\in J^c}} D_{(\alpha_j)_{j\in J^c}} \prod_{s=1}^{q}\Bigg(\prod_{\substack{j\in J^c\\ \mathrm{spin}(j)=s}} \varphi^{\mathfrak{z}}_{\alpha_j,s}(x_j)\Bigg), \tag{111}$$

for suitable coefficients $D_{(\alpha_j)_{j\in J^c}}$. Recall that $\varphi^{\mathfrak{z}}_{\alpha s}$ is supported entirely in $Q+\mathfrak{z}$ when $\alpha>0$, and in the complement of $Q+\mathfrak{z}$ when $\alpha\le 0$.

Hence, $\prod_{s=1}^{q}\Bigg(\prod_{\substack{j\in J^c\\ \text{spin}(j)=s}}\varphi^{\mathfrak{z}}_{\alpha_j,s}(x_j)\Bigg)$ is supported in the set of $(x_j)_{j\in J^c}$ for which $\mathcal{N}^{\text{extra}}_{s\mathfrak{z}}((x_j)_{j\in J^c})=$ [Number of $\alpha_j>0$ with $j\in J^c$ of spin s]. This shows that

$$\Phi^{\mathfrak{z},(n_s)}_{extra}((x_j)_{j\in J^c})=\sum_{(\alpha_j)_{j\in J^c}}\widetilde{D}_{(\alpha_j)_{j\in J^c}}\prod_{s=1}^{q}\Bigg(\prod_{\substack{j\in J^c\\ \text{spin}(j)=s}}\varphi^{\mathfrak{z}}_{\alpha_j s}(x_j)\Bigg),\tag{112}$$

where

$$\widetilde{D}_{(\alpha_j)_{j\in J^c}}=\begin{cases}D_{(\alpha_j)_{j\in J^c}} & \text{if for each } s\ (1\le s\le q) \text{ there}\\ & \text{are precisely } n_s \text{ indices } j\in J^c\\ & \text{with } \alpha_j>0 \text{ and spin}(j)=s\\ 0 & \text{otherwise.}\end{cases}$$

Comparing (111) with (82), (83), we see that each non-zero coefficient $D_{(\alpha_j)_{j\in J^c}}$ has the property that $\alpha_j\notin\{1\ldots\underline{N}_s\}$ for $j\in J^c$ of spin s. The $\widetilde{D}_{(\alpha_j)_{j\in J^c}}$ therefore have the same property, by definition. In particular, for $j_2\in J^c$ of spin s_0 and fixed $(x_j)_{j\in J^c\smallsetminus\{j_2\}}$, the function $x_{j_2}\mapsto\Phi^{\mathfrak{z},(n_s)}_{\text{extra}}((x_j)_{j\in J^c})$ belongs to the span of the $\varphi^{\mathfrak{z}}_{\alpha,s_0}$ for $\alpha\notin\{1\ldots\underline{N}_{s_0}\}$, as we see from (112). On the other hand, for $j_1\in J$ of spin s_0 and fixed $(x_j)_{j\in J\smallsetminus\{j_1\}}$ the function $x_{j_1}\mapsto\Phi^{\mathfrak{z}}_{\text{basic}}((x_j)_{j\in J})$ belongs to the span of the $\varphi^{\mathfrak{z}}_{\alpha,s_0}$ for $\alpha\in\{1\ldots\underline{N}_s\}$. Hence, the orthogonality of $x_{j_1}\mapsto\Phi^{\mathfrak{z}}_{\text{basic}}((x_j)_{j\in J})$ and $x_{j_2}\mapsto\Phi^{\mathfrak{z},(n_s)}_{\text{extra}}((x_j)_{j\in J^c})$ follows from the orthogonality of the $\varphi^{\mathfrak{z}}_{\alpha s_0}$ for fixed $\mathfrak{z}$ and s_0. So $\Phi^{\mathfrak{z}}_{\text{basic}}$ and $\Phi^{\mathfrak{z},(n_s)}_{\text{extra}}$ are strongly orthogonal, as asserted in Lemma 12.

It remains to check the assertion of Lemma 12 on the support of $\Phi^{\mathfrak{z}}_{\text{basic}}\wedge\Phi^{\mathfrak{z},(n_s)}_{\text{extra}}$. In general, suppose $\Phi_1((x_j)_{j\in J})$ is supported in the set where there are precisely $\underline{N}_s$ particles of spin s in $Q+\mathfrak{z}$; and suppose $\Phi_2((x_j)_{j\in J^c})$ is supported in the set where there are precisely n_s particles of spin s in $Q+\mathfrak{z}$. For any permutation σ of $\{1\ldots N\}$, the function

$$\Phi_1((x_{\sigma j})_{j\in J})\Phi_2((x_{\sigma j})_{j\in J^c})$$

is supported in the set where there are precisely $(\underline{N}_s+n_s)$ particles of spin s in $(Q+\mathfrak{z})$. Hence the antisymmetrized product $\Phi_1\wedge\Phi_2$ is also supported in the set where there are $\underline{N}_s+n_s$ particles of spin s in $Q+\mathfrak{z}$. Applying this observation to $\Phi_1=\Phi^{\mathfrak{z}}_{\text{basic}}$, $\Phi_2=\Phi^{\mathfrak{z},(n_s)}_{\text{extra}}$, we get the assertion of Lemma 12 on the support of $\Phi^{\mathfrak{z}}_{\text{basic}}\wedge\Phi^{\mathfrak{z},(n_s)}_{\text{extra}}$. □

Set $\mathcal{E}^{\mathfrak{z},(n_s)}=\{(x_1\ldots x_N)\in T^N\mid \mathcal{N}_{s\mathfrak{z}}(x_1\ldots x_N)=n_s\text{ for all }s\}$. Then since

$$\Phi^{\mathfrak{z}}_{\text{basic}}\wedge\Phi^{\mathfrak{z}}_{\text{extra}}=\sum_{(n_s)}\Phi^{\mathfrak{z}}_{\text{basic}}\wedge\Phi^{\mathfrak{z},(n_s)}_{\text{extra}},$$

the assertion of Lemma 12 about the support shows that

$$\chi_{\mathcal{E}_{\mathfrak{z}},(n_s)} \cdot (\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}) = \begin{cases} \Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z},(n_s - \underline{N}_s)}_{\text{extra}} & \text{if } n_s \geq \underline{N}_s \quad (\text{all } s) \\ 0 & \text{otherwise} \end{cases} \tag{113}$$

Lemma 13: *Suppose $K(x,y)$ is defined on $T \times T$, and satisfies $K(x,y) = K(y,x) \geq 0$ for all $x, y \in T$. Assume $K(x,y)$ is supported in $(Q + \mathfrak{z}) \times (Q + \mathfrak{z})$. Let $\underline{N}_*$ be a given integer, with $\underline{N}_* \geq \underline{N}_1 + \cdots + \underline{N}_s$. Define a potential*

$$V(x_1 \dots x_N) = \left[\begin{array}{ll} \sum\limits_{1 \leq j < k \leq N} K(x_j, x_k) & \text{if at most } \underline{N}_* \text{ of the } x_j \text{ belong to } Q + \mathfrak{z} \\ \qquad 0 & \text{otherwise.} \end{array} \right.$$

Then

$$\left\langle V(\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}), (\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}) \right\rangle \geq$$

$$V^{\mathfrak{z}}_{\text{basic}} \|\Phi^{\mathfrak{z}}_{\text{extra}}\|^2 - C V^{\mathfrak{z}}_{\text{basic}} (\underline{N}_* - [\underline{N}_1 + \cdots + \underline{N}_q])^{-5/3} \sum_{s=1}^{q} \left\langle (\mathcal{N}^{\text{extra}}_{s\mathfrak{z}})^{5/3} \Phi^{\mathfrak{z}}_{\text{extra}}, \Phi^{\mathfrak{z}}_{\text{extra}} \right\rangle$$

where

$$V^{\mathfrak{z}}_{\text{basic}} = \left\langle \frac{1}{2} \sum_{\substack{j,k \in J \\ j \neq k}} K(x_j, x_k) \Phi^{\mathfrak{z}}_{\text{basic}}, \Phi^{\mathfrak{z}}_{\text{basic}} \right\rangle$$

Proof:

$$\left\langle V(\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}), (\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}) \right\rangle =$$

$$\int_{T^N} V |\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}|^2 dx_1 \dots dx_N = \sum_{n_1 \dots n_q} \int_{\mathcal{E}_{\mathfrak{z}},(n_s)} V |\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}|^2 dx_1 \dots dx_N$$

$$= \sum_{n_1 + \cdots + n_q \leq \underline{N}_*} \int_{\mathcal{E}_{\mathfrak{z}},(n_s)} \left(\frac{1}{2} \sum_{j \neq k} K(x_j, x_k) \right) |\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}|^2 dx_1 \dots dx_N$$

$$= \sum_{n_1 + \cdots + n_q \leq \underline{N}} \int_{T^N} \left(\frac{1}{2} \sum_{j \neq k} K(x_j, x_k) \right) |\chi_{\mathcal{E}_{\mathfrak{z}},(n_s)} \cdot (\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}})|^2 dx_1 \dots dx_N$$

$$= \sum_{\substack{n_1 + \cdots + n_q \leq \underline{N}_* \\ \text{all } n_s \geq \underline{N}_s}} \int_{T^N} \left(\frac{1}{2} \sum_{j \neq k} K(x_j, x_k) \right) |\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z},(n_s - \underline{N}_s)}_{\text{extra}}|^2 dx_1 \dots dx_N$$

(by (113))

$$\geq \sum_{\substack{n_1 + \cdots + n_q \leq \underline{N}_* \\ \text{all } n_s \geq \underline{N}_s}} V^{\mathfrak{z}}_{\text{basic}} \|\Phi^{\mathfrak{z},(n_s - \underline{N}_s)}_{\text{extra}}\|^2,$$

by the Corollary to Lemma 10. The hypotheses of that Corollary hold, by virtue of the strong orthogonality assertion of Lemma 12.

Changing dummy indices on the right from n_s to $\tilde{n}_s = n_s - \underline{N}_s$, we rewrite the above inequality as

$$\Big\langle V(\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}), (\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}})\Big\rangle \geq V^{\mathfrak{z}}_{\text{basic}} \cdot \sum_{\tilde{n}_1+\cdots+\tilde{n}_q \leq \underline{N}_* - (\underline{N}_1+\cdots+\underline{N}_q)} \|\Phi^{\mathfrak{z},(\tilde{n}_s)}_{\text{extra}}\|^2$$

$$= V^{\mathfrak{z}}_{\text{basic}}\|\Phi^{\mathfrak{z}}_{\text{extra}}\|^2 - V^{\mathfrak{z}}_{\text{basic}} \sum_{\tilde{n}_1+\cdots+\tilde{n}_q > \underline{N}_* - (\underline{N}_1+\cdots+\underline{N}_q)} \|\Phi^{\mathfrak{z},(\tilde{n}_s)}_{\text{extra}}\|^2$$

$$\geq V^{\mathfrak{z}}_{\text{basic}}\|\Phi^{\mathfrak{z}}_{\text{extra}}\|^2 - V^{\mathfrak{z}}_{\text{basic}} \cdot (\underline{N}_* - (\underline{N}_1 + \cdots + \underline{N}_q))^{-5/3} \sum_{\tilde{n}_1 \ldots \tilde{n}_q \geq 0} (\tilde{n}_1 + \cdots + \tilde{n}_q)^{5/3} \|\Phi^{\mathfrak{z},(\tilde{n}_s)}_{\text{extra}}\|^2$$

$$= V^{\mathfrak{z}}_{\text{basic}}\|\Phi^{\mathfrak{z}}_{\text{extra}}\|^2 - V^{\mathfrak{z}}_{\text{basic}}(\underline{N}_* - (\underline{N}_1 + \cdots + \underline{N}_q))^{-5/3}\Big\langle (\mathcal{N}^{\text{extra}}_{1\mathfrak{z}} + \cdots + \mathcal{N}^{\text{extra}}_{q\mathfrak{z}})^{5/3}\Phi^{\mathfrak{z}}_{\text{extra}}, \Phi^{\mathfrak{z}}_{\text{extra}}\Big\rangle$$

$$\geq V^{\mathfrak{z}}_{\text{basic}}\|\Phi^{\mathfrak{z}}_{\text{extra}}\|^2 - C V^{\mathfrak{z}}_{\text{basic}}(\underline{N}_* - (\underline{N}_1 + \cdots + \underline{N}_q))^{-5/3} \sum_{s=1}^{q} \Big\langle (\mathcal{N}^{\text{extra}}_{s\mathfrak{z}})^{5/3}\Phi^{\mathfrak{z}}_{\text{extra}}, \Phi^{\mathfrak{z}}_{\text{extra}}\Big\rangle .$$

The proof of Lemma 13 is complete. □

We introduced the cutoff $\underline{N}_*$ and proved Lemma 13 because the full two-body potential $\frac{1}{2}\sum_{j\neq k} K(x_j, x_k)$ may grow so large that $\Big\langle \frac{1}{2}\sum_{j\neq k} K(x_j, x_k)\Phi, \Phi\Big\rangle$ is highly unstable under small perturbations of Φ. Consequently, changing from $\Phi^{\mathfrak{z}}_{\text{main}} = \Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}$ to $\Psi = \Phi^{\mathfrak{z}}_{\text{main}} + \Phi^{\mathfrak{z}}_{\text{error}}$ will lead to disaster unless we first pass to the more stable potential V of Lemma 13.

From the statement of Lemma 13, it is clear that we must estimate $\Big\langle (\mathcal{N}^{\text{extra}}_{s\mathfrak{z}})^{5/3}\Phi^{\mathfrak{z}}_{\text{extra}}, \Phi^{\mathfrak{z}}_{\text{extra}}\Big\rangle$. We will also need to understand $\langle \mathcal{N}^{\text{extra}}_{s\mathfrak{z}}\Phi^{\mathfrak{z}}_{\text{extra}}, \Phi^{\mathfrak{z}}_{\text{extra}}\rangle$. Therefore, we give the following result.

Lemma 14: *We have the identities*

$$\Big\langle (\mathcal{N}^{\text{extra}}_{s\mathfrak{z}})^{5/3}\Phi^{\mathfrak{z}}_{\text{extra}}, \Phi^{\mathfrak{z}}_{\text{extra}}\Big\rangle = \Big\langle (\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s)^{5/3}_{+}(\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}), (\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}})\Big\rangle$$

and

$$\langle (\mathcal{N}^{\text{extra}}_{s\mathfrak{z}})\Phi^{\mathfrak{z}}_{\text{extra}}, \Phi^{\mathfrak{z}}_{\text{extra}}\rangle = \langle (\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s)(\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}), (\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}})\rangle$$

Proof: If $g(n)$ is any real-valued function on the integers, then we have

$$\langle g(\mathcal{N}_{s_0\mathfrak{z}})(\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}), (\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}})\rangle =$$

$$\sum_{n_1\dots n_q} g(n_{s_0}) \int\limits_{\mathcal{E}^{\mathfrak{z},(n_s)}} |\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}|^2 dx_1 \dots dx_N =$$

$$\sum_{n_1\dots n_q} g(n_{s_0}) \int\limits_{T^N} |\chi_{\mathcal{E}^{\mathfrak{z},(n_s)}} \cdot (\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}})|^2 dx_1 \dots dx_N =$$

$$\sum_{\substack{n_1\dots n_q \\ n_s \geq \underline{N}_s \text{ (all } s)}} g(n_{s_0}) \int\limits_{T^N} |\Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z},(n_s - \underline{N}_s)}_{\text{extra}}|^2 dx_1 \dots dx_N =$$

$$\sum_{\substack{n_1\dots n_q \\ n_s \geq \underline{N}_s \text{ (all } s)}} g(n_{s_0}) \|\Phi^{\mathfrak{z},(n_s - \underline{N}_s)}_{\text{extra}}\|^2 \text{ (by Lemmas 9 and 12)}$$

$$= \sum_{\tilde{n}_1\dots\tilde{n}_q} g(\tilde{n}_{s_0} + \underline{N}_{s_0}) \|\Phi^{\mathfrak{z},(\tilde{n}_s)}_{\text{extra}}\|^2 = \left\langle g(\mathcal{N}^{\text{extra}}_{s_0\mathfrak{z}} + \underline{N}_{s_0}) \Phi^{\mathfrak{z}}_{\text{extra}}, \Phi^{\mathfrak{z}}_{\text{extra}} \right\rangle.$$

Taking $g(n) = n - \underline{N}_{s_0}$ and $g(n) = (n - \underline{N}_{s_0})_+^{5/3}$, we obtain the conclusions of Lemma 14. □

We can use Lemmas 13 and 14 to derive a lower bound for $\left\langle \sum_{1\leq j<k\leq N} K_{\mathfrak{z}}(x_j, x_k)\Psi, \Psi \right\rangle$ for suitable $K_{\mathfrak{z}}(x,y)$, thus returning to our original wave function. Recall that $\Psi = \Phi^{\mathfrak{z}}_{\text{main}} + \Phi^{\mathfrak{z}}_{\text{error}}$; $\Phi^{\mathfrak{z}}_{\text{main}} = \Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}$; and $\Phi^{\mathfrak{z}}_{\text{basic}}, \Phi^{\mathfrak{z}}_{\text{extra}}$ are strongly orthogonal. Since $\Phi^{\mathfrak{z}}_{\text{basic}}$ has norm 1, Lemma 9 gives $\|\Phi^{\mathfrak{z}}_{\text{main}}\| = \|\Phi^{\mathfrak{z}}_{\text{extra}}\|$, so that (77) implies

$$\|\Phi^{\mathfrak{z}}_{\text{extra}}\|^2 + \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 = 1 \quad \text{for} \quad \mathfrak{z} \in T. \tag{114}$$

Let $\underline{N}_* > 2(\underline{N}_1 + \cdots \underline{N}_q)$ and $0 < \tau < 1$ be parameters to be picked later.

Lemma 15: *Suppose $K_{\mathfrak{z}}(x,y) = K_{\mathfrak{z}}(y,x) \geq 0$, and suppose $K_{\mathfrak{z}}(\,\cdot\,,\,\cdot\,)$ is supported in $(Q_0 + \mathfrak{z}) \times (Q_0 + \mathfrak{z})$, where Q_0 is the middle $3/4$ of Q. Then we have the inequality*

$$\left\langle \sum_{1\leq j<k\leq N} K_{\mathfrak{z}}(x_j, x_k)\Psi, \Psi \right\rangle \geq$$

$$V^{\mathfrak{z}}_{\text{basic}} -$$

$$\left\{ \tau V^{\mathfrak{z}}_{\text{basic}} + \frac{C}{\tau}(\underline{N}_*)^2 \|K_{\mathfrak{z}}\|_{L^\infty} \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 + C V^{\mathfrak{z}}_{\text{basic}} (\underline{N}_*)^{-5/3} \sum_{s=1}^{q} \left\langle \mathcal{N}^{5/3}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle \right\},$$

with

$$V^{\mathfrak{z}}_{\text{basic}} = \left\langle \frac{1}{2} \sum_{\substack{j,k\in J \\ j\neq k}} K_{\mathfrak{z}}(x_j, x_k) \Phi^{\mathfrak{z}}_{\text{basic}}, \Phi^{\mathfrak{z}}_{\text{basic}} \right\rangle$$

Proof: Set

$$V(x_1 \dots x_N) = \left[\begin{array}{ll} \displaystyle\sum_{1\leq j<k\leq N} K_{\mathfrak{z}}(x_j, x_k) & \text{if at most } \underline{N}_* \text{ of the } x_j \text{ be-} \\ & \text{long to } (Q + \mathfrak{z}) \\ 0 & \text{otherwise.} \end{array} \right.$$

Lemmas 13, 14 and the fact that $\Phi^{\mathfrak{z}}_{\text{main}} = \Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}$ show that

$$\left\langle V\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle \geq$$

$$V^{\mathfrak{z}}_{\text{basic}} \|\Phi^{\mathfrak{z}}_{\text{extra}}\|^2 - C V^{\mathfrak{z}}_{\text{basic}} (\underset{\sim}{N}_* - [\underset{\sim}{N}_1 + \cdots + \underset{\sim}{N}_q])^{-5/3} \sum_{s=1}^{q} \left\langle (\mathcal{N}_{s\mathfrak{z}} - \underset{\sim}{N}_s)_+^{5/3} \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle .$$

From (114) and our assumption that $\underset{\sim}{N}_* > 2(\underset{\sim}{N}_1 + \cdots + \underset{\sim}{N}_q)$, we conclude that

$$\left\langle V\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle \geq \tag{115}$$

$$V^{\mathfrak{z}}_{\text{basic}} - V^{\mathfrak{z}}_{\text{basic}} \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 - C' V^{\mathfrak{z}}_{\text{basic}} (\underset{\sim}{N}_*)^{-5/3} \sum_{s=1}^{q} \left\langle \mathcal{N}^{5/3}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle .$$

For any positive semidefinite quadratic form $|||\ \cdot\ |||$ on a vector space, we have

$$|||x+y|||^2 \geq (1-\tau)|||x|||^2 - \frac{C}{\tau}|||y|||^2.$$

We use this for

$$|||\Phi|||^2 = \langle V\Phi, \Phi\rangle\,,\ x = \Phi^{\mathfrak{z}}_{\text{main}},\ y = \Phi^{\mathfrak{z}}_{\text{error}}.$$

Thus

$$\langle V\Psi, \Psi\rangle \geq (1-\tau) \left\langle V\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle - \frac{C}{\tau} \left\langle V\Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}} \right\rangle . \tag{116}$$

To control $\langle V\Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}}\rangle$, suppose we are given $x_1 \ldots x_N \in T$. If more than $\underset{\sim}{N}_*$ of the x_j belong to $(Q+\mathfrak{z})$, then $V(x_1 \ldots x_N) = 0$ by definition. If at most $\underset{\sim}{N}_*$ of the x_j belong to $(Q+\mathfrak{z})$, then the sum $\sum_{j \neq k} K_{\mathfrak{z}}(x_j, x_k)$ contains at most $(\underset{\sim}{N}_*)^2$ non-zero terms, since $K_{\mathfrak{z}}(\ \cdot\ )$ is supported in $(Q+\mathfrak{z}) \times (Q+\mathfrak{z})$. Therefore, $|V(x_1 \ldots x_N)| \leq (\underset{\sim}{N}_*)^2 \|K_{\mathfrak{z}}\|_{L^\infty}$ for almost all $x_1 \ldots x_N$, which shows that

$$\langle V\Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}}\rangle \leq (\underset{\sim}{N}_*)^2 \|K_{\mathfrak{z}}\|_{L^\infty} \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2.$$

Combining this with (115), (116), we see that

$$\langle V\Psi, \Psi\rangle \geq \tag{117}$$

$$(1-\tau) V^{\mathfrak{z}}_{\text{basic}} - V^{\mathfrak{z}}_{\text{basic}} \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 - C V^{\mathfrak{z}}_{\text{basic}} (\underset{\sim}{N}_*)^{-5/3} \sum_{s=1}^{q} \left\langle \mathcal{N}^{5/3}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle$$

$$- \frac{C}{\tau} (\underset{\sim}{N}_*)^2 \|K_{\mathfrak{z}}\|_{L^\infty} \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2.$$

Since

$$\sum_{\substack{j,k \in J \\ j \neq k}} K_{\mathfrak{z}}(x_j, x_k) \leq \|K_{\mathfrak{z}}\|_{L^\infty} \cdot (\text{Number of } j \in J)^2 = \|K_{\mathfrak{z}}\|_{L^\infty} \cdot (\underset{\sim}{N}_1 + \cdots + \underset{\sim}{N}_q)^2$$

$\leq \|K_{\mathfrak{z}}\|_{L^\infty} (\underset{\sim}{N}_*)^2$ for almost all $(x_j)_{j \in J}$, it follows that $V^{\mathfrak{z}}_{\text{basic}} \leq \|K_{\mathfrak{z}}\|_{L^\infty} (\underset{\sim}{N}_*)^2$.

Therefore, the right-hand side of (117) simplifies, and we have

$$\langle V\Psi,\Psi\rangle \geq V^{\mathfrak{z}}_{\text{basic}} - \Big\{\tau V^{\mathfrak{z}}_{\text{basic}} + \frac{C}{\tau}(\underline{\mathrm{N}}_*)^2 \|K_{\mathfrak{z}}\|_{L^\infty} \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 + CV^{\mathfrak{z}}_{\text{basic}}(\underline{\mathrm{N}}_*)^{-5/3} \sum_{s=1}^{q} \Big\langle \mathcal{N}^{5/3}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \Big\rangle \Big\}.$$

This immediately implies the conclusion of Lemma 15, since $\sum_{1\leq j<k\leq N} K_{\mathfrak{z}}(x_j,x_k) \geq V(x_1 \dots x_N)$. □

To apply Lemma 15, we have to compute $V^{\mathfrak{z}}_{\text{basic}}$.

Lemma 16: *Let $K_{\mathfrak{z}}(x,y)$ and $V^{\mathfrak{z}}_{\text{basic}}$ be as in the previous lemma, and assume also that $K_{\mathfrak{z}}(x,y)$ is supported in $\{|x-y| \leq C\underline{N}^{3\epsilon-\frac{1}{9}} \operatorname{diam} Q\}$. Then*

$$V^{\mathfrak{z}}_{\text{basic}} = \frac{1}{2} \int\limits_{T\times T} K_{\mathfrak{z}}(x,y) \left\{ \rho^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2 \right\} dxdy + V_{\text{error}}(\mathfrak{z}),$$

with

$$|V_{\text{error}}(\mathfrak{z})| \leq C_\epsilon \rho^2 \underline{N}^{3\epsilon - \frac{1}{9}} \int\limits_{T\times T} K_{\mathfrak{z}}(x,y) dxdy.$$

Proof: Recall that

$$\Phi^{\mathfrak{z}}_{\text{basic}}((x_j)_{j\in J}) = \left(\prod_{s=1}^{q} \underline{\mathrm{N}}_s!\right)^{-1/2} \sum_{\sigma} (\operatorname{sgn}\sigma) \left(\prod_{s=1}^{q} \prod_{\substack{j\in J \\ \text{spin}(j)=s}} \varphi^{\mathfrak{z}}_{\widetilde{\beta}_{\sigma j},s}(x_j) \right)$$

where σ runs over spin-preserving permutations of J. Hence

(118)

$$V^{\mathfrak{z}}_{\text{basic}} = \left\langle \frac{1}{2} \sum_{\substack{a,b\in J \\ a\neq b}} K_{\mathfrak{z}}(x_a,x_b) \Phi^{\mathfrak{z}}_{\text{basic}}, \Phi^{\mathfrak{z}}_{\text{basic}} \right\rangle =$$

$$\frac{1}{2}\left(\prod_{s=1}^{q} \underline{\mathrm{N}}_s!\right)^{-1} \sum_{\substack{a,b\in J \\ a\neq b \\ \sigma,\pi}} (\operatorname{sgn}\sigma)\cdot(\operatorname{sgn}\pi) \int\limits_{T^{|J|}} K_{\mathfrak{z}}(x_a,x_b) \prod_{s=1}^{q} \left(\prod_{\substack{j\in J \\ \text{spin}(j)=s}} \varphi^{\mathfrak{z}}_{\widetilde{\beta}_{\sigma j},s}(x_j) \overline{\varphi^{\mathfrak{z}}_{\widetilde{\beta}_{\pi j},s}(x_j)} \right)$$

$$\cdot \prod_{j\in J} dx_j$$

For fixed $\mathfrak{z}$, s, the $\varphi^{\mathfrak{z}}_{\alpha s}$ are orthonormal, and for fixed s, the $\widetilde{\beta}_j$ with $j \in J$ of spin s are all distinct. Hence in (118) we may carry out all the integrations except for the dx_a and dx_b-integrals; and the only non-zero terms are those with $\sigma j = \pi j$ for all $j \neq a,b$.

Thus, a non-zero term in (118) has $\pi = \sigma$ or else $\pi = \sigma\tau_{ab}$, where τ_{ab} denotes the transposition that interchanges a and b, and fixes the other $j \in J$. Since in (118) σ and π vary only over spin-preserving permutations, we can have $\pi = \sigma\tau_{ab}$ only when a and b have the same spin. These remarks allow us to rewrite (118) as follows.

$$
\begin{aligned}
V^{\mathfrak{z}}_{\text{basic}} = \\
&\frac{1}{2}\left(\prod_{s=1}^{q} \underset{\sim}{\mathrm{N}}_s!\right)^{-1} \sum_{\substack{a,b\in J\\ a\neq b\\ \sigma}} \int_{T^2} K_{\mathfrak{z}}(x_a,x_b)|\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma a},\mathrm{spin}(a)}(x_a)|^2|\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma b},\mathrm{spin}(b)}(x_b)|^2 dx_a dx_b - \\
&\frac{1}{2}\left(\prod_{s=1}^{q} \underset{\sim}{\mathrm{N}}_s!\right)^{-1} \sum_{\substack{a,b\in J\\ a\neq b\\ \mathrm{spin}(a)=\mathrm{spin}(b)\\ \sigma}} \int_{T^2} K_{\mathfrak{z}}(x_a,x_b)\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma a},\mathrm{spin}(a)}(x_a)\overline{\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma b},\mathrm{spin}(a)}(x_a)}\cdot \\
&\qquad\qquad \varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma b},\mathrm{spin}(b)}(x_b)\overline{\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma a},\mathrm{spin}(b)}(x_b)} dx_a dx_b.
\end{aligned}
$$

We can remove the restriction $a \neq b$ from the two sums on the right, since the contributions to those sums from $a = b$ will cancel each other. Therefore,

$$
\begin{aligned}
V^{\mathfrak{z}}_{\text{basic}} = \\
&\frac{1}{2}\left(\prod_{s=1}^{q} \underset{\sim}{\mathrm{N}}_s!\right)^{-1} \sum_{\substack{a,b\in J\\ \sigma}} \int_{T^2} K_{\mathfrak{z}}(x,y)|\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma a},\mathrm{spin}(a)}(x)|^2|\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma b},\mathrm{spin}(b)}(y)|^2 dx dy - \\
&\frac{1}{2}\left(\prod_{s=1}^{q} \underset{\sim}{\mathrm{N}}_s!\right)^{-1} \sum_{s=1}^{q} \sum_{\substack{a,b\in J\\ \mathrm{spin}(a)=s\\ \mathrm{spin}(b)=s\\ \sigma}} \int_{T^2} K_{\mathfrak{z}}(x,y)\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma a},s}(x)\overline{\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma b},s}(x)}\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma b},s}(y)\overline{\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\sigma a},s}(y)} dx dy
\end{aligned}
$$

For fixed σ, we change dummy indices from a, b to $\mu = \sigma a$, $\nu = \sigma b$. Thus,

$$
\begin{aligned}
(119)\quad V^{\mathfrak{z}}_{\text{basic}} = \\
&\frac{1}{2}\left(\prod_{s=1}^{q} \underset{\sim}{\mathrm{N}}_s!\right)^{-1} \sum_{\substack{\mu,\nu\in J\\ \sigma}} \int_{T^2} K_{\mathfrak{z}}(x,y)|\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\mu},\mathrm{spin}(\mu)}(x)|^2|\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\nu},\mathrm{spin}(\nu)}(y)|^2 dx dy - \\
&\frac{1}{2}\left(\prod_{s=1}^{q} \underset{\sim}{\mathrm{N}}_s!\right)^{-1} \sum_{s=1}^{q} \sum_{\substack{\mu,\nu\in J\\ \mathrm{spin}(\mu)=s\\ \mathrm{spin}(\nu)=s\\ \sigma}} \int_{T^2} K_{\mathfrak{z}}(x,y)\left[\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\mu},s}(x)\overline{\varphi_{\underset{\sim}{\beta}_{\mu},s}(y)}\right]\left[\overline{\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\nu},s}(x)}\varphi^{\mathfrak{z}}_{\underset{\sim}{\beta}_{\nu},s}(y)\right] dx dy
\end{aligned}
$$

The summands here are independent of σ, and the number of possible σ is $\prod_{s=1}^{q} \underset{\sim}{\mathrm{N}}_s!$. Hence the factors $\left(\prod_{s=1}^{q} \underset{\sim}{\mathrm{N}}_s!\right)^{-1}$ cancel the summations over σ.

So, with

$$\mathcal{S}_s^{\text{basic}}(x,y) = \sum_{\substack{j\in J\\ \text{spin}(j)=s}} \varphi_{\widetilde{\beta}_j,s}(x)\overline{\varphi_{\widetilde{\beta}_j,s}(y)} = \sum_{1\le\alpha\le\underline{\mathrm{N}}_s} \varphi_{\alpha,s}(x)\overline{\varphi_{\alpha,s}(y)} \tag{120}$$

and with

$$\rho_{\text{basic}}(x) = \sum_{j\in J} |\varphi_{\widetilde{\beta}_j,\text{spin}(j)}(x)|^2 = \sum_{s=1}^{q}\Big(\sum_{\substack{j\in J\\ \text{spin}(j)=s}} |\varphi_{\widetilde{\beta}_j,s}(x_j)|^2\Big) = \sum_{s=1}^{q} \mathcal{S}_s^{\text{basic}}(x,x), \tag{121}$$

we can rewrite (119) in the form

$$\begin{aligned} V^{\mathfrak{z}}_{\text{basic}} = \frac{1}{2}\int\limits_{T\times T} K_{\mathfrak{z}}(x,y)\rho_{\text{basic}}(x-\mathfrak{z})\rho_{\text{basic}}(y-\mathfrak{z})dxdy \\ -\frac{1}{2}\sum_{s=1}^{q}\int\limits_{T\times T} K_{\mathfrak{z}}(x,y)|\mathcal{S}_s^{\text{basic}}(x-\mathfrak{z},y-\mathfrak{z})|^2 dxdy. \end{aligned} \tag{122}$$

The second equality in (120) follows from the defining properties of $(\widetilde{\beta}_j)_{j\in J}$. To pass from (119) to (122), we recall that $\varphi^{\mathfrak{z}}_{\alpha,s}(x) = \varphi_{\alpha,s}(x-\mathfrak{z})$.

Equations (121), (122) reduce the computation of $V^{\mathfrak{z}}_{\text{basic}}$ to that of $\mathcal{S}_s^{\text{basic}}(x,y)$. From (41) we see that

$$|\mathcal{S}_s^{\text{basic}}(x,y) - \mathcal{S}_{\rho_s}(x-y)| \le C_\varepsilon \rho_s \cdot \underline{\mathrm{N}}^{3\varepsilon-1/9} \tag{123}$$

for $x,y\in Q_0$ and $|x-y| < \underline{\mathrm{N}}^{3\varepsilon-1/9}\operatorname{diam} Q$. Recall that $\mathcal{S}_{\rho_s}(x-y)$ is given by (18), (19). In particular, $\mathcal{S}_{\rho_s}(0)=\rho_s$.

From (123), we see that

$$|\mathcal{S}_s^{\text{basic}}(x-\mathfrak{z},y-\mathfrak{z}) - \mathcal{S}_{\rho_s}(x-y)| \le C_\varepsilon\rho_s\cdot\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}} \text{ for } (x,y)\in\operatorname{supp} K_{\mathfrak{z}}$$

and in particular,

$$|\mathcal{S}_s^{\text{basic}}(x-\mathfrak{z},x-\mathfrak{z}) - \rho_s| \le C_\varepsilon\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}}\rho_s \text{ for } x\in(Q_0+\mathfrak{z}).$$

Summing the last inequality over s, we get

$$|\rho_{\text{basic}}(x-\mathfrak{z}) - \rho| \le C_\varepsilon\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}}\rho \text{ for } x\in(Q_0+\mathfrak{z}).$$

Therefore, for $(x,y)\in\operatorname{supp}K_{\mathfrak{z}}$ we can write

$$\begin{aligned} &\rho_{\text{basic}}(x-\mathfrak{z}) = \rho + g_{\mathfrak{z}}(x),\ \ \rho_{\text{basic}}(y-\mathfrak{z}) = \rho + g_{\mathfrak{z}}(y),\\ &\mathcal{S}_s^{\text{basic}}(x-\mathfrak{z},y-\mathfrak{z}) = \mathcal{S}_{\rho_s}(x-y) + f_{\mathfrak{z}}(x,y), \end{aligned}$$

with

$$|g_{\mathfrak{z}}(x)|,\ |g_{\mathfrak{z}}(y)|\ |f_{\mathfrak{z}}(x-y)| \leq C_\varepsilon \underline{\mathrm{N}}^{3\varepsilon-1/9}\rho.$$

Since also $|\mathcal{S}_{\rho_s}(x-y)| \leq C\rho$, it follows that

(124)

$$\rho_{\,\text{basic}}(x-\mathfrak{z})\rho_{\,\text{basic}}(y-\mathfrak{z}) - \sum_{s=1}^{q} |\mathcal{S}_s^{\text{basic}}(x-\mathfrak{z}, y-\mathfrak{z})|^2 =$$

$$\rho^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2 + \mathrm{Error}_{\mathfrak{z}}(x,y) \text{ for } (x,y) \in \operatorname{supp} K_{\mathfrak{z}},$$

where

(125) $$|\mathrm{Error}_{\mathfrak{z}}(x,y)| \leq C_\varepsilon \underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}}\rho^2.$$

Putting (124) into (122), we get

(126) $$V^{\mathfrak{z}}_{\text{basic}} = \frac{1}{2}\int\limits_{T\times T} K_{\mathfrak{z}}(x,y)\left\{\rho^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2\right\} dxdy + V_{\text{error}}(\mathfrak{z}),$$

with

$$V_{\text{error}}(\mathfrak{z}) = \frac{1}{2}\int\limits_{T\times T} K_{\mathfrak{z}}(x,y)\mathrm{Error}_{\mathfrak{z}}(x,y)dxdy,$$

so that

(127) $$|V_{\text{error}}(\mathfrak{z})| \leq C_\varepsilon \underline{\mathrm{N}}^{3\varepsilon-1/9}\rho^2 \int\limits_{T\times T} K_{\mathfrak{z}}(x,y)dxdy.$$

Equations (126), (127) are the conclusions of Lemma 16. □

Corollary: $0 \leq V^{\mathfrak{z}}_{\text{basic}} \leq C\rho^2 \int\limits_{T\times T} K_{\mathfrak{z}}(x,y)dxdy.$

Proof: The second inequality follows by dropping the $\mathcal{S}_{\rho_s}(x-y)$-terms in the conclusion of Lemma 16. The first inequality is immediate from the definition of $V^{\mathfrak{z}}_{\text{basic}}$. □

To clarify the meaning of $\{(x,y) \mid |x-y| < C\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}}\operatorname{diam} Q\}$ in the statement of Lemma 16, recall that $\underline{\mathrm{N}} \sim \rho|Q|$. Hence, $|x-y| < C\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}}\operatorname{diam} Q$ means that

$$\rho^{1/3}|x-y| < C\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}}\rho^{1/3}\operatorname{diam} Q \sim C\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}}(\rho|Q|)^{1/3} \sim C\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}}\underline{\mathrm{N}}^{1/3}, \text{ i.e.}$$

$$\rho^{1/3}|x-y| \leq C\underline{\mathrm{N}}^{3\varepsilon+\frac{2}{9}}.$$

We are ready to apply Lemmas 15, 16 and equations (73), (75) to derive one of our main results. Suppose we are given $K(x,y)$ on $T \times T$, with $0 \leq K(x,y) = K(y,x) \leq \frac{C}{|x-y|}\chi_{|x-y|<r_{\max}}$. Say $\rho r_{\max}^3 \geq c$. Set

$$K_{\mathfrak{z}}(x,y) = K(x,y) \cdot \chi_{(Q_0+\mathfrak{z})}(x) \cdot \chi_{(Q_0+\mathfrak{z})}(y) \cdot \chi_{|x-y|>r_{\min}}$$

with $r_{\min}$ to be picked later. Then

$$\text{(127 bis)} \qquad \|K_{\mathfrak{z}}\|_{L^\infty} \leq \frac{C}{r_{\min}},$$

and

$$\text{(128)} \qquad \int\limits_{T\times T} K_{\mathfrak{z}}(x,y)dxdy \leq \int\limits_{\substack{x\in(Q_0+\mathfrak{z})\\ |y-x|<r_{\max}}} \frac{C}{|x-y|}dydx \leq C' r_{\max}^2|Q|.$$

Hence,

$$\text{(129)} \qquad 0 \leq V_{\text{basic}}^{\mathfrak{z}} \leq C'\rho^2|Q|r_{\max}^2 \leq C''\rho\underline{\mathrm{N}}r_{\max}^2,$$

by the Corollary to Lemma 16 (recall that $\underline{\mathrm{N}} \sim \rho|Q|$).

If $r_{\max} \leq C\underline{\mathrm{N}}^{-1/9}(\operatorname{diam} Q)$, then Lemma 16 applies, and we obtain

$$\begin{aligned} V_{\text{basic}}^{\mathfrak{z}} &\geq \frac{1}{2}\int\limits_{T\times T} K_{\mathfrak{z}}(x,y)\left\{\rho^2 - \sum_{s=1}^{q}|\mathcal{S}_{\rho_s}(x-y)|^2\right\}dxdy - C_\varepsilon\rho^2\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}}\cdot r_{\max}^2|Q| \\ &= \frac{1}{2}\int\limits_{T\times T} K_{\mathfrak{z}}(x,y)\left\{\rho^2 - \sum_{s=1}^{q}|\mathcal{S}_{\rho_s}(x-y)|^2\right\}dxdy - C_\varepsilon\rho r_{\max}^2\underline{\mathrm{N}}^{3\varepsilon+\frac{8}{9}}. \end{aligned}$$

Putting this, (127 bis) and (129) into Lemma 15, we learn that

$$\begin{aligned} \text{(130)} \quad &\left\langle \sum_{1\leq j<k\leq N} K_{\mathfrak{z}}(x_j,x_k)\Psi,\Psi\right\rangle \geq \\ &\left[\frac{1}{2}\iint\limits_{T\times T} K_{\mathfrak{z}}(x,y)\left\{\rho^2 - \sum_{s=1}^{q}|\mathcal{S}_{\rho_s}(x-y)|^2\right\}dxdy - C_\varepsilon\rho r_{\max}^2\underline{\mathrm{N}}^{3\varepsilon+\frac{8}{9}}\right] \\ &\quad - C\tau\rho\underline{\mathrm{N}}r_{\max}^2 - \frac{C(\underline{\mathrm{N}}_*)^2}{\tau r_{\min}}\|\Phi_{\text{error}}^{\mathfrak{z}}\|^2 - \frac{C\rho\underline{\mathrm{N}}r_{\max}^2}{(\underline{\mathrm{N}}_*)^{5/3}}\sum_{s=1}^{q}\left\langle \mathcal{N}_{s\mathfrak{z}}^{5/3}\Phi_{\text{main}}^{\mathfrak{z}},\Phi_{\text{main}}^{\mathfrak{z}}\right\rangle. \end{aligned}$$

Next, we integrate (130) over $\mathfrak{z} \in T$. Note that

$$\int_{\mathfrak{z}\in T} K_{\mathfrak{z}}(x,y)d\mathfrak{z} \leq \int_{\mathfrak{z}\in T} K(x,y)\chi_{Q_0+\mathfrak{z}}(x)d\mathfrak{z} = |Q_0|K(x,y),$$

and therefore

$$\int_{\mathfrak{z}\in T} \left\langle \sum_{1\leq j<k\leq N} K_{\mathfrak{z}}(x_j,x_k)\Psi,\Psi\right\rangle d\mathfrak{z} \leq |Q_0|\left\langle \sum_{1\leq j<k\leq N} K(x_j,x_k)\Psi,\Psi\right\rangle.$$

Hence, (130) yields

$$(131)\quad |Q_0|\cdot\left\langle \sum_{1\leq j<k\leq N} K(x_j,x_k)\Psi,\Psi\right\rangle \geq$$
$$\frac{1}{2}\iiint_{T\times T\times T} K_{\mathfrak{z}}(x,y)\left\{\rho^2 - \sum_{s=1}^{q}|\mathcal{S}_{\rho_s}(x-y)|^2\right\}dxdyd\mathfrak{z} -$$
$$L^3\cdot\left\{C_\varepsilon\rho r_{\max}^2\underline{\mathrm{N}}^{3\varepsilon+\frac{8}{9}} + C\tau\rho\underline{\mathrm{N}}r_{\max}^2\right\} - \frac{C(\underline{\mathrm{N}}_*)^2}{\tau r_{\min}}\int_{\mathfrak{z}\in T}\|\Phi^{\mathfrak{z}}_{\mathrm{error}}\|^2 d\mathfrak{z}$$
$$-\frac{C\rho\underline{\mathrm{N}}r_{\max}^2}{(\underline{\mathrm{N}}_*)^{5/3}}\sum_{s=1}^{q}\int_{\mathfrak{z}\in T}\left\langle \mathcal{N}_{s\mathfrak{z}}^{5/3}\Phi^{\mathfrak{z}}_{\mathrm{main}},\Phi^{\mathfrak{z}}_{\mathrm{main}}\right\rangle d\mathfrak{z}.\ \text{(Recall vol}\,T = L^3.\text{)}$$

From (73), (75) we have

$$\int_{\mathfrak{z}\in T}\|\Phi^{\mathfrak{z}}_{\mathrm{error}}\|^2 d\mathfrak{z} \leq L^3\cdot\left[C_{m\varepsilon}\underline{\mathrm{N}}^{-m} + C\underline{\mathrm{N}}^2\cdot(\delta+N^{-1/3})^{1/2}\right],\ \text{and}$$
$$\int_{\mathfrak{z}\in T}\left\langle \mathcal{N}_{s\mathfrak{z}}^{5/3}\Phi^{\mathfrak{z}}_{\mathrm{main}},\Phi^{\mathfrak{z}}_{\mathrm{main}}\right\rangle d\mathfrak{z} \leq CL^3\underline{\mathrm{N}}^{5/3}.$$

Putting these estimates into (131), we find that

$$(132)\quad |Q_0|\cdot\left\langle \sum_{1\leq j<k\leq N} K(x_j,x_k)\Psi,\Psi\right\rangle \geq$$
$$\frac{1}{2}\iiint_{T\times T\times T} K_{\mathfrak{z}}(x,y)\left\{\rho^2 - \sum_{s=1}^{q}|\mathcal{S}_{\rho_s}(x-y)|^2\right\}dxdyd\mathfrak{z} -$$
$$C_{m\varepsilon}L^3\cdot\left\{\rho r_{\max}^2\underline{\mathrm{N}}^{3\varepsilon+\frac{8}{9}} + \tau\rho r_{\max}^2\underline{\mathrm{N}} + \frac{(\underline{\mathrm{N}}_*)^2}{\tau r_{\min}}\underline{\mathrm{N}}^{-m} + \frac{(\underline{\mathrm{N}}_*)^2}{\tau r_{\min}}\underline{\mathrm{N}}^2(\delta+N^{-1/3})^{1/2}\right.$$
$$\left. + \frac{\rho r_{\max}^2(\underline{\mathrm{N}})^{8/3}}{(\underline{\mathrm{N}}_*)^{5/3}}\right\}.$$

Now

(133)

$$\left\{\rho^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2\right\} = \left(\sum_{s=1}^{q} \rho_s\right)^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2$$

$$\geq \sum_{s=1}^{q} (\rho_s^2 - |\mathcal{S}_{\rho_s}(x-y)|^2) \geq 0, \text{ by definition of } \mathcal{S}_{\rho_s}.$$

Also,

(134)

$$\frac{1}{2}\int_{\mathfrak{z}\in T} K_{\mathfrak{z}}(x,y)d\mathfrak{z} = \frac{1}{2}\int_{\mathfrak{z}\in T} \left[\chi_{|x-y|>r_{\min}} K(x,y)\right] \cdot \chi_{Q_0+\mathfrak{z}}(x) \cdot \chi_{Q_0+\mathfrak{z}}(y)d\mathfrak{z}$$

$$= \frac{1}{2}\chi_{|x-y|>r_{\min}} K(x,y) \cdot \mathrm{vol}\{(Q_0+x)\cap(Q_0+y)\} \geq$$

$$\frac{1}{2}\chi_{|x-y|>r_{\min}} K(x,y) \cdot |Q_0| \cdot \left(1 - \frac{C|x-y|}{\operatorname{diam} Q_0}\right) =$$

$$\frac{1}{2}K(x,y)|Q_0| \cdot \left(1 - \frac{C|x-y|}{\operatorname{diam} Q_0}\right) - \frac{1}{2}\chi_{|x-y|\leq r_{\min}} K(x,y) \cdot |Q_0| \cdot \left(1 - \frac{C|x-y|}{\operatorname{diam} Q_0}\right)$$

$$\geq \frac{1}{2}K(x,y)|Q_0| \cdot \left(1 - \frac{C|x-y|}{\operatorname{diam} Q_0}\right) - \frac{1}{2}\chi_{|x-y|\leq r_{\min}} K(x,y) \cdot |Q_0|$$

$$\geq \frac{1}{2}|Q_0|K(x,y) - C|Q_0| \cdot \left(\frac{\chi_{|x-y|<r_{\max}}}{|x-y|}\right) \cdot \frac{|x-y|}{\operatorname{diam} Q_0}$$

$$- C\chi_{|x-y|\leq r_{\min}} \left(\frac{1}{|x-y|}\right) |Q_0|$$

$$= \frac{1}{2}|Q_0|K(x,y) - C|Q_0|^{2/3}\chi_{|x-y|<r_{\max}} - \frac{C|Q_0|}{|x-y|}\chi_{|x-y|\leq r_{\min}}$$

From (133) and (134) we get

$$\frac{1}{2}\iiint_{T\times T\times T} K_{\mathfrak{z}}(x,y)\left\{\rho^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2\right\} dx dy d\mathfrak{z} \geq$$

$$\frac{1}{2}|Q_0| \iint_{T\times T} K(x,y)\left\{\rho^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2\right\} dx dy -$$

$$C|Q_0|^{2/3} \iint_{T\times T} \chi_{|x-y|<r_{\max}} \left\{\rho^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2\right\} dx dy -$$

$$C|Q_0| \iint_{T\times T} \frac{\chi_{|x-y|\leq r_{\min}}}{|x-y|} \cdot \left\{\rho^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2\right\} dx dy$$

$$
\begin{aligned}
&\geq \frac{1}{2}|Q_0| \iint\limits_{T\times T} K(x,y)\cdot \left\{ \rho^2 - \sum_{s=1}^{q} |\mathbb{S}_{\rho_s}(x-y)|^2 \right\} dxdy \\
&\qquad - C|Q_0|^{2/3} \iint\limits_{T\times T} \chi_{|x-y|<r_{\max}} \rho^2 dxdy \\
&\qquad - C|Q_0| \iint\limits_{T\times T} \frac{\chi_{|x-y|\leq r_{\min}}}{|x-y|} \rho^2 dxdy \\
&\geq \frac{1}{2}|Q_0| \iint\limits_{T\times T} K(x,y)\cdot \left\{ \rho^2 - \sum_{s=1}^{q} |\mathbb{S}_{\rho_s}(x-y)|^2 \right\} dxdy \\
&\qquad\qquad - C\rho^2 r_{\max}^3 L^3 |Q_0|^{2/3} - C\rho^2 r_{\min}^2 |Q_0| L^3
\end{aligned}
$$

Putting this into (132), we get

$$
\begin{aligned}
&|Q_0|\cdot \left\langle \sum_{1\leq j<k\leq N} K(x_j,x_k)\Psi,\Psi \right\rangle \geq \\
&\quad \frac{1}{2}|Q_0|\cdot \iint\limits_{T\times T} K(x,y) \left\{ \rho^2 - \sum_{s=1}^{q} |\mathbb{S}_{\rho_s}(x,y)|^2 \right\} dxdy - \\
&\quad C_{m\varepsilon} L^3 \cdot \Bigg\{ \rho^2 r_{\max}^3 |Q_0|^{2/3} + \rho^2 r_{\min}^2 |Q_0| + \rho r_{\max}^2 \underline{\mathrm{N}}^{3\varepsilon+\frac{8}{9}} \\
&\quad + \tau\rho r_{\max}^2 \underline{\mathrm{N}} + \frac{(\underline{\mathrm{N}}_*)^2 \underline{\mathrm{N}}^{-m}}{\tau r_{\min}} + \frac{(\underline{\mathrm{N}}_*)^2 \underline{\mathrm{N}}^2}{\tau r_{\min}} \cdot (\delta + N^{-1/3})^{1/2} \\
&\qquad\qquad + \rho r_{\max}^2 (\underline{\mathrm{N}})^{8/3} (\underline{\mathrm{N}}_*)^{-5/3} \Bigg\}.
\end{aligned}
$$

Dividing both sides by $|Q_0|$ and recalling that $\rho \sim \underline{\mathrm{N}}/|Q_0|$, we get

$$
\begin{aligned}
&\left\langle \sum_{1\leq j<k\leq N} K(x_j,x_k)\Psi,\Psi \right\rangle \geq \frac{1}{2} \iint\limits_{T\times T} K(x,y) \left\{ \rho^2 - \sum_{s=1}^{q} |\mathbb{S}_{\rho_s}(x-y)|^2 \right\} dxdy \\
&\quad - C_{m\varepsilon} L^3 \cdot \Bigg\{ \rho^2 r_{\max}^3 \cdot (\rho^{-1}\underline{\mathrm{N}})^{-1/3} + \rho^2 r_{\min}^2 + \rho r_{\max}^2 \underline{\mathrm{N}}^{3\varepsilon+8/9} (\rho \underline{\mathrm{N}}^{-1}) + \tau r_{\max}^2 \rho^2 \\
&\qquad + \frac{(\underline{\mathrm{N}}_*)^2 \underline{\mathrm{N}}^{-(m+1)}}{\tau r_{\min}} \rho + \frac{(\underline{\mathrm{N}}_*)^2 \underline{\mathrm{N}} \rho}{\tau r_{\min}} \cdot (\delta + N^{-1/3})^{1/2} + \rho^2 r_{\max}^2 (\underline{\mathrm{N}}/\underline{\mathrm{N}}_*)^{5/3} \Bigg\}.
\end{aligned}
$$

Since $\rho L^3 \sim N$, this can be rewritten in the form:

$$
\begin{aligned}
&\left\langle \sum_{1\leq j<k\leq N} K(x_j,x_k)\Psi,\Psi \right\rangle \geq \\
&\frac{1}{2} \iint\limits_{T\times T} K(x,y) \left\{ \rho^2 - \sum_{s=1}^{q} |\mathbb{S}_{\rho_s}(x-y)|^2 \right\} dxdy - C_{m\varepsilon} \rho^{1/3} N \widetilde{E},
\end{aligned}
\tag{135}
$$

with

(136)
$$\widetilde{E} = \rho r_{\max}^3 \underline{N}^{-1/3} + \rho^{2/3} r_{\min}^2 + \rho^{2/3} r_{\max}^2 \underline{N}^{3\varepsilon - 1/9} + \tau \rho^{2/3} r_{\max}^2 + \frac{(\underline{N}_*)^2 \underline{N}^{-(m+1)}}{\tau r_{\min} \rho^{1/3}} + \frac{(\underline{N}_*)^2 \underline{N}}{\tau r_{\min} \rho^{1/3}} \cdot (\delta + N^{-1/3})^{1/2} + \rho^{2/3} r_{\max}^2 (\underline{N}/\underline{N}_*)^{5/3}$$

These equations hold provided τ, $\underline{N}$ and $\underline{N}_*$ satisfy the constraints

$$0 < \tau < 1,\ \underline{N}_* > C\underline{N} > C' \quad \text{and} \quad r_{\max} \le C\underline{N}^{-1/9}(\operatorname{diam} Q), \rho r_{\max}^3 > c$$

which we assumed above in order to apply Lemmas 15 and 16. Since $\rho \sim \underline{N}/|Q|$, the constraints may be written as

$$0 < \tau < 1,\ \underline{N}_* > C\underline{N} > C',\ r_{\max} \le C\underline{N}^{-1/9} \cdot (\rho^{-1}\underline{N})^{1/3}, \rho r_{\max}^3 > c$$

i.e.

(137)
$$0 < \tau < 1,\ \underline{N}_* > C\underline{N},\ \underline{N} > C,\ \rho^{1/3} r_{\max} \le C\underline{N}^{2/9}, \rho r_{\max}^3 > c.$$

Thus, (137) implies (135), (136). If (137) holds, then

$$\rho r_{\max}^3 \underline{N}^{-1/3} = (\rho^{2/3} r_{\max}^2 \underline{N}^{3\varepsilon - 1/9}) \cdot (\rho^{1/3} r_{\max} \underline{N}^{-2/9 - 3\varepsilon}) \le C \rho^{2/3} r_{\max}^2 \underline{N}^{3\varepsilon - \frac{1}{9}}.$$

The left and right sides are both terms in the definition (136) of $\widetilde{E}$. Hence, deleting the term $\rho r_{\max}^3 \underline{N}^{-1/3}$ from (136) does not affect the order of magnitude of $\widetilde{E}$. Therefore, we have proven the following result.

Lemma 17: *Suppose we have τ, $\underline{N}$, $\underline{N}_*$, $r_{\min}, r_{\max}$ with $0 < \tau < 1$, $\underline{N} > C$, $\underline{N}_* > C\underline{N}$, $\rho^{1/3} r_{\max} \le C\underline{N}^{2/9}$. Suppose $K(x,y)$ is defined on $T \times T$ and satisfies $0 \le K(x,y) = K(y,x) \le C|x-y|^{-1}\chi_{|x-y|<r_{\max}}$, with $\rho r_{\max}^3 > c$. Then*

$$\left\langle \sum_{1 \le j < k \le N} K(x_j, x_k)\Psi, \Psi \right\rangle \ge \frac{1}{2} \iint_{T \times T} K(x,y) \left\{ \rho^2 - \sum_{s=1}^{q} |\mathbb{S}_{\rho_s}(x-y)|^2 \right\} dxdy - C_{m\varepsilon} \rho^{1/3} N E_{\#}$$

with

(138)
$$E_{\#} = \rho^{2/3} r_{\max}^2 \underline{N}^{3\varepsilon - 1/9} + \rho^{2/3} r_{\min}^2 + \tau \rho^{2/3} r_{\max}^2 + \frac{(\underline{N}_*)^2 \underline{N}^{-(m+1)}}{\tau r_{\min} \rho^{1/3}} + \frac{(\underline{N}_*)^2 \underline{N}}{\tau r_{\min} \rho^{1/3}} \cdot (\delta + N^{-1/3})^{1/2} + \rho^{2/3} r_{\max}^2 (\underline{N}/\underline{N}_*)^{5/3}.$$

In (138), the numbers δ, N, ρ, $r_{\max}$ are given. However, by varying the size of the cube Q, we may control the order of magnitude of $\underset{\sim}{\mathrm{N}}$. We can arrange for any order of magnitude for which

$$C_\varepsilon < \underset{\sim}{\mathrm{N}} < cN. \tag{139}$$

We may also pick τ, $\underset{\sim}{\mathrm{N}}_*$ and $r_{\min}$. In order to use Lemma 17, we need to assure that

$$0 < \tau < 1,\ \underset{\sim}{\mathrm{N}}_* > C\underset{\sim}{\mathrm{N}},\ \rho^{1/3} r_{\max} \leq C\underset{\sim}{\mathrm{N}}^{2/9}. \tag{140}$$

With $S = (\rho r_{\max}^3) \cdot (\delta + N^{-1/3})^{-1/2}$, we take

$$\underset{\sim}{\mathrm{N}} \sim S^{\frac{90}{307}},\ \underset{\sim}{\mathrm{N}}_* \sim S^{\frac{96}{307}}\ \tau = S^{-\frac{10}{307}},\ r_{\min} = r_{\max} \cdot S^{-\frac{5}{307}}. \tag{141}$$

Then

$$\rho^{2/3} r_{\max}^2 \underset{\sim}{\mathrm{N}}^{3\varepsilon - 1/9} \sim (\rho r_{\max}^3)^{2/3} S^{\left(\frac{270}{307}\right)\varepsilon - \frac{10}{307}} \tag{142}$$

$$\rho^{2/3} r_{\min}^2 = \rho^{2/3} r_{\max}^2 S^{-\frac{10}{307}} = (\rho r_{\max}^3)^{2/3} S^{-\frac{10}{307}} \tag{143}$$

$$\tau \rho^{2/3} r_{\max}^2 = (\rho r_{\max}^3)^{2/3} S^{-\frac{10}{307}} \tag{144}$$

$$\begin{aligned} \frac{(\underset{\sim}{\mathrm{N}}_*)^2 \underset{\sim}{\mathrm{N}}}{\tau r_{\min} \rho^{1/3}} \cdot (\delta + N^{-1/3})^{\frac{1}{2}} &\sim \frac{S^{\frac{2\cdot 96}{307} + \frac{90}{307}}}{S^{-\frac{10}{307}} \cdot r_{\max} S^{-\frac{5}{307}} \rho^{1/3}} \cdot (\delta + N^{-1/3})^{1/2} \\ &= \frac{S^{\frac{2\cdot 96 + 90 + 10 + 5}{307}} \cdot (\rho r_{\max}^3)^{2/3}}{(\rho r_{\max}^3) \cdot (\delta + N^{-1/3})^{-1/2}} = \frac{S^{\frac{2\cdot 96 + 90 + 10 + 5}{307}} \cdot (\rho r_{\max}^3)^{2/3}}{S} \\ &= (\rho r_{\max}^3)^{2/3} S^{-\frac{10}{307}} \end{aligned} \tag{145}$$

$$\rho^{2/3} r_{\max}^2 (\underset{\sim}{\mathrm{N}}/\underset{\sim}{\mathrm{N}}_*)^{5/3} \sim (\rho r_{\max}^3)^{2/3} \cdot \left(S^{-\frac{6}{307}}\right)^{5/3} = (\rho r_{\max}^3)^{2/3} S^{-\frac{10}{307}} \tag{146}$$

If we take m large, then for suitable large $\tilde{m}$, m_1, m_2 we have

$$\begin{aligned} \frac{(\underset{\sim}{\mathrm{N}}_*)^2 \underset{\sim}{\mathrm{N}}^{-(m+1)}}{\tau r_{\min} \rho^{1/3}} &\sim \frac{S^{\frac{2\cdot 96}{307} - (m+1)\cdot\left(\frac{90}{307}\right)}}{S^{-\frac{10}{307}} \cdot r_{\max} S^{-\frac{5}{307}} \cdot \rho^{1/3}} = \frac{S^{-\tilde{m}}}{(\rho r_{\max}^3)^{1/3}} \\ &= (\rho r_{\max}^3)^{-m_1} \cdot (\delta + N^{-1/3})^{m_2} S^{-\frac{10}{307}} \leq C(\rho r_{\max}^3)^{2/3} S^{-\frac{10}{307}}, \end{aligned} \tag{147}$$

provided $\rho r_{\max}^3 > c$ and $\delta + N^{-1/3} < c'$. Putting (142)...(147) into the definition of $E_\#$, and noting that $S > 1$ for $\rho r_{\max}^3 > c$ and $\delta + N^{-1/3} < c'$, we get

$$E_\# \leq C_\varepsilon (\rho r_{\max}^3)^{2/3} S^{-\frac{10}{307} + 2\varepsilon} = C_\varepsilon (\rho r_{\max}^3)^{\frac{584}{921} + 2\varepsilon} \cdot (\delta + N^{-1/3})^{\frac{5}{307} - \varepsilon}. \tag{148}$$

Next, we verify the constraints (139), (140).

If $\rho r_{\max}^3 > c$ and $\delta + N^{-1/3} < c'_\varepsilon$, then $S > C'_\varepsilon$, so that $\underline{\mathrm{N}} > C_\varepsilon$, $\underline{\mathrm{N}}_* > C\underline{\mathrm{N}}$, $0 < \tau < 1$. The remaining inequalities of (139), (140) are

$$\underline{\mathrm{N}} < cN \quad \text{and} \quad \rho^{1/3} r_{\max} \leq C\underline{\mathrm{N}}^{2/9}. \tag{149}$$

The first estimate of (149) asserts that

$$S^{\frac{90}{307}} < cN, \quad \text{i.e.} \quad (\rho r_{\max}^3)^{\frac{90}{307}} < cN \cdot (\delta + N^{-1/3})^{\frac{45}{307}},$$

which follows from

$$(\rho r_{\max}^3)^{\frac{90}{307}} < cN \cdot (N^{-1/3})^{\frac{45}{307}} = cN^{1-\frac{15}{307}} = cN^{\frac{292}{307}}, \quad \text{i.e.}$$

$N > C(\rho r_{\max}^3)^{\frac{90}{292}}$. That is, the first estimate in (149) follows from the assumption $N > C(\rho r_{\max}^3)^{\frac{90}{292}}$.

The second estimate of (149) asserts that

$$(\rho r_{\max}^3)^{1/3} \leq C\left[S^{\frac{90}{307}}\right]^{\frac{2}{9}} = CS^{\frac{20}{307}} = C(\rho r_{\max}^3)^{\frac{20}{307}} \cdot (\delta + N^{-1/3})^{-\frac{10}{307}},$$

i.e.

$$\delta + N^{-1/3} \leq C\left[(\rho r_{\max}^3)^{\frac{20}{307}-\frac{1}{3}}\right]^{\frac{307}{10}} = C(\rho r_{\max}^3)^{-\frac{247}{30}},$$

i.e. $\delta < C(\rho r_{\max}^3)^{-\frac{247}{30}}$ and $N \geq C(\rho r_{\max}^3)^{+\frac{247}{10}}$. Consequently, the constraints (139), (140) hold, provided

$$\rho r_{\max}^3 > c', \ \delta < c'_\varepsilon (\rho r_{\max}^3)^{-\frac{247}{30}}, \ N \geq C'_\varepsilon (\rho r_{\max}^3)^{+\frac{247}{10}}.$$

Lemma 17 and (148) therefore yield the following theorem, which is one of our main results.

Theorem 1: *Let $T = \mathbb{R}^3/L\mathbb{Z}^3$ and spin: $\{1 \dots N\} \to \{1 \dots q\}$ be given. Define $N_s =$ (number of $j \in \{1 \dots N\}$ with spin$(j) = s$), $\rho_s = N_s L^{-3}$, $\rho = NL^{-3}$. Assume $\rho_s > c\rho$.*

Let $K(x,y)$ be defined on $T \times T$, satisfying $0 \leq K(x,y) = K(y,x) \leq C|x-y|^{-1} \chi_{|x-y|<r_{\max}}$, with $\rho r_{\max}^3 > c$.

Let $\varepsilon > 0$ be given.

Let $\Psi(x_1 \dots x_N) \in L^2(T^N)$ have norm 1 and satisfy $\Psi(x_{\sigma 1} \dots x_{\sigma N}) = (\operatorname{sgn}\sigma)\Psi(x_1 \dots x_N)$ for spin-preserving permutations σ.

Assume $\|\nabla\Psi\|^2 \leq (1+\delta)c_{TF}\sum_{s=1}^{q} \rho_s^{5/3} L^3$ with $c_{TF} = \frac{(6\pi^2)^{5/3}}{10\pi^2}$. Finally, assume that

$$\delta < c'_\varepsilon \cdot (\rho r_{\max}^3)^{-\frac{247}{30}} \quad \text{and} \quad N > C'_\varepsilon \cdot (\rho r_{\max}^3)^{+\frac{247}{10}},$$

with c'_ε, C'_ε depending only on c, C, q, ε.

Then

$$\left\langle \sum_{1\le j<k\le N} K(x_j,x_k)\Psi,\Psi \right\rangle \ge$$
$$\frac{1}{2}\iint_{T\times T} K(x,y)\left\{\rho^2-\sum_{s=1}^{q}|\mathcal{S}_{\rho_s}(x-y)|^2\right\}dxdy - C''_\varepsilon E_\# \rho^{1/3}N,$$

with $E_\# = (\rho r^3_{\max})^{\frac{584}{921}+2\varepsilon}\cdot(\delta+N^{-1/3})^{\frac{5}{307}-\varepsilon}$ and $\mathcal{S}_\rho$ defined by (18), (19). The constant C''_ε depends only on c, C, q, ε.

We drop the assumption (141) about the parameters τ, $\underline{\mathrm{N}}$, $\underline{\mathrm{N}}_*$, $r_{\min}$.

The ideas in the proof of Theorem 1 also allow us to control the correlation function $\mathcal{S}_s(x,y,\Psi)$. We need two simple additional results. The first concerns a bilinear variant for $\mathcal{S}_s(x,y,\Psi)$.

Lemma 18: *If $\Phi(x_1\dots x_N)$ and $\Theta(x_1\dots x_N)$ are defined on T^N, then define*

$$\mathcal{S}_s(x,y,\Phi,\Theta)=\sum_{\mathrm{spin}(j)=s}\int_{T^{N-1}}\Phi(x_1\dots x_{j-1}xx_{j+1}\dots x_N)\cdot$$
$$\bar{\Theta}(x_1\dots x_{j-1}yx_{j+1}\dots x_N)dx_1\dots dx_{j-1}dx_{j+1}\dots dx_N.$$

For $h\in\mathbb{R}^3$ with $|h|<c\,\mathrm{diam}\,Q$, and for $\tau>0$, we have

$$\int_{x\in Q_{00}+\mathfrak{z}}|\mathcal{S}_s(x,x+h,\Phi,\Theta)|dx \le \frac{\tau}{2}\langle \mathcal{N}_{s\mathfrak{z}}\Phi,\Phi\rangle + \frac{\tau^{-1}}{2}\langle \mathcal{N}_{s\mathfrak{z}}\Theta,\Theta\rangle,$$

where Q_{00} is the middle half of Q.

Proof: Since

$$|\Phi(x_1\dots x_{j-1}xx_{j+1}\dots x_N)\bar{\Theta}(x_1\dots x_{j-1}x+h\;x_{j+1}\dots x_N)|\le$$
$$\frac{1}{2}\tau|\Phi(x_1\dots x_{j-1}xx_{j+1}\dots x_N)|^2+\frac{1}{2}\tau^{-1}|\Theta(x_1\dots x_{j-1}x+h\;x_{j+1}\dots x_N)|^2,$$

it follows that

$$(150)\qquad \int\limits_{x\in(Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x,x+h,\Phi,\Theta)|dx \le$$

$$\frac{\tau}{2}\int\limits_{T^N}\sum_{\mathrm{spin}(j)=s}\chi_{x\in(Q_{00}+\mathfrak{z})}|\Phi(x_1\ldots x_{j-1}xx_{j+1}\ldots x_N)|^2dx_1\ldots dx_{j-1}dxdx_{j+1}\ldots dx_N$$

$$+\frac{\tau^{-1}}{2}\int\limits_{T^N}\sum_{\mathrm{spin}(j)=s}\chi_{x\in(Q_{00}+\mathfrak{z})}|\Theta(x_1\ldots x_{j-1}x{+}h\ x_{j+1}\ldots x_N)|^2dx_1\ldots dx_{j-1}dxdx_{j+1}\ldots dx_N$$

$$=\frac{\tau}{2}\int\limits_{T^N}\Bigg[\sum_{\mathrm{spin}(j)=s}\chi_{Q_{00}+\mathfrak{z}}(x_j)\Bigg]|\Phi(x_1\ldots x_N)|^2dx_1\ldots dx_N$$

$$+\frac{\tau^{-1}}{2}\int\limits_{T^N}\Bigg[\sum_{\mathrm{spin}(j)=s}\chi_{Q_{00}+\mathfrak{z}}(x_j-h)\Bigg]|\Theta(x_1\ldots x_N)|^2dx_1\ldots dx_N,$$

as follows from renaming the dummy variable x in the two integrals. (Set $x_j = x$ in the first integral and $x_j = x+h$ in the second.) Since $(Q_{00}+\mathfrak{z})$ and $(Q_{00}+\mathfrak{z}\pm h)$ are contained in $Q+\mathfrak{z}$ for $|h| < c\,\mathrm{diam}\,Q$, it follows that

$$\sum_{\mathrm{spin}(j)=s}\chi_{Q_{00}+\mathfrak{z}}(x_j)\quad\text{and}\quad\sum_{\mathrm{spin}(j)=s}\chi_{Q_{00}+\mathfrak{z}}(x_j-h)$$

are less than or equal to $\mathcal{N}_{s\mathfrak{z}}(x_1\ldots x_N)=\sum\limits_{\mathrm{spin}(j)=s}\chi_{Q+\mathfrak{z}}(x_j)$. Therefore, (150) implies

$$\int\limits_{x\in Q_{00}+\mathfrak{z}}|\mathcal{S}_s(x,x+h,\Phi,\Theta)|dx\le\frac{\tau}{2}\int\limits_{T^N}\mathcal{N}_{s\mathfrak{z}}(x_1\ldots x_N)|\Phi(x_1\ldots x_N)|^2dx_1\ldots dx_N$$

$$+\frac{\tau^{-1}}{2}\int\limits_{T^N}\mathcal{N}_{s\mathfrak{z}}(x_1\ldots x_N)|\Theta(x_1\ldots x_N)|^2dx_1\ldots dx_N,$$

which is the conclusion of Lemma 18. □

Corollary: *If $|h| < c\,\mathrm{diam}\,Q$, then*

$$\int\limits_{x\in(Q_{00}+\mathfrak{z})}|\mathcal{S}_s(x,x+h,\Phi)|dx\le\langle\mathcal{N}_{s\mathfrak{z}}\Phi,\Phi\rangle\,.$$

Proof: Take $\Theta=\Phi$ and $\tau=1$ in Lemma 18. □

The second additional result we need is the calculation of the correlation function for $\Phi^{\mathfrak{z}}_{\mathrm{basic}}$.

Lemma 19: $\mathcal{S}_{s_0}(x, y, \Phi^{\mathfrak{z}}_{\text{basic}}) = \sum_{1 \le \alpha \le \underline{N}_{s_0}} \varphi^{\mathfrak{z}}_{\alpha s_0}(x) \overline{\varphi^{\mathfrak{z}}_{\alpha s_0}(y)}$.

Proof: By definition of $\Phi^{\mathfrak{z}}_{\text{basic}}$ and $\mathcal{S}_{s_0}$ we have

(151) $\mathcal{S}_{s_0}(x, y, \Phi^{\mathfrak{z}}_{\text{basic}}) =$

$$\sum_{\substack{i \in J \\ \text{spin}(i) = s_0}} \int \Phi^{\mathfrak{z}}_{\text{basic}}((x_j)_{j \in J}) \cdot \bar{\Phi}^{\mathfrak{z}}_{\text{basic}}((y_j)_{j \in J}) \cdot \delta(x_i - x)\delta(y_i - y) \cdot \prod_{j \in J \smallsetminus \{i\}} \delta(x_j - y_j) \cdot \prod_{j \in J} dx_j dy_j$$

$$= \left(\prod_{s=1}^{q} \underline{N}_s! \right)^{-1} \cdot \sum_{\substack{i \in J \\ \text{spin}(i) = s_0}} \sum_{\sigma, \tau} (\operatorname{sgn} \sigma)(\operatorname{sgn} \tau) \cdot \text{Term}(\sigma, \tau, i)$$

with

(152)

$$\text{Term}(\sigma, \tau, i) = \int \prod_{s=1}^{q} \prod_{\substack{j \in J \\ \text{spin}(j) = s}} \varphi_{\widetilde{\beta}_{\sigma j} s}(x_j) \overline{\varphi_{\widetilde{\beta}_{\tau j} s}}(y_j)$$

$$\cdot \delta(x_i - x)\delta(y_i - y) \prod_{j \in J \smallsetminus \{i\}} \delta(x_j - y_j) \cdot \prod_{j \in J} dx_j dy_j$$

Here, σ and τ run over spin-preserving permutations of J. If i, σ, τ are given, and if $\sigma j_0 \neq \tau j_0$ for some $j_0 \in J \smallsetminus \{i\}$, then since σj_0 and τj_0 have the same spin, and since the $\widetilde{\beta}_\ell$ with $\ell \in J$ of fixed spin are all distinct, it follows that $\widetilde{\beta}_{\sigma j_0} \neq \widetilde{\beta}_{\tau j_0}$. Hence, by performing the $dx_{j_0} dy_{j_0}$ integral first in (152), we see that $\text{Term}(\sigma, \tau, i) = 0$. Thus, $\text{Term}(\sigma, \tau, i) \neq 0$ implies $\sigma j = \tau j$ for all $j \in J \smallsetminus \{i\}$, hence $\sigma = \tau$. So we may restrict the sum on the right of (151) to $\sigma = \tau$. From (152) and the orthonormality of the $\varphi^{\mathfrak{z}}_{\alpha, s}$ for $\mathfrak{z}$, s fixed, we obtain

$$\text{Term}(\sigma, \sigma, i) = \varphi^{\mathfrak{z}}_{\widetilde{\beta}_{\sigma i}, s_0}(x) \overline{\varphi^{\mathfrak{z}}_{\widetilde{\beta}_{\sigma i}, s_0}}(y).$$

Hence (151) implies

$$\mathcal{S}_{s_0}(x, y, \Phi^{\mathfrak{z}}_{\text{basic}}) = \left(\prod_{s=1}^{q} \underline{N}_s! \right)^{-1} \sum_{\sigma} \sum_{\substack{i \in J \\ \text{spin}(i) = s_0}} \varphi_{\widetilde{\beta}_{\sigma i}, s_0}(x) \overline{\varphi^{\mathfrak{z}}_{\widetilde{\beta}_{\sigma i}, s_0}}(y)$$

Changing the dummy index on the right from i to $j = \sigma i$, we get the equivalent formula

$$\mathcal{S}_{s_0}(x, y, \Phi^{\mathfrak{z}}_{\text{basic}}) = \left(\prod_{s=1}^{q} \underline{N}_s! \right)^{-1} \sum_{\sigma} \sum_{\substack{j \in J \\ \text{spin}(j) = s_0}} \varphi^{\mathfrak{z}}_{\widetilde{\beta}_j s_0}(x) \overline{\varphi^{\mathfrak{z}}_{\widetilde{\beta}_j s_0}}(y).$$

The summand is independent of σ, and the number of possible σ is $\prod_{s=1}^{q} \underline{N}_s!$. Hence

$$\mathcal{S}_{s_0}(x, y, \Phi^{\mathfrak{z}}_{\text{basic}}) = \sum_{\substack{j \in J \\ \text{spin}(j)=s_0}} \varphi^{\mathfrak{z}}_{\widetilde{\beta}_j s_0}(x)\overline{\varphi^{\mathfrak{z}}_{\widetilde{\beta}_j s_0}}(y) \tag{153}$$

As j runs through the indices of spin s_0 in J, the $\widetilde{\beta}_j$ take on each of the values $1 \ldots \underline{N}_{s_0}$ once – that is the defining property of the $(\widetilde{\beta}_j)_{j \in J}$. So (153) is equivalent to

$$\mathcal{S}_{s_0}(x, y, \Phi^{\mathfrak{z}}_{\text{basic}}) = \sum_{1 \leq \alpha \leq \underline{N}_{s_0}} \varphi^{\mathfrak{z}}_{\alpha s_0}(x)\overline{\varphi^{\mathfrak{z}}_{\alpha s_0}}(y),$$

which is the conclusion of Lemma 19. □

Corollary: *If $x, y \in (Q_0 + \mathfrak{z})$, then*

$$|\mathcal{S}_s(x, y, \Phi^{\mathfrak{z}}_{\text{basic}}) - \mathcal{S}_{\rho_s}(x - y)| \leq C_\varepsilon \rho \cdot \left(\underline{N}^{3\varepsilon - \frac{1}{9}} + \frac{|x-y|}{\operatorname{diam} Q}\right).$$

Proof: Immediate from Lemma 19 and (41). □

Now we can control $\mathcal{S}_s(x, y, \Psi)$. In fact, since $\Psi = \Phi^{\mathfrak{z}}_{\text{main}} + \Phi^{\mathfrak{z}}_{\text{error}}$, we have

$$\begin{aligned}\mathcal{S}_s(x, y, \Psi) = \mathcal{S}_s(x, y, \Phi^{\mathfrak{z}}_{\text{main}}) + \mathcal{S}_s(x, y, \Phi^{\mathfrak{z}}_{\text{error}}) + \mathcal{S}_s(x, y, \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{error}}) \\ + \mathcal{S}_s(x, y, \Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{main}}).\end{aligned}$$

Setting $y = x + h$, and applying Lemma 18 and its Corollary, we obtain the following estimate, valid for $0 < \tau < 1$ and $|h| < c \operatorname{diam} Q$.

$$\begin{aligned}\int_{x \in (Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x, x+h, \Psi) - \mathcal{S}_s(x, x+h, \Phi^{\mathfrak{z}}_{\text{main}})| dx \leq \\ C\tau^{-1} \left\langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}} \right\rangle + C\tau \left\langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle.\end{aligned} \tag{154}$$

Since $\Phi^{\mathfrak{z}}_{\text{main}} = \Phi^{\mathfrak{z}}_{\text{basic}} \wedge \Phi^{\mathfrak{z}}_{\text{extra}}$ with $\|\Phi^{\mathfrak{z}}_{\text{basic}}\| = 1$, Lemma 11 yields

$$\begin{aligned}\mathcal{S}_s(x, x+h, \Phi^{\mathfrak{z}}_{\text{main}}) &= \|\Phi^{\mathfrak{z}}_{\text{extra}}\|^2 \mathcal{S}_s(x, x+h, \Phi^{\mathfrak{z}}_{\text{basic}}) + \mathcal{S}_s(x, x+h, \Phi^{\mathfrak{z}}_{\text{extra}}) \\ &= \mathcal{S}_s(x, x+h, \Phi^{\mathfrak{z}}_{\text{basic}}) - \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 \mathcal{S}_s(x, x+h, \Phi^{\mathfrak{z}}_{\text{basic}}) \\ &\quad + \mathcal{S}_s(x, x+h, \Phi^{\mathfrak{z}}_{\text{extra}}),\end{aligned}$$

in view of (114). Therefore,

$$\int_{x \in (Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x, x+h, \Phi^{\mathfrak{z}}_{\text{main}}) - \mathcal{S}_s(x, x+h, \Phi^{\mathfrak{z}}_{\text{basic}})| dx \leq$$

$$\|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 \int\limits_{x\in(Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x,x+h,\Phi^{\mathfrak{z}}_{\text{basic}})|dx + \int\limits_{x\in(Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x,x+h,\Phi^{\mathfrak{z}}_{\text{extra}})|dx$$

$$\leq \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 \int\limits_{x\in(Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x,x+h,\Phi^{\mathfrak{z}}_{\text{basic}})|dx + \left\langle \mathcal{N}^{\text{extra}}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{extra}}, \Phi^{\mathfrak{z}}_{\text{extra}} \right\rangle,$$

by the analogue of Lemma 18 for wave functions $\Phi((x_j)_{j\in J})$. These inequalities imply

(155)

$$\int\limits_{x\in(Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x,x+h,\Phi^{\mathfrak{z}}_{\text{main}}) - \mathcal{S}_s(x,x+h,\Phi^{\mathfrak{z}}_{\text{basic}})|dx \leq$$

$$\|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 \int\limits_{(Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x,x+h,\Phi^{\mathfrak{z}}_{\text{basic}})|dx + \left\langle (\mathcal{N}_{s\mathfrak{z}} - \underline{\mathrm{N}}_s)\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle,$$

by virtue of Lemma 14.

The Corollary to Lemma 19 shows that

$$\int\limits_{x\in(Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x,x+h,\Phi^{\mathfrak{z}}_{\text{basic}}) - \mathcal{S}_{\rho_s}(h)|dx \leq C_\varepsilon \rho |Q| \cdot \left(\underline{\mathrm{N}}^{3\varepsilon - \frac{1}{9}} + \frac{|h|}{\operatorname{diam} Q} \right). \tag{156}$$

Adding (154), (155), (156), we obtain the estimate

$$\int\limits_{x\in(Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x,x+h,\Psi) - \mathcal{S}_{\rho_s}(h)|dx \leq$$

$$C\tau^{-1} \langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}} \rangle + C\tau \left\langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle +$$

$$\|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 \int\limits_{(Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x,x+h,\Phi^{\mathfrak{z}}_{\text{basic}})|dx + \left\langle (\mathcal{N}_{s\mathfrak{z}} - \underline{\mathrm{N}}_s)\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle$$

$$+ C_\varepsilon \rho |Q| \cdot \left(\underline{\mathrm{N}}^{3\varepsilon - \frac{1}{9}} + \frac{|h|}{\operatorname{diam} Q} \right).$$

Integrate this estimate over all $\mathfrak{z} \in T$, and we get:

$$|Q_{00}| \int\limits_T |\mathcal{S}_s(x,x+h,\Psi) - \mathcal{S}_{\rho_s}(h)|dx \leq$$

$$C\tau^{-1} L^3 Av_{\mathfrak{z}\in T} \langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{error}} \Phi^{\mathfrak{z}}_{\text{error}} \rangle + C\tau L^3 Av_{\mathfrak{z}\in T} \left\langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle$$

$$+ Av_{\mathfrak{z}\in T} \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 L^3 \int\limits_{Q_{00}} |\mathcal{S}_s(x,x+h,\Phi^{0}_{\text{basic}})|dx + L^3 Av_{\mathfrak{z}\in T} \left\langle (\mathcal{N}_{s\mathfrak{z}} - \underline{\mathrm{N}}_s)\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle$$

$$+ C_\varepsilon \rho |Q| L^3 \cdot \left(\underline{\mathrm{N}}^{3\varepsilon - \frac{1}{9}} + \frac{|h|}{\operatorname{diam} Q} \right).$$

Here we use the fact that $\int\limits_{x\in(Q_{00}+\mathfrak{z})} |\mathcal{S}_s(x, x+h, \Phi^{\mathfrak{z}}_{\text{basic}})|dx$ is independent of $\mathfrak{z}$.

The Corollary to Lemma 19 with $\mathfrak{z} = 0$ gives

$$\int\limits_{Q_{00}} |\mathcal{S}_s(x, x+h, \Phi^0_{\text{basic}})|dx \leq |\mathcal{S}_{\rho_s}(h)| \cdot |Q_{00}| + C_\varepsilon \rho |Q| \left(\underline{N}^{3\varepsilon - \frac{1}{9}} + \frac{|h|}{\operatorname{diam} Q} \right).$$

Substituting this in the preceding inequality, we find that

$$\begin{aligned} |Q_{00}| \int\limits_T |\mathcal{S}_s(x, x+h, \Psi) - \mathcal{S}_{\rho_s}(h)|dx \leq \\ C\tau^{-1} L^3 Av_{\mathfrak{z}\in T} \langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}} \rangle + C\tau L^3 Av_{\mathfrak{z}\in T} \left\langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle \\ + Av_{\mathfrak{z}\in T} \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 L^3 \cdot \left\{ |\mathcal{S}_{\rho_s}(h)| \cdot |Q_{00}| + C_\varepsilon \rho |Q| \left(\underline{N}^{3\varepsilon - \frac{1}{9}} + \frac{|h|}{\operatorname{diam} Q} \right) \right\} \\ + L^3 Av_{\mathfrak{z}\in T} \left\langle (\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s) \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle \\ + C_\varepsilon \rho |Q| L^3 \cdot \left(\underline{N}^{3\varepsilon - \frac{1}{9}} + \frac{|h|}{\operatorname{diam} Q} \right). \end{aligned}$$

Since $\|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 \leq 1$ by (114), this is equivalent to

$$\begin{aligned} (157) \quad |Q_{00}| \int\limits_T |\mathcal{S}_s(x, x+h, \Psi) - \mathcal{S}_{\rho_s}(h)|dx \leq \\ C\tau^{-1} L^3 Av_{\mathfrak{z}\in T} \langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}} \rangle + C\tau L^3 Av_{\mathfrak{z}\in T} \left\langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{main}} \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle + \\ Av_{\mathfrak{z}\in T} \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 L^3 \cdot |\mathcal{S}_{\rho_s}(h)| \cdot |Q_{00}| + L^3 Av_{\mathfrak{z}\in T} \left\langle (\mathcal{N}_{s\mathfrak{z}} - \underline{N}_s) \Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}} \right\rangle \\ + C_\varepsilon \rho |Q| L^3 \cdot \left(\underline{N}^{3\varepsilon - \frac{1}{9}} + \frac{|h|}{\operatorname{diam} Q} \right). \end{aligned}$$

Let us estimate the various terms on the right in (157). For an $\underline{N}_* > C\underline{N}$ to be picked later, we use the obvious inequality $\mathcal{N}_{s\mathfrak{z}} \leq \underline{N}_* + \underline{N}_*^{-2/3} \mathcal{N}_{s\mathfrak{z}}^{5/3}$ and (73), (74) to conclude that

$$\begin{aligned} Av_{\mathfrak{z}\in T} \langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}} \rangle &\leq \underline{N}_* Av_{\mathfrak{z}\in T} \|\Phi^{\mathfrak{z}}_{\text{error}}\|^2 \\ &\quad + \underline{N}_*^{-2/3} Av_{\mathfrak{z}\in T} \left\langle \mathcal{N}_{s\mathfrak{z}}^{5/3} \Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}} \right\rangle \\ &\leq \underline{N}_* [C_{m\varepsilon} \underline{N}^{-m} + C\underline{N}^2 \cdot (\delta + N^{-1/3})^{1/2}] + C\underline{N}_*^{-2/3} \underline{N}^{5/3}, \quad \text{i.e.} \end{aligned}$$

$$\begin{aligned} (158) \quad \tau^{-1} L^3 Av_{\mathfrak{z}\in T} \langle \mathcal{N}_{s\mathfrak{z}} \Phi^{\mathfrak{z}}_{\text{error}}, \Phi^{\mathfrak{z}}_{\text{error}} \rangle \leq \\ \tau^{-1} L^3 \underline{N}_* [C_{m\varepsilon} \underline{N}^{-m} + C\underline{N}^2 \cdot (\delta + N^{-1/3})^{1/2}] + C\tau^{-1} L^3 \underline{N}_*^{-2/3} \underline{N}^{5/3}. \end{aligned}$$

Next, we have

$$Av_{\mathfrak{z}\in T}\left\langle \mathcal{N}_{s\mathfrak{z}}\Phi^{\mathfrak{z}}_{main}, \Phi^{\mathfrak{z}}_{\text{main}}\right\rangle =$$
$$Av_{\mathfrak{z}\in T}\left\langle (\mathcal{N}_{s\mathfrak{z}} - \underline{\mathrm{N}}_s)\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}}\right\rangle + \underline{\mathrm{N}}_s Av_{\mathfrak{z}\in T}\|\Phi^{\mathfrak{z}}_{\text{main}}\|^2$$
$$\leq C\underline{\mathrm{N}}^2\cdot(\delta + N^{-1/3})^{1/2} + C\underline{\mathrm{N}}^{\frac{8}{9}+3\varepsilon} + \underline{\mathrm{N}}_s,$$

by (76) and (114). Hence,

$$\tau L^3 Av_{\mathfrak{z}\in T}\left\langle \mathcal{N}_{s\mathfrak{z}}\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}}\right\rangle \leq C\tau L^3\cdot\underline{\mathrm{N}}^2\cdot(\delta+N^{-1/3})^{1/2} + C_\varepsilon\tau L^3\underline{\mathrm{N}}^{\frac{8}{9}+3\varepsilon} + \tau L^3\underline{\mathrm{N}}_s. \tag{159}$$

Since $|\mathcal{S}_{\rho_s}(h)| \leq \rho_s$, equation (73) implies

$$Av_{\mathfrak{z}\in T}\|\Phi^{\mathfrak{z}}_{\text{error}}\|^2\cdot L^3\cdot|\mathcal{S}_{\rho_s}(h)|\cdot|Q_{00}| \leq$$
$$\rho L^3|Q_{00}|\cdot[C_{m\varepsilon}\underline{\mathrm{N}}^{-m} + C\underline{\mathrm{N}}^2\cdot(\delta + N^{-1/3})^{1/2}]. \tag{160}$$

Again using (76), we have

$$L^3 Av_{\mathfrak{z}\in T}\left\langle (\mathcal{N}_{s\mathfrak{z}} - \underline{\mathrm{N}}_s)\Phi^{\mathfrak{z}}_{\text{main}}, \Phi^{\mathfrak{z}}_{\text{main}}\right\rangle \leq CL^3\underline{\mathrm{N}}^2(\delta + N^{-1/3})^{1/2} + C_\varepsilon L^3\underline{\mathrm{N}}^{\frac{8}{9}+3\varepsilon}. \tag{161}$$

Putting (158) ... (161) into (157), we obtain

$$|Q_{00}|\int_T |\mathcal{S}_s(x, x+h, \Psi) - \mathcal{S}_{\rho_s}(h)|dx \leq$$
$$\tau^{-1}L^3\underline{\mathrm{N}}_*[C_{m\varepsilon}\underline{\mathrm{N}}^{-m} + C\underline{\mathrm{N}}^2\cdot(\delta + N^{-1/3})^{1/2}] + C\tau^{-1}L^3\underline{\mathrm{N}}_*^{-2/3}\underline{\mathrm{N}}^{5/3} \tag{162}$$
$$+ C\tau L^3\underline{\mathrm{N}}^2(\delta + N^{-1/3})^{1/2} + C_\varepsilon\tau L^3\underline{\mathrm{N}}^{\frac{8}{9}+3\varepsilon} + \tau L^3\underline{\mathrm{N}}_s$$
$$+ \rho L^3|Q_{00}|\cdot[C_{m\varepsilon}\underline{\mathrm{N}}^{-m} + C\underline{\mathrm{N}}^2\cdot(\delta + N^{-1/3})^{1/2}]$$
$$+ CL^3\underline{\mathrm{N}}^2(\delta + N^{-1/3})^{1/2} + C_\varepsilon L^3\underline{\mathrm{N}}^{\frac{8}{9}+3\varepsilon}$$
$$+ C_\varepsilon\rho|Q|L^3\cdot\left(\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}} + \frac{|h|}{\operatorname{diam} Q}\right)$$

We are assuming that $0 < \tau < 1$ and $\underline{\mathrm{N}}_* > C\underline{\mathrm{N}}$. Hence,

$$\rho L^3|Q_{00}|\cdot[C_{m\varepsilon}\underline{\mathrm{N}}^{-m} + C\underline{\mathrm{N}}^2\cdot(\delta + N^{-1/3})^{1/2}] \sim \underline{\mathrm{N}}L^3[C_{m\varepsilon}\underline{\mathrm{N}}^{-m} + \text{etc.}]$$
$$\leq \tau^{-1}L^3\underline{\mathrm{N}}_*\cdot[C_{m\varepsilon}\underline{\mathrm{N}}^{-m} + \text{etc.}],$$

which shows that the term $\rho L^3|Q_{00}|\cdot[C_{m\varepsilon}\underline{\mathrm{N}}^{-m} + C\underline{\mathrm{N}}^2\cdot(\delta + N^{-1/3})^{1/2}]$ may be dropped from the right-hand side of (162). Recalling that $L^3\underline{\mathrm{N}}/|Q_{00}| \sim L^3\rho \sim N$ and dividing both sides of (162) by $|Q_{00}|$, we obtain

$$\int_T |\mathcal{S}_s(x, x+h, \Psi) - \mathcal{S}_{\rho_s}(h)|dx \leq$$
$$C_{m\varepsilon}\tau^{-1}N\underline{\mathrm{N}}_*[\underline{\mathrm{N}}^{-(m+1)} + \underline{\mathrm{N}}\cdot(\delta + N^{-1/3})^{1/2}] + C\tau^{-1}N(\underline{\mathrm{N}}/\underline{\mathrm{N}}_*)^{2/3}$$
$$+ C\tau N\underline{\mathrm{N}}(\delta + N^{-1/3})^{1/2} + C_\varepsilon\tau N\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}} + \tau N$$
$$+ CN\underline{\mathrm{N}}(\delta + N^{-1/3})^{1/2} + C_\varepsilon N\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}}$$
$$+ C_\varepsilon N\cdot\left(\underline{\mathrm{N}}^{3\varepsilon-\frac{1}{9}} + \frac{|h|}{\operatorname{diam} Q}\right).$$

Since $0 < \tau < 1$ and $\underline{N}_* > C\underline{N} > C$, the right-hand side simplifies, and we have

(163)
$$\int_T |\mathcal{S}_s(x, x+h, \Psi) - \mathcal{S}_{\rho_s}(h)| dx \leq$$
$$C_{m\varepsilon} N \cdot \Big[\tau^{-1} \underline{N}_* \underline{N}^{-(m+1)} + \tau^{-1} \underline{N}_* \underline{N} \cdot (\delta + N^{-1/3})^{1/2} + \tau^{-1} (\underline{N}/\underline{N}_*)^{2/3}$$
$$+ \underline{N}^{3\varepsilon - \frac{1}{9}} + \tau + \frac{|h|}{\operatorname{diam} Q} \Big].$$

This holds provided $|h| < c \operatorname{diam} Q$, $\underline{N}_* > C\underline{N}$, $\underline{N} > C$, $0 < \tau < 1$. We may again pick the order of magnitude of $\underline{N}$ by varying the size of the cube Q. We take

$$\text{(164)} \qquad \underline{N} \sim (\delta + N^{-1/3})^{-9/46}, \ \underline{N}_* \sim (\delta + N^{-1/3})^{-12/46}, \ \tau \sim (\delta + N^{-1/3})^{1/46}.$$

If $\delta < c'$ and $N > C'$ for suitable c', C', then the constraints $0 < \tau < 1$, $\underline{N}_* > C\underline{N}$ and $\underline{N} > C$ are satisfied. Note also that $\underline{N} \ll N$, so that $\operatorname{diam} Q \ll L$. With parameters (164), we have:

$$\tau^{-1} \underline{N}_* \underline{N} \cdot (\delta + N^{-1/3})^{1/2} \sim (\delta + N^{-1/3})^{-\frac{1}{46} - \frac{12}{46} - \frac{9}{46} + \frac{1}{2}} = (\delta + N^{-1/3})^{\frac{1}{46}}$$
$$\tau^{-1} (\underline{N}/\underline{N}_*)^{2/3} \sim (\delta + N^{-1/3})^{-\frac{1}{46}} [(\delta + N^{-1/3})^{+\frac{3}{46}}]^{\frac{2}{3}} = (\delta + N^{-1/3})^{\frac{1}{46}}$$
$$\underline{N}^{3\varepsilon - \frac{1}{9}} \sim (\delta + N^{-1/3})^{-\frac{27}{46}\varepsilon + \frac{1}{46}}$$
$$\tau \sim (\delta + N^{-1/3})^{\frac{1}{46}}$$

If m is large, then

$$\tau^{-1} \underline{N}_* \underline{N}^{-(m+1)} = (\delta + N^{-1/3})^{\text{large positive power}} \ll (\delta + N^{-1/3})^{\frac{1}{46}}.$$

So (163) implies

$$\text{(165)} \qquad \int_T |\mathcal{S}_s(x, x+h, \Psi) - \mathcal{S}_{\rho_s}(h)| dx \leq C_\varepsilon N \cdot \left[(\delta + N^{-1/3})^{\frac{1}{46} - \varepsilon} + \frac{|h|}{\operatorname{diam} Q} \right].$$

This holds for $\delta < c'$, $N > C'$ and $|h| < c \operatorname{diam} Q$. Since $\rho^{1/3} \operatorname{diam} Q \sim (\rho |Q|)^{1/3} \sim \underline{N}^{1/3} \sim (\delta + N^{-1/3})^{-3/46}$ by (164), the condition $|h| < c \operatorname{diam} Q$ means that $\rho^{1/3} |h| \leq c(\delta + N^{-1/3})^{-3/46}$, and (165) may be rewritten as

$$\text{(166)} \quad \int_T |\mathcal{S}_s(x, x+h, \Psi) - \mathcal{S}_{\rho_s}(h)| dx \leq C_\varepsilon N \cdot \left[(\delta + N^{-1/3})^{\frac{1}{46} - \varepsilon} + (\delta + N^{-1/3})^{\frac{3}{46}} \rho^{1/3} |h| \right]$$

Thus, we have proven (166) for $\delta < c'$, $N > C'$, $\rho^{1/3} |h| < c(\delta + N^{-1/3})^{-\frac{3}{46}}$. We state this result as the second main theorem of the present section.

Theorem 2: *Let $T = \mathbb{R}^3/L\mathbb{Z}^3$ and spin: $\{1\dots N\} \to \{1\dots q\}$ be given. Define $N_s =$ (number of $j \in \{1\dots N\}$ with spin$(j) = s$), $\rho_s = N_s L^{-3}$, $\rho = NL^{-3}$. Assume $\rho_s > c\rho$. Let $\varepsilon > 0$ be given. Let $\Psi(x_1\dots x_N) \in L^2(T^N)$ have norm 1 and satisfy $\Psi(x_{\sigma 1}\dots x_{\sigma N}) = (\operatorname{sgn}\sigma)\Psi(x_1\dots x_N)$ for spin-preserving permutations σ. Assume*

$$\|\nabla\Psi\|^2 \le (1+\delta)c_{TF}\sum_{s=1}^{q}\rho_s^{5/3}L^3 \quad \textit{with} \quad c_{TF} = \frac{(6\pi^2)^{5/3}}{10\pi^2}.$$

Finally, assume $0 < \delta < c'$, $N > C'$. Then

$$\begin{aligned}&\mathcal{S}_s(x,y,\Psi) = \\ &\sum_{\mathrm{spin}(j)=s}\ \int_{T^{N-1}} \Psi(x_1\dots x_{j-1}xx_{j+1}\dots x_N)\bar{\Psi}(x_1\dots x_{j-1}yx_{j+1}\dots x_N) \\ &dx_1\dots dx_{j-1}dx_{j+1}\dots dx_N\end{aligned}$$

satisfies the estimate

$$\int_T |\mathcal{S}_s(x,x+h,\Psi) - \mathcal{S}_{\rho_s}(h)|dx \le C''N\cdot\left[(\delta+N^{-1/3})^{\frac{1}{46}-\varepsilon} + (\delta+N^{-1/3})^{\frac{3}{46}}\rho^{1/3}|h|\right]$$

for all $h \in T$ with $\rho^{1/3}|h| < c''(\delta+N^{-1/3})^{-\frac{3}{46}}$. Here, $\mathcal{S}_{\rho_s}(h)$ is defined by (18), (19). The constants c', C', C'', c'' depend only on q, ε, c.

Removing Periodic Boundary Conditions

In the previous section, we studied N quantized particles in a flat torus T. Now we will apply what we have learned, to study N particles in $\mathbb{R}^3$. Our setting is as follows. We take as given a small positive number ε, a positive real number ρ_0 (the density of particles of a fixed spin), a positive integer q (the number of possible spins), a large positive integer N (the total number of particles), and a cube $Q \subset \mathbb{R}^3$.

In addition, we are given a function spin: $\{1, \dots, N\} \to \{1, \dots, q\}$, and a wave function $\Psi(x_1 \dots x_N) \in L^2(\mathbb{R}^{3N})$ of norm 1, satisfying $\Psi(x_{\sigma 1} \dots x_{\sigma N}) = (\mathrm{sgn}\sigma)\Psi(x_1 \dots x_N)$ for spin-preserving permutations σ.

Under an assumption on the kinetic energy of Ψ, we want to control the behavior of all the particles x_j belonging to Q. In fact, we want to compare Ψ with the state Ψ_0 in which approximately $\underline{\mathrm{N}} = \rho_0|Q|$ particles of each spin are placed in Q with the lowest possible kinetic energy. We will derive analogues of Theorems 1 and 2 in the preceding section.

In this section, c, C etc. denote constants depending only on ε and q. We assume $\underline{\mathrm{N}}$ is greater than a large constant C.

We prepare to state our basic assumption on the kinetic energy of Ψ. Define

$$KE(Q,\Psi) = \sum_{j=1}^{N} \int_{\mathbb{R}^{3N}} |\nabla_{x_j}\Psi(x_1 \dots x_N)|^2 \chi_Q(x_j)\, dx_1 \dots dx_N \tag{1}$$

$$\mathcal{N}_{sQ}(x_1 \dots x_N) = [\text{no. of particles of spin } s \text{ in } Q] = \sum_{\mathrm{spin}(j)=s} \chi_Q(x_j) \tag{2}$$

$$\mathcal{N}_Q(x_1 \dots x_N) = [\text{no. of particles in } Q] = \sum_{j=1}^{N} \chi_Q(x_j) \tag{3}$$

Then set

$$\begin{aligned} \mathcal{E}(Q,\rho_0,\Psi) = & KE(Q,\Psi) - \frac{5}{3} c_{TF} \rho_0^{2/3} \langle \mathcal{N}_Q \Psi, \Psi \rangle \\ & + \frac{2}{3} q c_{TF} \rho_0^{5/3} |Q| + C_1 q \rho_0^{5/3} |Q| \underline{\mathrm{N}}^{-1/3} \end{aligned} \tag{4}$$

for a large constant C_1. Here, as in the previous section,

$$c_{TF} = \frac{(6\pi^2)^{5/3}}{10\pi^2} \tag{5}$$

For the ground-state Ψ_0 above, we have

$$KE(Q, \Psi_0) \approx q c_{TF} \rho_0^{5/3} |Q| \quad \text{and} \quad \langle \mathcal{N}_Q \Psi, \Psi \rangle \approx q \rho_0 |Q|,$$

so that

$$\begin{aligned} \text{(6)} \qquad \mathcal{E}(Q, \rho_0, \Psi_0) &\approx q c_{TF} \rho_0^{5/3} |Q| - \frac{5}{3} c_{TF} \rho_0^{2/3} \cdot q \rho_0 |Q| + \frac{2}{3} q c_{TF} \rho_0^{5/3} |Q|, \\ &+ C_1 q \rho_0^{5/3} |Q| \underset{\sim}{N}^{-1/3} = C_1 q \rho_0^{5/3} |Q| \underset{\sim}{N}^{-1/3} \\ &\ll \rho_0^{5/3} |Q|. \end{aligned}$$

Our basic assumption on the kinetic energy of Ψ is that

$$\text{(7)} \qquad \mathcal{E}(Q, \rho_0, \Psi) \leq \delta \rho_0^{5/3} |Q| \quad \text{with} \quad 0 < \delta < c.$$

It is plausible that (7) forces Ψ to approximate Ψ_0 on Q, in view of (6) and the following result.

Lemma 1: $\mathcal{E}(Q, \rho_0, \Psi) \geq 0$.

Sketch of Proof: Suppose spin*: $\{1 \ldots n\} \to \{1 \ldots q\}$, and let $\Phi(x_1 \ldots x_n) \in L^2(Q^n)$ be antisymmetric under permutations that preserve spin*. Then if $n \geq C$, we have

(8)

$$\int_{Q^n} \sum_{j=1}^{n} |\nabla_{x_j} \Phi(x_1 \ldots x_n)|^2 dx_1 \ldots dx_n \geq$$

$$\sum_{s=1}^{q} \left(c_{TF} \left(\frac{n_s}{|Q|} \right)^{5/3} |Q| - C n_s^{4/3} (\operatorname{diam} Q)^{-2} \right) \cdot \int_{Q^n} |\Phi(x_1 \ldots x_n)|^2 dx_1 \ldots dx_n$$

where $n_s =$ (number of $j \in \{1 \ldots n\}$ with spin*$(j) = s$).

Estimate (8) follows by expanding $\Phi(x_1 \ldots x_n)$ in terms of the Neumann eigenfunctions of the Laplacian on Q, and then using a slight variant of equation (11) from the preceding section. (Here, we must restrict attention to lattice points $\xi = (\xi_1, \xi_2, \xi_3) \in \mathbb{R}^3$ with non-negative coordinates ξ_i.) If $n < C$, then at least the left-hand side of (8) is non-negative.

Fix a subset $A \subset \{1 \ldots N\}$. Then fix all the x_j for $j \notin A$, and regard $\Phi = \Psi(x_1 \ldots x_N) \cdot \prod_{j \in A} \chi_Q(x_j) \cdot \prod_{j \notin A} \chi_{c_Q}(x_j)$ as a function of the x_j for $j \in A$. Applying (8) and integrating over the x_j ($j \notin A$), we obtain the estimate

$$\text{(9)} \qquad \int_{\mathbb{R}^{3N}} \sum_{k \in A} |\nabla_{x_k} \Psi(x_1 \ldots x_N)|^2 \cdot \prod_{j \in A} \chi_Q(x_j) \cdot \prod_{j \notin A} \chi_{c_Q}(x_j) dx_1 \ldots dx_N$$

$$\geq \sum_{s=1}^{q} \left\{ c_{TF} \left(\frac{n_s}{|Q|} \right)^{5/3} |Q| - C n_s^{4/3} (\operatorname{diam} Q)^{-2} \right\} \cdot \int_{\mathbb{R}^{3N}} |\Psi(x_1 \ldots x_N)|^2 \prod_{j \in A} \chi_Q(x_j) \prod_{j \notin A} \chi_{c_Q}(x_j) \cdot$$

$$dx_1 \ldots dx_N$$

for A containing at least C indices, where $n_s = $ (number of $j \in A$ with spin s).

If A contains fewer than C indices, then at least the left-hand side of (9) is non-negative. In the support of the integrand in (9), we have $\mathcal{N}_{sQ}(x_1 \dots x_N) = n_s$, and $\chi_{\mathcal{N}_Q \geq C} = \chi_{A \text{ contains at least } C \text{ indices}}$. Hence, (9) implies

$$\int_{\mathbb{R}^{3N}} \sum_{k \in A} |\nabla_{x_k} \Psi(x_1 \dots x_N)|^2 \cdot \prod_{j \in A} \chi_Q(x_j) \cdot \prod_{j \notin A} \chi_{c_Q}(x_j) dx_1 \dots dx_N \geq$$

$$\int_{\mathbb{R}^{3N}} \sum_{s=1}^{q} \left\{ c_{TF} \left(\frac{\mathcal{N}_{sQ}}{|Q|} \right)^{5/3} |Q| - C \mathcal{N}_{sQ}^{4/3} (\operatorname{diam} Q)^{-2} \right\} \chi_{\mathcal{N}_Q \geq C} \cdot$$
$$|\Psi(x_1 \dots x_N)|^2 \cdot \prod_{j \in A} \chi_Q(x_j) \cdot \prod_{j \notin A} \chi_{c_Q}(x_j) dx_1 \dots dx_N$$

for any subset $A \subset \{1 \dots N\}$. Summing over all possible A, we obtain

$$\int_{\mathbb{R}^{3N}} \sum_{k=1}^{N} |\nabla_{x_k} \Psi(x_1 \dots x_N)|^2 \chi_Q(x_k) dx_1 \dots dx_N \geq$$
$$\int_{\mathbb{R}^{3N}} \sum_{s=1}^{q} \left\{ c_{TF} \left(\frac{\mathcal{N}_{sQ}}{|Q|} \right)^{5/3} |Q| - C \mathcal{N}_{sQ}^{4/3} (\operatorname{diam} Q)^{-2} \right\} \chi_{\mathcal{N}_Q \geq C} \cdot |\Psi(x_1 \dots x_N)|^2 dx_1 \dots dx_N,$$

i.e.

$$\text{(10)} \qquad KE(Q, \Psi) \geq \left\langle \sum_{s=1}^{q} \left\{ c_{TF} \left(\frac{\mathcal{N}_{sQ}}{|Q|} \right)^{5/3} |Q| - C \mathcal{N}_{sQ}^{4/3} (\operatorname{diam} Q)^{-2} \right\} \chi_{\mathcal{N}_Q \geq C} \Psi, \Psi \right\rangle$$

Substituting (10) into the definition of $\mathcal{E}(Q, \rho_0, \Psi)$ and recalling that $\mathcal{N}_Q = \sum_{s=1}^{q} \mathcal{N}_{sQ}$, we obtain the lower bound

$$\text{(11)} \qquad \mathcal{E}(Q, \rho_0, \Psi) \geq \langle X \Psi, \Psi \rangle, \quad \text{where}$$

$$\text{(12)} \quad X = \sum_{s=1}^{q} \left\{ c_{TF} \left(\frac{\mathcal{N}_{sQ}}{|Q|} \right)^{5/3} |Q| - C \mathcal{N}_{sQ}^{4/3} (\operatorname{diam} Q)^{-2} \right\} \chi_{\mathcal{N}_Q \geq C}$$
$$- \frac{5}{3} c_{TF} \rho_0^{2/3} \sum_{s=1}^{q} \mathcal{N}_{sQ} + \frac{2}{3} q c_{TF} \rho_0^{5/3} |Q| + C_1 q \rho_0^{5/3} |Q| \underline{\mathrm{N}}^{-1/3}.$$

We shall check that $X \geq 0$. The conclusion of Lemma 1 will then follow immediately from (11).

If the characteristic function $\chi_{\mathcal{N}_Q \geq C}$ in (12) is equal to zero, then $X \geq -\frac{5}{3}c_{TF}\rho_0^{2/3}C + \frac{2}{3}qc_{TF}\rho_0^{5/3}|Q| = -\frac{5}{3}c_{TF}\rho_0^{2/3}C + \frac{2}{3}qc_{TF}\rho_0^{2/3}\underline{N} \geq 0$, since we have assumed $\underline{N}$ exceeds a large constant. On the other hand, if the characteristic function in (12) is equal to 1, then

$$X = \sum_{s=1}^{q} X_s, \quad \text{with} \tag{13}$$

$$X_s = c_{TF}\left(\frac{\mathcal{N}_{sQ}}{|Q|}\right)^{5/3}|Q| - C\mathcal{N}_{sQ}^{4/3}(\operatorname{diam} Q)^{-2} - \frac{5}{3}c_{TF}\rho_0^{2/3}\mathcal{N}_{sQ} + \frac{2}{3}c_{TF}\rho_0^{5/3}|Q| + C_1\rho_0^{5/3}|Q|\underline{N}^{-1/3}. \tag{14}$$

So, to complete the proof of Lemma 1, it is enough to check that each $X_s \geq 0$.

The function $f(\rho) = c_{TF}\rho^{5/3}|Q| - \frac{5}{3}c_{TF}\rho_0^{2/3}\rho|Q| + \frac{2}{3}c_{TF}\rho_0^{5/3}|Q|$ takes its minimum at $\rho = \rho_0$, where we have $f(\rho_0) = 0$. Hence $f(\rho) \geq 0$. Setting $\rho = \mathcal{N}_{sQ}/|Q|$ and comparing $f(\rho) \geq 0$ with (14), we see that $X_s \geq 0$ provided

$$-C\mathcal{N}_{sQ}^{4/3}(\operatorname{diam} Q)^{-2} + C_1\rho_0^{5/3}|Q|\underline{N}^{-1/3} \geq 0. \tag{15}$$

Since $\underline{N} = \rho_0|Q|$, we may take C_1 large enough to make (15) hold whenever $\mathcal{N}_{sQ} \leq 100\bar{N}$. Therefore, $X_s \geq 0$ for $\mathcal{N}_{sQ} \leq 100\underline{N}$. If instead $\mathcal{N}_{sQ} > 100\bar{N}$, then $\rho = \mathcal{N}_{sQ}/|Q| > 100\rho_0$, so that

$$f(\rho) = c_{TF}\rho^{5/3}|Q| - \frac{5}{3}c_{TF}\rho_0^{2/3}\rho|Q| + \frac{2}{3}c_{TF}\rho_0^{5/3}|Q| \geq c\rho^{5/3}|Q|.$$

Comparing this with (14), we see that

$$X_s \geq c\rho^{5/3}|Q| - C\mathcal{N}_{sQ}^{4/3}(\operatorname{diam} Q)^{-2} = c'\mathcal{N}_{sQ}^{5/3}(\operatorname{diam} Q)^{-2} - C\mathcal{N}_{sQ}^{4/3}(\operatorname{diam} Q)^{-2} \geq 0,$$

since here $\mathcal{N}_{sQ} \geq 100\underline{N}$ and $\underline{N}$ is assumed to exceed a large constant. Hence in all cases, $X_s \geq 0$, and the proof of Lemma 1 is complete. □

Corollary: $\mathcal{E}(Q, 2\rho_0, \Psi) \geq 0$.

Proof: Repeat the above argument. □

Before we come to the main ideas, we prove a technical result that tells us that not too many particles can accumulate near the boundary of Q. Specifically, let

$$\Omega = \{x \in Q \mid \operatorname{dist}(x, \partial Q) < \rho_0^{-1/3}\}, \tag{16}$$

and define

$$\mathcal{N}_\Omega(x_1 \ldots x_N) = (\text{no. of particles in } \Omega) = \sum_{j=1}^{N} \chi_\Omega(x_j) \tag{17}$$

Lemma 2: $\langle \mathcal{N}_\Omega \Psi, \Psi\rangle \leq C\underline{N}^{13/15}$.

Sketch of Proof: Cover Ω by cubes $Q_\nu \subset Q$ of diameter $\sim \rho_0^{-1/3}$. The number of Q_ν needed to cover Ω will be of the order of magnitude $\underline{N}^{2/3}$. (To see this, note that $\rho_0 \mathrm{vol}\, Q_\nu \sim 1$, while $\rho_0 \mathrm{vol}\, \Omega \sim \rho_0 \cdot \rho_0^{-1/3} \mathrm{area}\, Q \sim \rho_0^{2/3}|Q|^{2/3} = \underline{N}^{2/3}$.) We can assume that the sum of the characteristic functions of the Q_ν is bounded. Let $\mathcal{N}_{Q_\nu} =$ (number of particles in Q_ν) $= \sum_{j=1}^{N} \chi_{Q_\nu}(x_j)$. The proof of equation (10) applies also to Q_ν, and shows in particular that

$$KE(Q_\nu, \Psi) \geq c \left\langle \mathcal{N}_{Q_\nu}^{5/3} \chi_{\mathcal{N}_{Q_\nu} \geq C} (\mathrm{diam}\, Q_\nu)^{-2} \Psi, \Psi \right\rangle$$

Since $\mathrm{diam}\, Q_\nu \sim \rho_0^{-1/3}$, this means that

$$KE(Q_\nu, \Psi) \geq c\rho_0^{2/3} \left\langle \mathcal{N}_{Q_\nu}^{5/3} \chi_{\mathcal{N}_{Q_\nu} \geq C} \Psi, \Psi \right\rangle. \tag{18}$$

Since the sum of the characteristic functions of the Q_ν is bounded, and since the $Q_\nu \subset Q$, it follows from (1) that

$$KE(Q, \Psi) \geq c \sum_\nu KE(Q_\nu, \Psi).$$

Therefore, (18) yields

$$KE(Q, \Psi) \geq c' \rho_0^{2/3} \left\langle \sum_\nu \mathcal{N}_{Q_\nu}^{5/3} \chi_{\mathcal{N}_{Q_\nu} \geq C} \Psi, \Psi \right\rangle \tag{19}$$

On the other hand, the Corollary to Lemma 1 gives $\mathcal{E}(Q, 2\rho_0, \Psi) \geq 0$, i.e.

$$KE(Q, \Psi) - \frac{5}{3} c_{TF} (2\rho_0)^{2/3} \langle \mathcal{N}_Q \Psi, \Psi\rangle + \frac{2}{3} q c_{TF} (2\rho_0)^{5/3} |Q| + C_1 q \cdot 2^{4/3} \rho_0^{5/3} |Q| \underline{N}^{-1/3} \geq 0.$$

Hence

$$KE(Q, \Psi) - \frac{5}{3} c_{TF} (2\rho_0)^{2/3} \langle \mathcal{N}_Q \Psi, \Psi\rangle + C\rho_0^{5/3}|Q| \geq 0.$$

So

$$\begin{aligned}
&(1 - 2^{-2/3}) KE(Q, \Psi) \leq \\
&\qquad (1 - 2^{-2/3}) KE(Q, \Psi) + 2^{-2/3} \{ KE(Q, \Psi) - \frac{5}{3} c_{TF} (2\rho_0)^{2/3} \langle \mathcal{N}_Q \Psi, \Psi\rangle \\
&\qquad + C\rho_0^{5/3}|Q| \} = KE(Q, \Psi) - \frac{5}{3} c_{TF} \rho_0^{2/3} \langle \mathcal{N}_Q \Psi, \Psi\rangle + C' \rho_0^{5/3} |Q| \\
&\qquad = \mathcal{E}(Q, \rho_0, \Psi) - \frac{2}{3} q c_{TF} \rho_0^{5/3} |Q| - C_1 q \rho_0^{5/3} |Q| \underline{N}^{-1/3} + C' \rho_0^{5/3} |Q| \\
&\qquad \text{(by (4))} \quad \leq \mathcal{E}(Q, \rho_0, \Psi) + C' \rho_0^{5/3} |Q| \leq (\delta + C') \rho_0^{5/3} |Q| \quad \text{by (7)}
\end{aligned}$$

Hence,

$$KE(Q,\Psi) \le C''\rho_0^{5/3}|Q|. \tag{20}$$

Comparing this with (19), we get

$$\left\langle \sum_\nu \mathcal{N}_{Q_\nu}^{5/3}\chi_{\mathcal{N}_{Q_\nu}\ge C}\Psi,\Psi\right\rangle \le C\rho_0|Q| = C\underline{\mathrm{N}}. \tag{21}$$

Since the number of Q_ν is $\sim \underline{\mathrm{N}}^{2/3}$, we have

$$\sum_\nu \mathcal{N}_{Q_\nu} \le S^{-2/3}\sum_\nu \mathcal{N}_{Q_\nu}^{5/3}\chi_{\mathcal{N}_{Q_\nu}\ge S} + CS\underline{\mathrm{N}}^{2/3}, \quad \text{for} \quad S>0.$$

Therefore, if $S > C$, then (21) implies

$$\left\langle \sum_\nu \mathcal{N}_{Q_\nu}\Psi,\Psi\right\rangle \le C\underline{\mathrm{N}}S^{-2/3} + CS\underline{\mathrm{N}}^{2/3}.$$

Taking $S = \underline{\mathrm{N}}^{1/5}$, we get

$$\left\langle \sum_\nu \mathcal{N}_{Q_\nu}\Psi,\Psi\right\rangle \le C\underline{\mathrm{N}}^{13/15}. \tag{22}$$

Since the Q_ν cover Ω, we have $\mathcal{N}_\Omega \le \sum_\nu \mathcal{N}_{Q_\nu}$, so (22) implies the conclusion of Lemma 2.□

After introducing a little more notation, we can give the main idea of this section. Make a partition of unity $\theta_0^2(x)+\theta_1^2(x) = 1$ on $\mathbb{R}^3$, with the following properties.

$\operatorname{supp}\theta_0 \subset\subset Q$.

$\theta_0(x) = 1$ in $Q \setminus \Omega$.

$|\partial_x^\alpha \theta_i(x)| \le C_\alpha(\rho_0^{1/3})^{|\alpha|}$ for $i = 0,1$.

θ_0 and θ_1 are real-valued.

If $A \subset \{1\dots N\}$ consists of $j_1 < j_2 < \cdots < j_s$ and ${}^cA$ consists of $i_1 < i_2 < \cdots < i_t$, then for $(x_1\dots x_N) \in \mathbb{R}^{3N}$ given, we define $x_A = (x_{j_1}\dots x_{j_s})$ and $x'_A = (x_{i_1}\dots x_{i_t})$. Let $\mathcal{M}$ be the space of all pairs (A, x'_A), and define

$$\Psi^{\#}_{A,x'_A}(x_A) = \Psi(x_1\dots x_N)\cdot\prod_{j\in A}\theta_0(x_j)\cdot\prod_{i\notin A}\theta_1(x_i). \tag{23}$$

On $\mathcal{M}$ we define a probability measure μ by

$$d\mu(A,x'_A) = \|\Psi^{\#}_{A,x'_A}\|^2\cdot\prod_{i\notin A}dx_i. \tag{24}$$

To check that μ is indeed a probability measure, we note that the total μ-measure of $\mathcal{M}$ is given by

$$\sum_A \int_{\mathbb{R}^{3|{}^cA|}} \|\Psi^\#_{A,x'_A}\|^2 \cdot \prod_{i\notin A} dx_i =$$

$$\sum_A \int_{\mathbb{R}^{3|{}^cA|}} \left\{ \int_{\mathbb{R}^{3|A|}} \left| \Psi(x_1 \dots x_N) \prod_{j\in A} \theta_0(x_j) \prod_{i\notin A} \theta_1(x_i) \right|^2 \cdot \prod_{j\in A} dx_j \right\} \prod_{i\notin A} dx_i$$

$$= \sum_A \int_{\mathbb{R}^{3N}} |\Psi(x_1 \dots x_N)|^2 \prod_{j\in A} \theta_0^2(x_j) \prod_{i\notin A} \theta_1^2(x_i) dx_1 \dots dx_N$$

$$= \int_{\mathbb{R}^{3N}} |\Psi(x_1 \dots x_N)|^2 dx_1 \dots dx_N = 1.$$

Thus $\mu(\mathcal{M}) = 1$.

Since μ is obviously non-negative by (24), we know that μ is a probability measure.

For those $(A, x'_A) \in \mathcal{M}$ with $\|\Psi^\#_{A,x'_A}\| \neq 0$, define

$$\Psi_{A,x'_A}(x_A) = \|\Psi^\#_{A,x'_A}\|^{-1} \cdot \Psi^\#_{A,x'_A}(x_A). \tag{25}$$

If $\|\Psi^\#_{A,x'_A}\| = 0$, then Ψ_{A,x'_A} is undefined.

Immediately from the definitions (23), (25) we see that Ψ_{A,x'_A} has the following properties whenever it is defined.

(26) $\|\Psi_{A,x'_A}\| = 1$

(27) $\Psi_{A,x'_A}(x_A)$ is antisymmetric under spin-preserving permutations of the x_j $(j \in A)$

(28) $\Psi_{A,x'_A}(x_A) = 0$ unless $x_j \in \operatorname{supp}\theta_0 \subset\subset Q$ for all $j \in A$.

In view of (26)…(28), we may regard Ψ_{A,x'_A} as an $|A|$-particle wave function on the flat torus T obtained from Q by identifying opposite faces of ∂Q. The identifications create no problems, by virtue of (28).

The main idea of this section is to apply Theorems 1 and 2 of the previous section to Ψ_{A,x'_A}, viewed as a many-particle wave function on a flat torus. To carry this out, we begin as follows.

Lemma 3: *For μ-almost every $(A, x'_A) \in \mathcal{M}$, the wave function Ψ_{A,x'_A} is well-defined. We* *have also the following relations*

$$(29) \qquad KE(Q,\Psi) \geq \int_{\mathcal{M}} \|\nabla_{x_A}\Psi_{A,x'_A}\|^2 d\mu(A,x'_A) - C\rho_0^{2/3}\langle \mathcal{N}_\Omega\Psi,\Psi\rangle$$

$$(30) \qquad \mathcal{S}_s(x,y,\Psi) = \int_{\mathcal{M}} \mathcal{S}_s(x,y,\Psi_{A,x'_A})d\mu(A,x'_A) \text{ for } x,y\in Q\setminus\Omega$$

$$(31) \qquad \Big\langle \sum_{1\leq i<j\leq N} K(x_i,x_j)\Psi,\Psi\Big\rangle = \int_{\mathcal{M}} \Big\langle \sum_{\substack{i<j\\ i,j\in A}} K(x_i,x_j)\Psi_{A,x'_A},\Psi_{A,x'_A}\Big\rangle d\mu(A,x'_A)$$

for symmetric $K(x,y)$ supported in $(Q\setminus\Omega)\times(Q\setminus\Omega)$

$$(32) \qquad \langle \mathcal{N}_Q\Psi,\Psi\rangle \leq \int_{\mathcal{M}} |A|d\mu(A,x'_A) + \langle \mathcal{N}_\Omega\Psi,\Psi\rangle.$$

Note: In (30), $\mathcal{S}_s(x,y,\Psi_{A,x'_A})$ is defined as

$$\sum_{\substack{\text{spin}(k)=s\\ k\in A}} \int \Psi_{A,x'_A}((x_j)_{j\in A})\bar{\Psi}_{A,x'_A}((y_j)_{j\in A})\delta(x_k-x)\delta(y_k-y)\prod_{\substack{\ell\neq k\\ \ell\in A}}\delta(x_\ell-y_\ell)\prod_{i\in A}dx_i dy_i.$$

We trust that the meaning of this expression is clear, even when Ψ is not smooth.

Proof of Lemma 3: Set $\mathcal{M}_+ = \{(A,x'_A)\in\mathcal{M} \mid \|\Psi^{\#}_{A,x'_A}\|\neq 0\}$, $\mathcal{M}_0(A) = \{x'_A \mid \|\Psi^{\#}_{A,x'_A}\| = 0\}$. Then

$$\mu(\mathcal{M}\setminus\mathcal{M}_+) = \sum_A \int_{\mathcal{M}_0(A)} \|\Psi^{\#}_{A,x'_A}\|^2 \prod_{i\notin A} dx_i = 0,$$

since the integrand is zero on $\mathcal{M}_0(A)$. So Ψ_{A,x'_A} is defined μ-almost everywhere, since it is defined on $\mathcal{M}_+$.

Next we check (30). Again, we use delta-functions, and we trust that the reader will understand the meaning of our integrals. For $x,y\in Q\setminus\Omega$, we have

$$\mathcal{S}_s(x,y,\Psi) = \sum_{\text{spin}(j)=s} \int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} \Psi(x_1\dots x_N)\bar{\Psi}(y_1\dots y_N)\delta(x_j-x)\delta(y_j-y)\prod_{i\neq j}\delta(x_i-y_i)\cdot \prod_{i=1}^N dx_i dy_i$$

$$= \sum_A \sum_{\text{spin}(j)=s} \int \prod_{i\in A}\theta_0^2(x_i)\prod_{i\notin A}\theta_1^2(x_i)\Psi(x_1\dots x_N)\bar{\Psi}(y_1\dots y_N)\delta(x_j-x)\delta(y_j-y)\prod_{i\neq j}\delta(x_i-y_i)\cdot$$

$$\prod_{i=1}^{N} dx_i dy_i \equiv \sum_{A} \sum_{\text{spin}(j)=s} \text{Term}(A,j).$$

If $j \notin A$, then $\text{Term}(A,j) = 0$ since the integrand in $\text{Term}(A,j)$ contains the factor $\theta_1^2(x_j)\delta(x_j - x)$, and $\theta_1^2(x) = 0$ for $x \in Q \setminus \Omega$. If $j \in A$, then in the support of $\delta(x_j - x)\delta(y_j - y) \prod_{i \neq j} \delta(x_i - y_i)$ we have

$$\prod_{i\in A} \theta_0^2(x_i) \prod_{i\notin A} \theta_1^2(x_i) = \Big[\prod_{i\in A} \theta_0(x_i) \prod_{i\notin A} \theta_1(x_i)\Big] \cdot \Big[\prod_{i\in A} \theta_0(y_i) \prod_{i\notin A} \theta_1(y_i)\Big]. \tag{33}$$

(To check this, we note that $\theta_0^2(x_j) = 1 = \theta_0(x_j)\theta_0(y_j)$ in $\text{supp}\,\delta(x_j - x)\delta(y_j - y)$ with $x, y \in Q \setminus \Omega$.)

Using (33) to rewrite the integral defining $\text{Term}(A,j)$, we obtain

(34) $\mathcal{S}_s(x,y,\Psi) =$

$$\sum_{A} \sum_{\substack{j\in A \\ \text{spin}(j)=s}} \int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} \Big[\prod_{i\in A} \theta_0(x_i) \prod_{i\notin A} \theta_1(x_i) \Psi(x_1 \dots x_N)\Big] \cdot \Big[\prod_{i\in A} \theta_0(y_i) \prod_{i\notin A} \theta_1(y_i) \bar{\Psi}(y_1 \dots y_N)\Big] \cdot$$

$$\delta(x_j - x)\delta(y_j - y) \prod_{i\neq j} \delta(x_i - y_i) \prod_{i=1}^{N} dx_i dy_i =$$

$$\sum_{A} \sum_{\substack{j\in A \\ \text{spin}(j)=s}} \int \Psi^{\#}_{A,x'_A}(x_A) \overline{\Psi^{\#}_{A,y'_A}(y_A)} \delta(x_j - x)\delta(y_j - y) \prod_{i\neq j} \delta(x_i - y_i) \prod_{i=1}^{N} dx_i dy_i =$$

$$\sum_{A} \sum_{\substack{j\in A \\ \text{spin}(j)=s}} \int \Big[\int \Psi^{\#}_{A,x'_A}(x_A) \overline{\Psi^{\#}_{A,y'_A}(y_A)} \delta(x_j - x)\delta(y_j - y) \prod_{i\in A\setminus\{j\}} \delta(x_i - y_i) \prod_{i\in A} dx_i dy_i\Big] \cdot$$

$$\prod_{i\notin A} \delta(x_i - y_i) dx_i dy_i =$$

$$\sum_{A} \sum_{\substack{j\in A \\ \text{spin}(j)=s}} \int \Big[\int \Psi^{\#}_{A,x'_A}(x_A) \overline{\Psi^{\#}_{A,x'_A}(y_A)} \delta(x_j - x)\delta(y_j - y) \prod_{i\in A\setminus\{j\}} \delta(x_i - y_i) \prod_{i\in A} dx_i dy_i\Big] \cdot$$

$$\prod_{i\notin A} dx_i$$

The integral in square brackets is zero for $(A, x'_A) \notin \mathcal{M}_+$, so

$\mathcal{S}_s(x,y,\Psi) =$

$$\sum_{A} \int_{(A,x'_A)\in\mathcal{M}_+} \Big[\sum_{\substack{j\in A \\ \text{spin}(j)=s}} \int \Psi^{\#}_{A,x'_A}(x_A) \overline{\Psi^{\#}_{A,x'_A}(y_A)} \delta(x_j - x)\delta(y_j - y) \prod_{i\in A\setminus\{j\}} \delta(x_i - y_i) \prod_{i\in A} dx_i dy_i\Big] \cdot$$

$$\prod_{i\notin A} dx_i =$$

$$\sum_A \int_{(A,x'_A)\in\mathcal{M}_+} \Big[\sum_{\substack{j\in A\\ \mathrm{spin}(j)=s}} \int \Psi_{A,x'_A}(x_A)\overline{\Psi_{A,x'_A}(y_A)}\delta(x_j-x)\delta(y_j-y) \prod_{i\in A\setminus\{j\}} \delta(x_i-y_i)\prod_{i\in A} dx_i dy_i\Big]\cdot$$

$$\|\Psi^{\#}_{A,x'_A}\|^2 \prod_{i\notin A} dx_i =$$

$$\sum_A \int_{(A,x'_A)\in\mathcal{M}_+} \mathcal{S}_s(x,y,\Psi_{A,x'_A})\|\Psi^{\#}_{A,x'_A}\|^2 \prod_{i\notin A} dx_i =$$

$$\int_{(A,x'_A)\in\mathcal{M}_+} \mathcal{S}_s(x,y,\Psi_{A,x'_A})d\mu(A,x'_A).$$

This proves (30), since $\mathcal{M}_+$ has full μ-measure in $\mathcal{M}$.

Next, we check (31). With $K(x,y)$ supported in $(Q\setminus\Omega)\times(Q\setminus\Omega)$ we have

$$(35)\quad \Big\langle \sum_{i<j} K(x_i,x_j)\Psi,\Psi\Big\rangle = \sum_{i<j}\int_{\mathbb{R}^{3N}} K(x_i,x_j)|\Psi(x_1\dots x_N)|^2 dx_1\dots dx_N$$

$$\sum_A\sum_{i<j}\int_{\mathbb{R}^{3N}} K(x_i,x_j)\prod_{k\in A}\theta_0^2(x_k)\prod_{k\notin A}\theta_1^2(x_k)|\Psi(x_1\dots x_N)|^2 dx_1\dots dx_N =$$

$$\equiv \sum_A\sum_{i<j}\mathrm{Term}(A,i,j).$$

If $i\notin A$, then the integrand in $\mathrm{Term}(A,i,j)$ contains the factor $K(x_i,x_j)\theta_1^2(x_i)$. Since $K(x_i,x_j)$ is supported in $\{x_i\in Q\setminus\Omega\}$, and since $\theta_1(x_i)=0$ for $x_i\in Q\setminus\Omega$, it follows that $K(x_i,x_j)\theta_1^2(x_i)\equiv 0$. Hence $\mathrm{Term}(A,i,j)=0$ for $i\notin A$. Similarly, $\mathrm{Term}(A,i,j)=0$ for $j\notin A$. Therefore (35) implies

$$(36)\quad \Big\langle \sum_{i<j} K(x_i,x_j)\Psi,\Psi\Big\rangle =$$

$$\sum_A \sum_{\substack{i<j\\ i,j\in A}} \int_{\mathbb{R}^{3N}} K(x_i,x_j)|\Psi(x_1\dots x_N)\prod_{k\in A}\theta_0(x_k)\prod_{k\notin A}\theta_1(x_k)|^2 dx_1\dots dx_N$$

$$= \sum_A \sum_{\substack{i<j\\ i,j\in A}} \int_{\mathbb{R}^{3N}} K(x_i,x_j)|\Psi^{\#}_{A,x'_A}(x_A)|^2 dx_1\dots dx_N =$$

$$\sum_A \int\Big[\int \sum_{\substack{i<j\\ i,j\in A}} K(x_i,x_j)|\Psi^{\#}_{A,x'_A}(x_A)|^2 \prod_{k\in A} dx_k\Big]\cdot\prod_{k\notin A} dx_k.$$

If $(A, x'_A) \notin \mathcal{M}_+$, then the integral in square brackets in (36) is zero. Hence (36) is equivalent to

$$\left\langle \sum_{i<j} K(x_i,x_j)\Psi,\Psi \right\rangle = \sum_A \int\limits_{(A,x'_A)\in\mathcal{M}_+} \left[\int \sum_{\substack{i<j\\ i,j\in A}} K(x_i,x_j)|\Psi^{\#}_{A,x'_A}(x_A)|^2 \prod_{k\in A} dx_k \right] \prod_{k\notin A} dx_k$$

$$= \sum_A \int\limits_{(A,x'_A)\in\mathcal{M}_+} \left[\int \sum_{\substack{i<j\\ i,j\in A}} K(x_i,x_j)|\Psi_{A,x'_A}(x_A)|^2 \prod_{k\in A} dx_k \right] \cdot \|\Psi^{\#}_{A,x'_A}\|^2 \prod_{k\notin A} dx_k$$

$$= \int\limits_{(A,x'_A)\in\mathcal{M}_+} \left\langle \sum_{\substack{i<j\\ i,j\in A}} K(x_i,x_j)\Psi_{A,x'_A},\Psi_{A,x'_A} \right\rangle d\mu(A,x').$$

This proves (31), since $\mathcal{M}_+$ has full μ-measure in $\mathcal{M}$.

Next we prove (29). By definition of $d\mu(A,x'_A)$ and of Ψ_{A,x'_A}, we have

$$(37) \quad \int\limits_{\mathcal{M}} \|\nabla_{x_A}\Psi_{A,x'_A}(x_A)\|^2 d\mu(A,x'_A) =$$

$$\sum_A \int \left[\sum_{j\in A} \int |\nabla_{x_j}\Psi_{A,x'_A}(x_A)|^2 \prod_{i\in A} dx_i \right] \cdot \|\Psi^{\#}_{A,x'_A}\|^2 \prod_{i\notin A} dx_i =$$

$$\sum_A \sum_{j\in A} \int \left[|\nabla_{x_j}\Psi^{\#}_{A,x'_A}(x_A)|^2 \prod_{i\in A} dx_i \right] \prod_{i\notin A} dx_i =$$

$$\sum_A \sum_{j\in A} \int \left| \nabla_{x_j} \left\{ \Psi(x_1\dots x_N) \prod_{i\in A}\theta_0(x_i) \prod_{i\notin A}\theta_1(x_i) \right\} \right|^2 dx_1\dots dx_N =$$

$$\sum_A \sum_{j\in A} \int |\nabla_{x_j} \left\{ \Psi(x_1\dots x_N)\theta_0(x_j) \right\}|^2 \prod_{i\in A\setminus\{j\}} \theta_0^2(x_i) \prod_{i\notin A}\theta_1^2(x_i) dx_1\dots dx_N =$$

$$\sum_{j=1}^N \int \left| \nabla_{x_j} \left\{ \Psi(x_1\dots x_N)\theta_0(x_j) \right\} \right|^2 \cdot \sum_{A\ni j} \left[\prod_{i\in A\setminus\{j\}} \theta_0^2(x_i) \prod_{i\notin A}\theta_1^2(x_i) \right] dx_1\dots dx_N =$$

$$\sum_{j=1}^N \int |\nabla_{x_j}\{\Psi(x_1\dots x_N)\theta_0(x_j)\}|^2 dx_1\dots dx_N =$$

$$\sum_{j=1}^N \int \left[\theta_0^2(x_j)|\nabla_{x_j}\Psi|^2 + |\nabla_{x_j}\theta_0(x_j)|^2|\Psi|^2 + 2\mathrm{Re}(\theta_0(x_j)\nabla_{x_j}\theta_0(x_j)\cdot\bar{\Psi}\nabla_{x_j}\Psi) \right] dx_1\dots dx_N$$

Integration by parts gives

(38)

$$\int 2\mathrm{Re}[\theta_0(x_j)\nabla_{x_j}\theta_0(x_j)\cdot\bar{\Psi}\nabla_{x_j}\Psi] dx_1\dots dx_N = \frac{1}{2}\int \nabla_{x_j}\theta_0^2(x_j)\cdot\nabla_{x_j}|\Psi|^2 dx_1\dots dx_N$$

$$= -\frac{1}{2}\int \{\nabla_{x_j}\cdot\nabla_{x_j}\theta_0^2(x_j)\}|\Psi|^2 dx_1\dots dx_N = \int\{-|\nabla_{x_j}\theta_0(x_j)|^2 - \theta_0(x_j)\Delta_{x_j}\theta_0(x_j)\}\cdot |\Psi|^2 dx_1\dots dx_N$$

since $\frac{1}{2}\nabla_{x_j}\cdot\nabla_{x_j}\theta_0^2(x_j) = \nabla_{x_j}\cdot[\theta_0(x_j)\nabla_{x_j}\theta_0(x_j)] = |\nabla_{x_j}\theta_0(x_j)|^2 + \theta_0(x_j)\Delta_{x_j}\theta_0(x_j)$. Substituting (38) into the right-hand side of (37), we get

$$(39)\quad \int_{\mathcal{M}} \|\nabla_{x_A}\Psi_{A,x'_A}(x_A)\|^2 d\mu(A,x'_A) = \sum_{j=1}^{N}\int_{\mathbb{R}^{3N}} \theta_0^2(x_j)|\nabla_{x_j}\Psi(x_1\dots x_N)|^2 dx_1\dots dx_N - \sum_{j=1}^{N}\int_{\mathbb{R}^{3N}} \theta_0(x_j)\Delta_{x_j}\theta_0(x_j)|\Psi(x_1\dots x_N)|^2 dx_1\dots dx_N.$$

Our estimates on the derivatives of θ_0 show that $|\theta_0(x_j)\Delta_{x_j}\theta_0(x_j)| \le C\rho_0^{2/3}$. Since $\theta_0 \equiv 1$ in $Q\setminus\Omega$ and $\theta_0\equiv 0$ outside Q, it follows that $\Delta_{x_j}\theta_0(x_j)$ is supported in Ω, so $|\theta_0(x_j)\Delta_{x_j}\theta_0(x_j)| \le C\rho_0^{2/3}\chi_\Omega(x_j)$. Summing on j, we conclude that

$$\left|\sum_{j=1}^{N}\theta_0(x_j)\Delta_{x_j}\theta_0(x_j)\right| \le C\rho_0^{2/3}\mathcal{N}_\Omega(x_1\dots x_N).$$

Therefore,

$$(40)\quad -\sum_{j=1}^{N}\int_{\mathbb{R}^{3N}} \theta_0(x_j)\Delta_{x_j}\theta_0(x_j)|\Psi(x_1\dots x_N)|^2 dx_1\dots dx_N \le C\rho_0^{2/3}\left\langle \mathcal{N}_\Omega\Psi,\Psi\right\rangle.$$

Also, $\theta_0^2(x_j)\le \chi_Q(x_j)$, so

$$(41)\quad \sum_{j=1}^{N}\int_{\mathbb{R}^{3N}} \theta_0^2(x_j)|\nabla_{x_j}\Psi(x_1\dots x_N)|^2 dx_1\dots dx_N \le \sum_{j=1}^{N}\int_{\mathbb{R}^{3N}} \chi_Q(x_j)|\nabla_{x_j}\Psi(x_1\dots x_N)|^2 dx_1\dots dx_N = KE(Q,\Psi).$$

Putting (40) and (41) into (39), we get

$$\int_{\mathcal{M}} \|\nabla_{x_A}\Psi_{A,x'_A}\|^2 d\mu(A,x'_A) \le KE(Q,\Psi) + C\rho_0^{2/3}\left\langle\mathcal{N}_\Omega\Psi,\Psi\right\rangle,$$

which completes the proof of (29).

Finally, we check (32). By definition of $d\mu(A, x'_A)$ and $\Psi^{\#}_{A,x'_A}$ we have

$$
\int\limits_{\mathcal{M}} |A| d\mu(A, x'_A) = \sum_A |A| \int \|\Psi^{\#}_{A,x'_A}\|^2 \prod_{i \notin A} dx_i = \tag{42}
$$

$$
\sum_A |A| \int \Big[\int |\Psi(x_1 \ldots x_N) \prod_{i \in A} \theta_0(x_i) \prod_{i \notin A} \theta_1(x_i)|^2 \prod_{i \in A} dx_i \Big] \prod_{i \notin A} dx_i =
$$

$$
\sum_A |A| \int |\Psi(x_1 \ldots x_N) \prod_{i \in A} \theta_0(x_i) \prod_{i \notin A} \theta_1(x_i)|^2 dx_1 \ldots dx_N =
$$

$$
\sum_A \sum_{j \in A} \int |\Psi(x_1 \ldots x_N)|^2 \prod_{i \in A} \theta_0^2(x_i) \prod_{i \notin A} \theta_1^2(x_i) dx_1 \ldots dx_N =
$$

$$
\int\limits_{\mathbb{R}^{3N}} \sum_{j=1}^{N} \Big[\sum_{A \ni j} \prod_{i \in A} \theta_0^2(x_i) \prod_{i \notin A} \theta_1^2(x_i) \Big] \cdot |\Psi(x_1 \ldots x_N)|^2 dx_1 \ldots dx_N =
$$

$$
\int\limits_{\mathbb{R}^{3N}} \sum_{j=1}^{N} \theta_0^2(x_j) |\Psi(x_1 \ldots x_N)|^2 dx_1 \ldots dx_N
$$

Since $\theta_0^2(x_j) = 1$ for $x_j \in Q \setminus \Omega$, and since $\Omega \subset Q$, we have $\theta_0^2(x_j) \geq \chi_{Q \setminus \Omega}(x_j) = \chi_Q(x_j) - \chi_\Omega(x_j)$. Summing on j, we get the inequality $\sum_{j=1}^{N} \theta_0^2(x_j) \geq \mathcal{N}_Q(x_1 \ldots x_N) - \mathcal{N}_\Omega(x_1 \ldots x_N)$, which implies

$$
\int\limits_{\mathbb{R}^{3N}} \sum_{j=1}^{N} \theta_0^2(x_j) |\Psi(x_1 \ldots x_N)|^2 dx_1 \ldots dx_N \geq \langle \mathcal{N}_Q \Psi, \Psi \rangle - \langle \mathcal{N}_\Omega \Psi, \Psi \rangle . \tag{43}
$$

Combining (42), (43), we get

$$
\int\limits_{\mathcal{M}} |A| d\mu(A, x'_A) \geq \langle \mathcal{N}_Q \Psi, \Psi \rangle - \langle \mathcal{N}_\Omega \Psi, \Psi \rangle ,
$$

which is equivalent to (32). The proof of Lemma 3 is complete. □

Next we show that our hypothesis (7) on $\mathcal{E}(Q, \rho_0, \Psi)$ controls the wave functions Ψ_{A,x'_A} for (A, x'_A) outside a subset of $\mathcal{M}$ with small μ-measure. Specifically, the number of particles of spin s in Ψ_{A,x'_A} will be close to $\rho_0|Q|$, and the kinetic energy $\|\nabla_{x_A} \Psi_{A,x'_A}\|^2$ will be close to the minimum possible for the given number of particles of each spin. To see this, we start with (7) and the definition of $\mathcal{E}(Q, \rho_0, \Psi)$, which imply that

$$
\delta \rho_0^{5/3} |Q| \geq \mathcal{E}(Q, \rho_0, \Psi) \geq KE(Q, \Psi) - \frac{5}{3} c_{TF} \rho_0^{5/3} \langle \mathcal{N}_Q \Psi, \Psi \rangle + \frac{2}{3} q c_{TF} \rho_0^{5/3} |Q|. \tag{44}
$$

Lemmas 2 and 3 yield

$$KE(Q,\Psi) \geq \int_{\mathcal{M}} \|\nabla_{x_A}\Psi_{A,x'_A}\|^2 d\mu(A,x'_A) - C\rho_0^{2/3}\underline{\mathrm{N}}^{13/15} \tag{45}$$

and

$$-\frac{5}{3}c_{TF}\rho_0^{2/3}\langle \mathcal{N}_Q\Psi,\Psi\rangle \geq -\frac{5}{3}c_{TF}\rho_0^{2/3}\int_{\mathcal{M}} |A| d\mu(A,x'_A) - C\rho_0^{2/3}\underline{\mathrm{N}}^{13/15}. \tag{46}$$

Also,

$$\frac{2}{3}qc_{TF}\rho_0^{5/3}|Q| = \int_{\mathcal{M}} \left(\frac{2}{3}qc_{TF}\rho_0^{5/3}|Q|\right) d\mu(A,x'_A) \tag{47}$$

since μ is a probability measure. Putting (45), (46), (47) into the right-hand side of (44), we obtain

$$\delta\rho_0^{5/3}|Q| \geq \int_{\mathcal{M}} Y(A,x'_A)d\mu(A,x'_A) - C\rho_0^{2/3}\underline{\mathrm{N}}^{13/15}, \tag{48}$$

with

$$Y(A,x'_A) = \|\nabla_{x_A}\Psi_{A,x'_A}\|^2 - \frac{5}{3}c_{TF}\rho_0^{2/3}|A| + \frac{2}{3}qc_{TF}\rho_0^{5/3}|Q|. \tag{49}$$

Since $\underline{\mathrm{N}} = \rho_0|Q|$, (48) can be rewritten as

$$\int_{\mathcal{M}} Y(A,x'_A)d\mu(A,x'_A) \leq C(\delta + \underline{\mathrm{N}}^{-2/15})\rho_0^{5/3}|Q|. \tag{50}$$

Let us explore the meaning of $Y(A,x'_A)$. We fix $(A,x'_A) \in \mathcal{M}_+$. As explained above, Ψ_{A,x'_A} may be viewed as a many-particle wave function on the flat torus T, obtained from Q by identifications. In the study of Ψ_{A,x'_A}, the number of particles of spin s is m_s = (number of $j \in A$ with spin$(j) = s$). Therefore, Lemma 3 in the previous section shows that

$$\|\nabla_{x_A}\Psi_{A,x'_A}\|^2 \geq \sum_{s=1}^{q}(c_{TF}m_s^{5/3} - C_2 m_s^{4/3})|Q|^{-2/3}. \tag{51}$$

This suggests that we rewrite $Y(A,x'_A)$ in (49) as

$$Y(A,x'_A) = \left[\|\nabla_{x_A}\Psi_{A,x'_A}\|^2 - \sum_{s=1}^{q}(c_{TF}m_s^{5/3} - C_2 m_s^{4/3})|Q|^{-2/3}\right] +$$
$$\sum_{s=1}^{q}(c_{TF}m_s^{5/3} - C_2 m_s^{4/3})|Q|^{-2/3} - \frac{5}{3}c_{TF}\rho_0^{2/3}\sum_{s=1}^{q} m_s + \frac{2}{3}qc_{TF}\rho_0^{5/3}|Q|.$$

Equivalently,

(52)
$$\left[\|\nabla_{x_A}\Psi_{A,x'_A}\|^2 - \sum_{s=1}^{q}(c_{TF}m_s^{5/3} - C_2 m_s^{4/3})|Q|^{-2/3}\right] + \sum_{s=1}^{q} Y_*(m_s) = Y(A,x'_A) + C_3 q\rho_0^{5/3}|Q|\underline{\mathrm{N}}^{-1/3}$$

with

(53)
$$Y_*(m_s) = (c_{TF}m_s^{5/3}|Q|^{-2/3} - \frac{5}{3}c_{TF}\rho_0^{2/3}m_s + \frac{2}{3}c_{TF}\rho_0^{5/3}|Q|) + (C_3\rho_0^{5/3}|Q|\underline{\mathrm{N}}^{-1/3} - C_2 m_s^{4/3}|Q|^{-2/3}) \equiv Y_{\mathrm{main}}(m_s) + Y_{\mathrm{extra}}(m_s).$$

The behavior of $Y_{\mathrm{main}}(m_s)$ is easily understood in terms of the elementary function $g(t) = t^{5/3} - \frac{5}{3}t + \frac{2}{3}$, which is comparable to $(t-1)^2\chi_{t\le 2} + t^{5/3}\chi_{t\ge 2}$ for $t \in [0,\infty)$. Putting $t = \frac{m_s}{\rho_0|Q|} = \frac{m_s}{\underline{\mathrm{N}}}$, we see that

$$Y_{\mathrm{main}}(m_s) \sim \rho_0^{5/3}|Q| \cdot \left(1 - \frac{m_s}{\underline{\mathrm{N}}}\right)^2 \chi_{m_s \le 2\underline{\mathrm{N}}} + m_s^{5/3}|Q|^{-2/3}\chi_{m_s \ge 2\underline{\mathrm{N}}}.$$

Regarding $Y_{\mathrm{extra}}(m_s) = (C_3\underline{\mathrm{N}}^{4/3} - C_2 m_s^{4/3})|Q|^{-2/3}$, we take $C_3 \gg C_2$ and assume that $\underline{\mathrm{N}}$ exceeds a large constant, so that

$$Y_{\mathrm{extra}}(m_s) \ge 0 \quad \text{if} \quad m_s \le 2\underline{\mathrm{N}},$$
$$|Y_{\mathrm{extra}}(m_s)| \sim m_s^{4/3}|Q|^{-2/3} \ll m_s^{5/3}|Q|^{-2/3} \sim Y_{\mathrm{main}}(m_s) \quad \text{if} \quad m_s \ge 2\underline{\mathrm{N}}.$$

In either case, we conclude that

$$Y_*(m_s) = Y_{\mathrm{main}}(m_s) + Y_{\mathrm{extra}}(m_s) \ge cY_{\mathrm{main}}(m_s), \quad \text{i.e.}$$
$$Y_*(m_s) \ge c\rho_0^{5/3}|Q| \cdot \left(1 - \frac{m_s}{\underline{\mathrm{N}}}\right)^2 \chi_{m_s \le 2\underline{\mathrm{N}}} + cm_s^{5/3}|Q|^{-2/3}\chi_{m_s \ge 2\underline{\mathrm{N}}}.$$

Putting this into (52), we get

(54)
$$\left[\|\nabla_{x_A}\Psi_{A,x'_A}\|^2 - \sum_{s=1}^{q}(c_{TF}m_s^{5/3} - C_2 m_s^{4/3})|Q|^{-2/3}\right] + c\rho_0^{5/3}|Q|\sum_{s=1}^{q}\left(1 - \frac{m_s}{\underline{\mathrm{N}}}\right)^2 \chi_{m_s \le 2\underline{\mathrm{N}}} + c|Q|^{-2/3}\sum_{s=1}^{q} m_s^{5/3}\chi_{m_s \ge 2\underline{\mathrm{N}}} \le Y(A,x'_A) + C_3 q\rho_0^{5/3}|Q|\underline{\mathrm{N}}^{-1/3} \equiv \widetilde{Y}(A,x'_A).$$

From (51) and (54), we see that $\widetilde{Y}(A, x'_A) \geq 0$, and from (50) we obtain

$$\int_{\mathcal{M}} \widetilde{Y}(A, x'_A) d\mu(A, x'_A) \leq C'(\delta + \underline{N}^{-2/15}) \rho_0^{5/3} |Q|. \tag{55}$$

Hence for $0 < \widetilde{\delta} < c$ to be picked later, we have

$$\widetilde{Y}(A, x'_A) \leq \widetilde{\delta} \rho_0^{5/3} |Q| \quad \text{for all} \quad (A, x'_A) \in \mathcal{M} \setminus F, \tag{56}$$

where F is a subset of $\mathcal{M}$ with μ-measure

$$\mu(F) \leq C \widetilde{\delta}^{-1} (\delta + \underline{N}^{-2/15}). \tag{57}$$

For $(A, x'_A) \in \mathcal{M} \setminus F$, estimates (51), (54), (56) imply

$$\|\nabla_{x_A} \Psi_{A, x'_A}\|^2 - \sum_{s=1}^{q} (c_{TF} m_s^{5/3} - C_2 m_s^{4/3}) |Q|^{-2/3} \leq \widetilde{\delta} \rho_0^{5/3} |Q|, \tag{58}$$

$$\sum_{s=1}^{q} \left(1 - \frac{m_s}{\underline{N}}\right)^2 \chi_{m_s \leq 2\underline{N}} \leq \widetilde{\delta}, \quad \text{and} \tag{59}$$

$$|Q|^{-2/3} \sum_{s=1}^{q} m_s^{5/3} \chi_{m_s \geq 2\underline{N}} \leq C \widetilde{\delta} \rho_0^{5/3} |Q| = C \widetilde{\delta} \underline{N}^{5/3} |Q|^{-2/3}. \tag{60}$$

If $C\widetilde{\delta} < 1$ in (60), then already (60) is violated if even one of the m_s exceeds $2\underline{N}$. Hence for $(A, x'_A) \in \mathcal{M} \setminus F$, we have $m_s \leq 2\underline{N}$ for all s, and therefore (59) implies

$$|1 - m_s/\underline{N}| \leq \widetilde{\delta}^{1/2} \quad \text{for} \quad (A, x'_A) \in \mathcal{M} \setminus F. \tag{61}$$

As an immediate consequence of (58) and (61), we have

$$\|\nabla_{x_A} \Psi_{A, x'_A}\|^2 \leq (1 + C\widetilde{\delta}) c_{TF} \sum_{s=1}^{q} \left(\frac{m_s}{|Q|}\right)^{5/3} |Q|, \quad \text{for} \quad (A, x'_A) \in \mathcal{M} \setminus F \tag{62}$$

and

$$\frac{1}{2} \leq m_s / m_{s'} \leq 2 \quad \text{for all } s,\ s', \text{ and all } (A, x'_A) \in \mathcal{M} \setminus F. \tag{63}$$

Thus, we have succeeded in controlling the particle numbers and kinetic energy of Ψ_{A, x'_A} for (A, x'_A) outside a set of small μ-measure.

Equations (61)...(63) allow us to use Theorems 1 and 2 from the preceding section. Thus, we obtain the following results.

Lemma 4: *Suppose* $\varepsilon > 0$ *and* $K(x,y)$ *is defined on* $Q \times Q$*, satisfying*

$$0 \le K(x,y) = K(y,x) \le C|x-y|^{-1}\chi_{|x-y|<r_{\max}}. \tag{64}$$

Assume also that

$$\rho_0 r_{\max}^3 \ge c,\ \widetilde{\delta} < c'_\varepsilon(\rho_0 r_{\max}^3)^{-\frac{247}{30}},\ \underline{N} > C'_\varepsilon(\rho_0 r_{\max}^3)^{+\frac{247}{10}}, \tag{65}$$

with c'_ε *and* C'_ε *depending only on* C, c, ε, q. *Then for* $(A, x'_A) \in \mathcal{M} \setminus F$*, we have*

$$\left\langle \sum_{\substack{j<k \\ j,k\in A}} K(x_j,x_k)\Psi_{A,x'_A}, \Psi_{A,x'_A} \right\rangle \ge \tag{66}$$

$$\frac{1}{2}\iint_{Q\times Q} K(x,y)\left\{\rho^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2\right\} dxdy - C''_\varepsilon E_\# \rho_0^{1/3}\underline{N},$$

with

$$\rho_s = \frac{m_s}{|Q|}, \quad \rho = \sum_{s=1}^{q} \rho_s, \quad \text{and} \tag{67}$$

$$E_\# = (\rho_0 r_{\max}^3)^{\frac{584}{921}+2\varepsilon} \cdot (\widetilde{\delta} + \underline{N}^{-1/3})^{\frac{5}{307}-\varepsilon}. \tag{68}$$

Here, $\mathcal{S}_\rho(\cdot)$ *is defined as in the previous section, and* C''_ε *depends only on* c, C, ε, q.

Proof: Equations (61)...(65) show that the hypotheses of Theorem 1 in the previous section are satisfied, with $\underline{N}$ in place of N, and with $\widetilde{\delta}$ in place of δ. The conclusion of Theorem 1 is equivalent to (66)...(68), since $\rho \sim \rho_0$. □

Lemma 5: *Let* $\varepsilon > 0$*, and assume that*

$$0 < \widetilde{\delta} < c', \quad \underline{N} > C', \quad \text{with } c' \text{ and } C' \text{ depending only on } \varepsilon,\ q. \tag{69}$$

Then for $(A, x'_A) \in \mathcal{M} \setminus F$ *and for* $h \in \mathbb{R}^3$ *with*

$$\rho_0^{1/3}|h| \le c''(\widetilde{\delta} + \underline{N}^{-1/3})^{-3/46}, \quad \text{we have} \tag{70}$$

$$\int_{Q_0} |\mathcal{S}_s(x, x+h, \Psi_{A,x'_A}) - \mathcal{S}_{\rho_s}(h)|dx \le \tag{71}$$

$$C''\underline{N} \cdot \left[\left(\widetilde{\delta} + \underline{N}^{-1/3}\right)^{\frac{1}{46}-\varepsilon} + \left(\widetilde{\delta} + \underline{N}^{-1/3}\right)^{\frac{3}{46}} \rho_0^{1/3}|h|\right].$$

Here, Q_0 denotes the middle half of Q, $\rho_s = \frac{m_s}{|Q|}$, and the constants c'', C'' depend only on ε and q.

Proof: Equations (61)...(63) and (69), (70) show that the hypotheses of Theorem 2 in the previous section are satisfied, with $\underset{\sim}{N}$ in place of N, and with $\widetilde{\delta}$ in place of δ. The conclusion of Theorem 2 implies (71), since $\rho \sim \rho_0$. □

To deal with $(A, x'_A) \in F$, we will need the following additional remarks. For $A \subset \{1 \dots N\}$ and $m_s =$ (number of $j \in A$ with spin s), we have $|A|^{5/3}\chi_{|A|>C\underset{\sim}{N}} \leq C' \sum_{s=1}^{q} m_s^{5/3}$ $\chi_{m_s \geq 2\underset{\sim}{N}}$. Hence, (51), (54), (55) imply

$$\int_{\mathcal{M}} c|Q|^{-2/3}|A|^{5/3}\chi_{|A|>C\underset{\sim}{N}} d\mu(A, x'_A) \leq$$

$$C'(\delta + \underset{\sim}{N}^{-2/15})\rho_0^{5/3}|Q| = C'(\delta + \underset{\sim}{N}^{-2/15})\underset{\sim}{N}^{5/3}|Q|^{-2/3}, \text{ i.e.}$$

(72)
$$\int_{\mathcal{M}} |A|^{5/3}\chi_{|A|>C\underset{\sim}{N}} d\mu(A, x'_A) \leq C''(\delta + \underset{\sim}{N}^{-2/15})\underset{\sim}{N}^{5/3}.$$

Now we can derive the analogues of Theorems 1 and 2 from the previous section. We begin with Theorem 1. Lemma 4 provides us with a lower bound (66) for

$$\left\langle \sum_{\substack{j<k \\ j,k \in A}} K(x_j, x_k)\Psi_{A,x'_A}, \Psi_{A,x'_A} \right\rangle \quad \text{when} \quad (A, x'_A) \in \mathcal{M} \setminus F.$$

In that lower bound, we want to replace ρ_s and ρ by ρ_0 and $q\rho_0$. To do so, note that

(73)
$$|\rho_0 - \rho_s| \leq \widetilde{\delta}^{1/2}\rho_0 \quad \text{and} \quad |\rho - q\rho_0| \leq q\widetilde{\delta}^{1/2}\rho_0,$$

when $(A, x'_A) \in \mathcal{M} \setminus F$, by virtue of (61), (67), and the definition $\underset{\sim}{N} = \rho_0|Q|$. Also, recall from (18), (19) in the previous section that

(74)
$$\mathcal{S}_\rho(\mathfrak{z}) = \int_{B(0,r_F)} e^{i\eta\cdot\mathfrak{z}} \frac{d\eta}{(2\pi)^3} \quad \text{with} \quad \rho = r_F^3/(6\pi^2).$$

From (73), we see that the Fermi radii associated to ρ_0 and ρ_s satisfy $(1 - C\widetilde{\delta}^{1/2})r_{F,0} \leq r_{F,s} \leq (1 + C\widetilde{\delta}^{1/2})r_{F,0}$, which together with (74) yields

(74 bis)
$$\begin{aligned} |\mathcal{S}_{\rho_s}(\mathfrak{z}) - \mathcal{S}_{\rho_0}(\mathfrak{z})| &\leq (2\pi)^{-3}\text{vol}\{B(0, (1 + C\widetilde{\delta}^{1/2})r_{F,0}) \setminus B(0, (1 - C\widetilde{\delta}^{1/2})r_{F,0})\} \\ &\leq C\widetilde{\delta}^{1/2}r_{F,0}^3 = C'\widetilde{\delta}^{1/2}\rho_0 \end{aligned}$$

Since also $|\mathcal{S}_{\rho_0}(\mathfrak{z})| \le \rho_0$, this implies

$$(75) \qquad \Big| |\mathcal{S}_{\rho_s}(\mathfrak{z})|^2 - |\mathcal{S}_{\rho_0}(\mathfrak{z})|^2 \Big| \le C\widetilde{\delta}^{1/2}\rho_0^2.$$

In addition, we note that

$$(76) \qquad |\rho^2 - (q\rho_0)^2| \le C\widetilde{\delta}^{1/2}\rho_0^2, \quad \text{by (73)}.$$

Hence, if $K(x,y)$ is as in Lemma 4, then (75), (76) show that

$$(77) \quad \frac{1}{2}\iint\limits_{Q\times Q} K(x,y)\Big\{\rho^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2\Big\}dxdy \ge$$
$$\frac{1}{2}\iint\limits_{Q\times Q} K(x,y)\Big\{(q\rho_0)^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_0}(x-y)|^2\Big\}dxdy - C\iint\limits_{Q\times Q} K(x,y)\widetilde{\delta}^{1/2}\rho_0^2 dxdy.$$

Since

$$\iint\limits_{Q\times Q} K(x,y)\widetilde{\delta}^{1/2}\rho_0^2 dxdy \le \iint_{\substack{x\in Q\\ |x-y|<r_{\max}}} \frac{C}{|x-y|}\widetilde{\delta}^{1/2}\rho_0^2 dxdy \le C'\widetilde{\delta}^{1/2}\rho_0^2 r_{\max}^2|Q|$$
$$= C'\widetilde{\delta}^{1/2}\rho_0 r_{\max}^2 \underline{\mathrm{N}} = C'\widetilde{\delta}^{1/2}(\rho_0 r_{\max}^3)^{2/3}\rho_0^{1/3}\underline{\mathrm{N}},$$

(77) implies

$$\frac{1}{2}\iint\limits_{Q\times Q} K(x,y)\Big\{\rho^2 - \sum_{s=1}^{q} |\mathcal{S}_{\rho_s}(x-y)|^2\Big\}dxdy \ge$$
$$\frac{1}{2}\iint\limits_{Q\times Q} K(x,y)\{q^2\rho_0^2 - q|\mathcal{S}_{\rho_0}(x-y)|^2\}dxdy - C\widetilde{\delta}^{1/2}(\rho_0 r_{\max}^3)^{2/3}\rho_0^{1/3}\underline{\mathrm{N}}$$

for $(A, x'_A) \in \mathcal{M} \setminus F$.

Putting this inequality into (66), we obtain

$$(78) \quad \Big\langle \sum_{\substack{j<k\\ j,k\in A}} K(x_j,x_k)\Psi_{A,x'_A}, \Psi_{A,x'_A}\Big\rangle \ge$$
$$\frac{1}{2}\iint\limits_{Q\times Q} K(x,y)\{q^2\rho_0^2 - q|\mathcal{S}_{\rho_0}(x-y)|^2\}dxdy - [C\widetilde{\delta}^{1/2}(\rho_0 r_{\max}^3)^{2/3} + C''_{\varepsilon}E_{\#}]\rho_0^{1/3}\underline{\mathrm{N}}$$

for $(A, x'_A) \in \mathcal{M} \setminus F$.

From (65) and (68) we get

$$[C\widetilde{\delta}^{1/2}(\rho_0 r_{\max}^3)^{2/3} + C''_\varepsilon E_\#] \le C_\varepsilon(\rho_0 r_{\max}^3)^{2/3}(\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{\frac{5}{307}-\varepsilon},$$

so that (78) implies the slightly simpler estimate

$$\text{(79)}\quad \Big\langle \sum_{\substack{j<k \\ j,k\in A}} K(x_j,x_k)\Psi_{A,x'_A}, \Psi_{A,x'_A}\Big\rangle \ge$$
$$\frac{1}{2}\iint\limits_{Q\times Q} K(x,y)\{q^2\rho_0^2 - q|\mathcal{S}_{\rho_0}(x-y)|^2\}dxdy - C_\varepsilon(\rho_0 r_{\max}^3)^{2/3}(\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{\frac{5}{307}-\varepsilon}\rho_0^{1/3}\underline{\mathrm{N}}$$

for $(A, x'_A) \in \mathcal{M} \smallsetminus F$.

For $(A, x'_A) \in F$, we use merely

$$\Big\langle \sum_{\substack{j<k \\ j,k\in A}} K(x_j,x_k)\Psi_{A,x'_A}, \Psi_{A,x'_A}\Big\rangle \ge 0.$$

Hence, if $K(x,y)$ is supported in $(Q \smallsetminus \Omega) \times (Q \smallsetminus \Omega)$, then (31) and (79) show that

$$\text{(80)}\quad \Big\langle \sum_{j<k} K(x_j,x_k)\Psi, \Psi\Big\rangle \ge \int\limits_{\mathcal{M}\smallsetminus F} \Big\langle \sum_{\substack{j<k \\ j,k\in A}} K(x_j,x_k)\Psi_{A,x'_A}, \Psi_{A,x'_A}\Big\rangle d\mu(A,x'_A)$$
$$\ge \mu(\mathcal{M}\smallsetminus F)\cdot\Big[\frac{1}{2}\iint\limits_{Q\times Q} K(x,y)\{q^2\rho_0^2 - q|\mathcal{S}_{\rho_0}(x-y)|^2\}dxdy\Big]$$
$$- C_\varepsilon(\rho_0 r_{\max}^3)^{2/3}(\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{\frac{5}{307}-\varepsilon}\rho_0^{1/3}\underline{\mathrm{N}}.$$

Since $0 \le q^2\rho_0^2 - q|\mathcal{S}_{\rho_0}(x-y)|^2 \le q^2\rho_0^2$ and $0 \le K(x,y) \le \frac{C}{|x-y|}\chi_{|x-y|<r_{\max}}$, the integral in square brackets in (80) is dominated by $C\rho_0^2 r_{\max}^2|Q| = C(\rho_0 r_{\max}^3)^{2/3}\rho_0^{1/3}\underline{\mathrm{N}}$. Therefore, (57) and (80) yield

$$\text{(81)}\quad \Big\langle \sum_{j<k} K(x_j,x_k)\Psi, \Psi\Big\rangle \ge \frac{1}{2}\iint\limits_{Q\times Q} K(x,y)\{q^2\rho_0^2 - q|\mathcal{S}_{\rho_0}(x-y)|^2\}dxdy -$$
$$- C\widetilde{\delta}^{-1}(\delta + \underline{\mathrm{N}}^{-2/15})\cdot(\rho_0 r_{\max}^3)^{2/3}\rho_0^{1/3}\underline{\mathrm{N}} - C_\varepsilon(\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{\frac{5}{307}-\varepsilon}\cdot(\rho_0 r_{\max}^3)^{2/3}\rho_0^{1/3}\underline{\mathrm{N}}.$$

This holds under the assumptions (64), (65) of Lemma 4, and the assumption $\operatorname{supp} K(x,y) \subset (Q \smallsetminus \Omega) \times (Q \smallsetminus \Omega)$. We take $\widetilde{\delta} = (\delta + \underline{\mathrm{N}}^{-2/15})^{\frac{307}{312}}$ to optimize (81). Note that $\widetilde{\delta} > \underline{\mathrm{N}}^{-\frac{2}{15}\cdot\frac{307}{312}} \gg \underline{\mathrm{N}}^{-\frac{1}{3}}$, so

$$(\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{\frac{5}{307}-\varepsilon} \sim (\widetilde{\delta})^{\frac{5}{307}-\varepsilon} = (\delta + \underline{\mathrm{N}}^{-\frac{2}{15}})^{\frac{307}{312}\cdot(\frac{5}{307}-\varepsilon)}$$
$$\le (\delta + \underline{\mathrm{N}}^{-2/15})^{\frac{5}{312}-\varepsilon},$$

and

$$\widetilde{\delta}^{-1}(\delta + \underline{\mathrm{N}}^{-2/15}) = (\delta + \underline{\mathrm{N}}^{-2/15})^{\frac{5}{312}}.$$

So (81) becomes

$$(82) \qquad \left\langle \sum_{j<k} K(x_j, x_k)\Psi, \Psi \right\rangle \geq \frac{1}{2} \iint\limits_{Q\times Q} K(x,y)\{q^2\rho_0^2 - q|\mathbb{S}_{\rho_0}(x-y)|^2\}dxdy$$
$$- C_\varepsilon(\delta + \underline{\mathrm{N}}^{-2/15})^{\frac{5}{312}-\varepsilon}(\rho_0 r_{\max}^3)^{2/3}\rho_0^{1/3}\underline{\mathrm{N}},$$

which holds proved (64), (65) are satisfied for our $\widetilde{\delta}$, and provided $\operatorname{supp} K \subset (Q \setminus \Omega) \times (Q \setminus \Omega)$.

One checks easily that (65) holds provided

$$(83) \qquad \rho_0 r_{\max}^3 > c, \ \delta < c_\varepsilon(\rho_0 r_{\max}^3)^{-\frac{42}{5}}, \ \underline{\mathrm{N}} > C_\varepsilon(\rho_0 r_{\max}^3)^{63}.$$

In fact, the only part of (65) that is not immediately contained in (83) is

$$\widetilde{\delta} < c'_\varepsilon(\rho_0 r_{\max}^3)^{-\frac{247}{30}}, \quad \text{i.e.}$$

$$(\delta + \underline{\mathrm{N}}^{-2/15})^{307/312} < c'_\varepsilon(\rho_0 r_{\max}^3)^{-\frac{247}{30}}, \quad \text{i.e.,}$$
$$\delta < c_\varepsilon(\rho_0 r_{\max}^3)^{-\frac{247}{30}\cdot\frac{312}{307}} \quad \text{and} \quad \underline{\mathrm{N}} > C_\varepsilon(\rho_0 r_{\max}^3)^{\frac{247}{30}\cdot\frac{312}{307}\cdot\frac{15}{2}}.$$

These inequalities follow from (83).

Hence, (64) and (83) imply (82), provided $\operatorname{supp} K \subset (Q \setminus \Omega) \times (Q \setminus \Omega)$. We formulate this result as a lemma.

Lemma 6: *Suppose $\varepsilon > 0$ and $K(x,y)$ is supported in $(Q \setminus \Omega) \times (Q \setminus \Omega)$, satisfying $0 \leq K(x,y) = K(y,x) \leq C|x-y|^{-1}\chi_{|x-y|<r_{\max}}$, with $\rho_0 r_{\max}^3 > c$. Assume also that*

$$\delta < c_\varepsilon(\rho_0 r_{\max}^3)^{-42/5}, \ \underline{\mathrm{N}} > C_\varepsilon(\rho_0 r_{\max}^3)^{63},$$

with c_ε and C_ε depending only on c, C, ε, q. Then

$$\left\langle \sum_{i<j} K(x_i, x_j)\Psi, \Psi \right\rangle \geq$$
$$\frac{1}{2} \iint\limits_{Q\times Q} K(x,y)\{q^2\rho_0^2 - q|\mathbb{S}_{\rho_0}(x-y)|^2\}dxdy - C'_\varepsilon(\delta + \underline{\mathrm{N}}^{-\frac{2}{15}})^{\frac{5}{312}-\varepsilon}(\rho_0 r_{\max}^3)^{2/3}\rho_0^{1/3}\underline{\mathrm{N}},$$

with C'_ε depending only on c, C, ε, q.

From here on, we drop our special choice of $\widetilde{\delta}$.

For $h \in \mathbb{R}^3$ with $\rho_0^{1/3}|h| < (\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{-\frac{2}{46}}$, Lemma 5 gives

(84)
$$\int\limits_{x \in Q_0} |\mathcal{S}_s(x, x+h, \Psi_{A,x'_A}) - \mathcal{S}_{\rho_s}(h) \mid dx \le C\underline{\mathrm{N}}(\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{\frac{1}{46}-\varepsilon}$$
$$\text{for } (A, x'_A) \in \mathcal{M} \setminus F.$$

Here, $\rho_s = m_s/|Q|$ depends on A, but we have

$$|\mathcal{S}_{\rho_s}(h) - \mathcal{S}_{\rho_0}(h)| \le C\widetilde{\delta}^{1/2}\rho_0 \quad \text{for } (A, x'_A) \in \mathcal{M} \setminus F, \text{ by (74 bis)}.$$

Therefore, $\int\limits_{x \in Q_0} |\mathcal{S}_{\rho_s}(h) - \mathcal{S}_{\rho_0}(h) \mid dx \le C\widetilde{\delta}^{1/2}\rho_0|Q| = C\widetilde{\delta}^{1/2}\underline{\mathrm{N}}$. The right-hand side is dominated by that of (84), so this inequality and (84) together show that

(85)
$$\int\limits_{x \in Q_0} |\mathcal{S}_s(x, x+h, \Psi_{A,x'_A}) - \mathcal{S}_{\rho_0}(h) \mid dx \le C'\underline{\mathrm{N}}(\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{\frac{1}{46}-\varepsilon}$$
$$\text{for } (A, x'_A) \in \mathcal{M} \setminus F.$$

For $(A, x'_A) \in F$, we use a trivial estimate in place of (85). Since Ψ_{A,x'_A} is an $|A|$-particle wave function, we have

$$\int\limits_{x \in Q_0} |\mathcal{S}_s(x, x+h, \Psi_{A,x'_A})| dx \le |A|.$$

Also,

$$\int\limits_{x \in Q_0} |\mathcal{S}_{\rho_0}(h)| dx \le \rho_0 |Q_0| \le \rho_0 |Q| = \underline{\mathrm{N}}.$$

Hence,

(86)
$$\int\limits_{x \in Q_0} |\mathcal{S}_s(x, x+h, \Psi_{A,x'_A}) - \mathcal{S}_{\rho_0}(h)| dx \le |A| + \underline{\mathrm{N}}$$
$$\text{for all } (A, x'_A).$$

We will use (85) for $(A, x'_A) \in \mathcal{M} \setminus F$ and (86) for $(A, x'_A) \in F$.

Lemma 3 relates $\mathcal{S}_s(x, x+h, \Psi)$ to the $\mathcal{S}_s(x, x+h, \Psi_{A,x'_A})$. It shows that

(87)
$$\int\limits_{x \in Q_0} |\mathcal{S}_s(x, x+h, \Psi) - \mathcal{S}_{\rho_0}(h)| dx =$$

$$\int_{x\in Q_0} \Big| \int_{\mathcal{M}} [\mathcal{S}_s(x,x+h,\Psi_{A,x'_A}) - \mathcal{S}_{\rho_0}(h)] d\mu(A,x'_A) \Big| dx \leq$$
$$\int_{x\in Q_0} \int_{\mathcal{M}} |\mathcal{S}_s(x,x+h,\Psi_{A,x'_A}) - \mathcal{S}_{\rho_0}(h)| d\mu(A,x'_A) dx =$$
$$\int_{\mathcal{M}\smallsetminus F} \left[\int_{x\in Q_0} |\mathcal{S}_s(x,x+h,\Psi_{A,x'_A}) - \mathcal{S}_{\rho_0}(h)| dx \right] d\mu(A,x'_A) +$$
$$\int_F \left[\int_{x\in Q_0} |\mathcal{S}_s(x,x+h,\Psi_{A,x'_A}) - \mathcal{S}_{\rho_0}(h)| dx \right] d\mu(A,x'_A) \leq$$
$$C'\underline{\mathrm{N}}(\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{\frac{1}{46}-\varepsilon} + \int_F (|A| + \underline{\mathrm{N}}) d\mu(A,x'_A)$$

(by (85) and (86))

$$\leq C'\underline{\mathrm{N}}(\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{\frac{1}{46}-\varepsilon} + (1+C)\underline{\mathrm{N}}\mu(F) + \int_F |A| \chi_{|A|\geq C\underline{\mathrm{N}}} d\mu(A,x'_A).$$

Note that $(1+C)\underline{\mathrm{N}}\mu(F) + \int_F |A| \chi_{|A|\geq C\underline{\mathrm{N}}} d\mu(A,x'_A)$

$$\leq (1+C)\underline{\mathrm{N}}\mu(F) + (\mu(F))^{2/5} \left(\int_F |A|^{5/3} \chi_{|A|\geq C\underline{\mathrm{N}}} d\mu(A,x'_A) \right)^{3/5}$$
$$\leq (1+C)\underline{\mathrm{N}} \cdot C\widetilde{\delta}^{-1}(\delta + \underline{\mathrm{N}}^{-2/15}) + C\widetilde{\delta}^{-2/5}(\delta + \underline{\mathrm{N}}^{-2/15})^{2/5} \cdot C''(\delta + \underline{\mathrm{N}}^{-2/15})^{3/5}\underline{\mathrm{N}}$$

(by (57) and (72)) $\leq C'\widetilde{\delta}^{-1}(\delta + \underline{\mathrm{N}}^{-\frac{2}{15}})\underline{\mathrm{N}}$.

Putting this into the right-hand side of (87), we find that

$$\int_{x\in Q_0} |\mathcal{S}_s(x,x+h,\Psi) - \mathcal{S}_{\rho_0}(h)| dx \leq C\underline{\mathrm{N}} \cdot \left[(\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{\frac{1}{46}-\varepsilon} + \widetilde{\delta}^{-1}(\delta + \underline{\mathrm{N}}^{-\frac{2}{15}}) \right]$$

for $\rho_0^{1/3}|h| < (\widetilde{\delta} + \underline{\mathrm{N}}^{-1/3})^{-2/46}$.

Take $\widetilde{\delta} = (\delta + \underline{\mathrm{N}}^{-2/15})^{\frac{46}{47}}$, and we obtain the following result.

Lemma 7: *Suppose* $\varepsilon > 0$, $\underline{N} > C'$, *and* $\rho_0^{1/3}|h| < (\delta + \underline{N}^{-2/15})^{-2/47}$. *Then*

$$\int_{x\in Q_0} |\mathcal{S}_s(x,x+h,\Psi) - \mathcal{S}_{\rho_0}(h)| dx \leq C''\underline{N} \cdot (\delta + \underline{N}^{-2/15})^{\frac{1}{47}-\varepsilon}.$$

The constants C', C'' *depend only on* q, ε.

The following result summarizes what we have done in this section.

Main Theorem on Free Particles: *Let ρ_0 be a positive number, and let Q be a cube in $\mathbb{R}^3$. Set $\underline{N} = \rho_0|Q|$, and $Q_0 =$ middle half of Q. Assume $\underline{N} > C$.*

Suppose we are given a map spin: $\{1 \dots N\} \to \{1 \dots q\}$ and a wave function $\Psi(x_1 \dots x_N) \in L^2(\mathbb{R}^{3N})$ with norm 1, satisfying $\Psi(x_{\sigma 1} \dots x_{\sigma N}) = (\operatorname{sgn} \sigma)\Psi(x_1 \dots x_N)$ for spin-preserving permutations σ. Define

$$\mathcal{E}(Q, \rho_0, \Psi) =$$
$$KE(Q, \Psi) - \frac{5}{3} c_{TF} \rho_0^{2/3} \langle \mathcal{N}_Q \Psi, \Psi \rangle + \frac{2}{3} q c_{TF} \rho_0^{5/3} |Q| \cdot (1 + C_1 \underline{N}^{-1/3})$$

with

$$KE(Q, \Psi) = \sum_{j=1}^{N} \int_{\mathbb{R}^{3N}} |\nabla_{x_j} \Psi(x_1 \dots x_N)|^2 \chi_Q(x_j) dx_1 \dots dx_N \quad \text{and}$$

$$\mathcal{N}_Q(x_1 \dots x_N) = \sum_{j=1}^{N} \chi_Q(x_j). \quad \left(\textit{Here, } c_{TF} = \frac{(6\pi^2)^{5/3}}{10\pi^2}.\right)$$

Then $\mathcal{E}(Q, \rho_0, \Psi) \geq 0$.

Moreover, suppose $\mathcal{E}(Q, \rho_0, \Psi) \leq \delta \rho_0^{5/3} |Q|$ with $0 < \delta < c$. Then Ψ has the following two properties:

(I) (Two-body interactions). *Suppose $K(x, y)$ is defined on $\mathbb{R}^3 \times \mathbb{R}^3$, with $0 \leq K(x, y) = K(y, x) \leq |x - y|^{-1}$ and $\operatorname{supp} K(x, y) \subset \{x, y \in Q_0, |x - y| < r_{\max}\}$. Assume*

$$\rho_0 r_{\max}^3 \geq 1, \ \delta < c(\rho_0 r_{\max}^3)^{-42/5}, \ \underline{N} > C(\rho_0 r_{\max}^3)^{63}.$$

Then

$$\left\langle \sum_{i<j} K(x_i, x_j) \Psi, \Psi \right\rangle \geq \frac{1}{2} \iint_{Q \times Q} K(x, y) \{q^2 \rho_0^2 - q |\mathcal{S}_{\rho_0}(x - y)|^2\} dx dy -$$
$$C(\delta + \underline{N}^{-\frac{2}{15}})^{\frac{1}{63}} (\rho_0 r_{\max}^3)^{2/3} \rho_0^{4/3} |Q|.$$

(II) (Correlation Functions). *Define*

$$\mathcal{S}_s(x, y, \Psi) =$$
$$\sum_{\operatorname{spin}(j)=s} \int_{\mathbb{R}^{3(N-1)}} \Psi(x_1 \dots x_{j-1} x x_{j+1} \dots x_N) \bar{\Psi}(x_1 \dots x_{j-1} y x_{j+1} \dots x_N)$$
$$dx_1 \dots dx_{j-1} dx_{j+1} \dots dx_N.$$

If $h \in \mathbb{R}^3$ and $\rho_0^{1/3}|h| \leq (\delta + \underline{N}^{-2/15})^{-\frac{2}{47}}$, then

$$\int_{x \in Q_0} |\mathcal{S}_s(x, x + h, \Psi) - \mathcal{S}_{\rho_0}(h)| dx \leq C(\delta + \underline{N}^{-2/15})^{\frac{1}{48}} \rho_0 |Q|,$$

where

$$\mathcal{S}_{\rho_0}(h) = \int\limits_{B(0,r_F)} e^{i\xi\cdot h} \frac{d\xi}{(2\pi)^3}, \quad \rho_0 = r_F^3/(6\pi^2).$$

The constants c, C, C_1 depend only on q.

Proof: $\mathcal{E} \geq 0$ by Lemma 1, (I) is immediate from Lemma 6, and (II) is immediate from Lemma 7. □

The precise exponents (eg. 1/63) appearing in this Theorem are of no importance for our purposes. Certainly they are not optimal.

Our main application of (II) is to give a lower bound for the integral

$$\int\limits_{x\in Q_0} \int\limits_{y\in\mathbb{R}^3} |\mathcal{S}_s(x,y,\Psi)|^2 \frac{dxdy}{|x-y|} \tag{87 bis}$$

To carry this out, note that $\mathcal{S}_{\rho_0}(h)$ is given by

$$\mathcal{S}_{\rho_0}(h) = \rho_0 \mathcal{S}_1(\rho_0^{1/3} h), \quad \text{with} \tag{88}$$

$$\mathcal{S}_1(x) = \int\limits_{\xi\in B(0,r_1)} e^{i\xi\cdot x} \frac{d\xi}{(2\pi)^3}, \quad r_1 = (6\pi^2)^{1/3}. \tag{89}$$

In particular, $\mathcal{S}_1(x) = c_1 \cdot \left[\frac{\cos(c_2|x|)}{(c_2|x|)^2} - \frac{\sin(c_2|x|)}{(c_2|x|)^3})\right]$, so

$$|\mathcal{S}_1(x)| \leq C(1+|x|)^{-2}, \quad \text{and} \tag{90}$$

$$\frac{1}{2}\int\limits_{\mathbb{R}^3} |\mathcal{S}_{\rho_0}(h)|^2 \frac{dh}{|h|} = c_D \rho_0^{4/3} \quad \text{with} \tag{91}$$

$$c_D = \frac{1}{2}\int\limits_{\mathbb{R}^3} |\mathcal{S}_1(x)|^2 \frac{dx}{|x|}. \quad \text{From (88), (90) we get} \tag{92}$$

$$|\mathcal{S}_{\rho_0}(h)| \leq C\rho_0(\rho_0^{1/3}|h|)^{-2} = C\rho_0^{1/3}|h|^{-2} \tag{93}$$

Now we can estimate the integral (87 bis).

Corollary to the Main Theorem on Free Particles: *Let ρ_0, Q, Ψ, δ, $\underline{N}$ be as in the Main Theorem on Free Particles. Define $\mathcal{S}_s(x,y,\Psi)$ as in (II). Then*

$$|Q_0|^{-1}\cdot\frac{1}{2}\int\limits_{x\in Q_0}\int\limits_{y\in\mathbb{R}^3}|\mathcal{S}_s(x,y,\Psi)|^2\frac{dxdy}{|x-y|}\geq c_D\rho_0^{4/3}-C(\delta+\underline{N}^{-2/15})^{\frac{1}{96}}\rho_0^{4/3},$$

with C depending only on q.

Proof: Set $\underline{d}=\rho_0^{-1/3}(\delta+\underline{N}^{-2/15})^{-\frac{1}{192}}$, and note that $\rho_0^{1/3}|h|\leq(\delta+\underline{N}^{-2/15})^{-\frac{2}{47}}$ for $h\in\mathbb{R}^3$, $|h|<\underline{d}$.

Therefore, part (II) of the Main Theorem above shows that

$$\int\limits_{x\in Q_0}|\mathcal{S}_s(x,x+h,\Psi)-\mathcal{S}_{\rho_0}(h)|dx\leq C(\delta+\underline{N}^{-2/15})^{\frac{1}{48}}\rho_0|Q| \tag{94}$$

for $|h|<\underline{d}$. On the other hand,

$$\begin{aligned}|\mathcal{S}_s(x,x+h,\Psi)|^2&=|\mathcal{S}_{\rho_0}(h)|^2+|\mathcal{S}_s(x,x+h,\Psi)-\mathcal{S}_{\rho_0}(h)|^2\\&\quad+2\mathrm{Re}(\overline{\mathcal{S}_{\rho_0}(h)}[\mathcal{S}_s(x,x+h,\Psi)-\mathcal{S}_{\rho_0}(h)])\\&\geq|\mathcal{S}_{\rho_0}(h)|^2-2|\mathcal{S}_{\rho_0}(h)|\cdot|\mathcal{S}_s(x,x+h,\Psi)-\mathcal{S}_{\rho_0}(h)|\geq\\&|\mathcal{S}_{\rho_0}(h)|^2-2\rho_0|\mathcal{S}_s(x,x+h,\Psi)-\mathcal{S}_{\rho_0}(h)|,\quad\text{so that}\end{aligned}$$

$$\begin{aligned}\frac{1}{2}\int\limits_{Q_0}|\mathcal{S}_s(x,x+h,\Psi)|^2dx&\geq\\\frac{1}{2}|\mathcal{S}_{\rho_0}(h)|^2|Q_0|&-\rho_0\int\limits_{x\in Q_0}|\mathcal{S}_s(x,x+h,\Psi)-\mathcal{S}_{\rho_0}(h)|dx.\end{aligned} \tag{95}$$

From (94) and (95) we conclude that

$$\begin{aligned}\frac{1}{2}|Q_0|^{-1}\int\limits_{x\in Q_0}&|\mathcal{S}_s(x,x+h,\Psi)|^2dx\geq\\&\frac{1}{2}|\mathcal{S}_{\rho_0}(h)|^2-C\rho_0^2(\delta+\underline{N}^{-2/15})^{1/48}\quad\text{for }|h|<\underline{d}.\end{aligned} \tag{96}$$

We multiply (96) by $|h|^{-1}$ and integrate over $h\in B(0,\underline{d})$. Thus,

$$\begin{aligned}\frac{1}{2}|Q_0|^{-1}\int\limits_{x\in Q_0}\int\limits_{h\in B(0,\underline{d})}&|\mathcal{S}_s(x,x+h,\Psi)|^2\frac{dxdh}{|h|}\geq\\&\frac{1}{2}\int\limits_{h\in B(0,\underline{d})}|\mathcal{S}_{\rho_0}(h)|^2\frac{dh}{|h|}-C\rho_0^2(\delta+\underline{N}^{-2/15})^{1/48}\underline{d}^2.\end{aligned} \tag{97}$$

From (91) and (93) follows

$$(98)\quad \frac{1}{2}\int_{h\in B(0,\underline{\mathrm{d}})} |\mathcal{S}_{\rho_0}(h)|^2\frac{dh}{|h|} = \frac{1}{2}\int_{\mathbb{R}^3} |\mathcal{S}_{\rho_0}(h)|^2\frac{dh}{|h|} - \frac{1}{2}\int_{|h|>\underline{\mathrm{d}}} |\mathcal{S}_{\rho_0}(h)|^2\frac{dh}{|h|}$$

$$= c_D\rho_0^{4/3} - \frac{1}{2}\int_{|h|>\underline{\mathrm{d}}} |\mathcal{S}_{\rho_0}(h)|^2\frac{dh}{|h|} \geq c_D\rho_0^{4/3} - C\int_{|h|>\underline{\mathrm{d}}} (\rho_0^{1/3}|h|^{-2})^2\frac{dh}{|h|}$$

$$= c_D\rho_0^{4/3} - C\rho_0^{2/3}\int_{|h|>\underline{\mathrm{d}}} \frac{dh}{|h|^5} = c_D\rho_0^{4/3} - C\rho_0^{2/3}\underline{\mathrm{d}}^{-2}.$$

Putting (98) into (97), we get

$$(99)\qquad |Q_0|^{-1}\cdot\frac{1}{2}\int_{x\in Q_0}\int_{h\in B(0,\underline{\mathrm{d}})} |\mathcal{S}_s(x,x+h,\Psi)|^2\frac{dxdh}{|h|} \geq$$

$$c_D\rho_0^{4/3} - C\rho_0^{2/3}\underline{\mathrm{d}}^{-2} - C\rho_0^2(\delta+\underline{\mathrm{N}}^{-2/15})^{\frac{1}{48}}\underline{\mathrm{d}}^2.$$

By definition of $\underline{\mathrm{d}}$, we have

$$C\rho_0^{2/3}\underline{\mathrm{d}}^{-2} = C\rho_0^{4/3}(\delta+\underline{\mathrm{N}}^{-2/15})^{\frac{1}{96}} \quad \text{and}$$
$$C\rho_0^2(\delta+\underline{\mathrm{N}}^{-2/15})^{\frac{1}{48}}\underline{\mathrm{d}}^2 = C\rho_0^{4/3}(\delta+\underline{\mathrm{N}}^{-2/15})^{\frac{1}{96}}.$$

So (99) is equivalent to

$$|Q_0|^{-1}\cdot\frac{1}{2}\int_{x\in Q_0}\int_{h\in B(0,\underline{\mathrm{d}})} |\mathcal{S}_s(x,x+h,\Psi)|^2\frac{dxdh}{|h|} \geq$$

$$c_D\rho_0^{4/3} - C(\delta+\underline{\mathrm{N}}^{-2/15})^{1/96}\rho_0^{4/3},$$

from which the present Corollary follows at once. □

Applications to Atoms

The goal of this section is to use the Main Theorem on Free Particles to derive information about atoms. Recall that the hypotheses of that theorem involve an "excess energy" $\mathcal{E}(Q, \rho_0, \Psi)$. We take Ψ to be a wave function for the electrons in an atom, having energy close to the ground-state energy. For ρ_0 we take the Thomas-Fermi density $\rho_{TF}(x)$, which is known to provide a good approximation to the density of particles of a given spin. Our cube Q will be a translate $\widehat{Q} + x$ of a fixed cube $\widehat{Q}$ centered at 0. We suppose $Z^{-2/3} \ll \operatorname{diam} \widehat{Q} \ll Z^{-1/3}$, so that $\widehat{Q} + x$ will be small compared to the whole atom, but large compared to the distance between nearest neighbor electrons. The main point is to note that $\mathcal{E}(\widehat{Q} + x, \rho_{TF}(x), \Psi) \ll \rho_{TF}^{5/3}(x)|\widehat{Q}|$ for all x outside a set $F \subset \mathbb{R}^3$, with $\int_F \rho_{TF}^{5/3}(x)dx \ll Z^{7/3}$. This estimate is essentially contained in Lieb-Simon [LS], but we provide details for the convenience of the reader. Applying the Main Theorem on Free Particles and its Corollary to $\widehat{Q} + x$ for $x \in \mathbb{R}^3 \smallsetminus F$, we will show that

$$(1) \qquad \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} |\mathcal{S}_s(x, y, \Psi)|^2 \frac{dxdy}{|x-y|} \geq c_D \int_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx - o(Z^{5/3})$$

and that

$$(2) \qquad \left\langle \sum_{i<j} K(x_i, x_j)\Psi, \Psi \right\rangle \geq \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} K(x, y)\{q^2 \rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy - o(Z^{5/3}).$$

Here, $\mathcal{S}_s(x, y, \Psi)$ is the correlation function, and $K(x, y)$ is a short-range interaction with $0 \leq K(x, y) = K(y, x) \leq |x - y|^{-1}$.

The purpose of this section is to prove (1) and (2). Later on, we will use (1) and (2) to compare the ground-state energy with its Hartree-Fock approximation.

We begin with the Thomas-Fermi density $\rho_{TF}(x)$ and the Thomas-Fermi potential $V_{TF}(x)$ on $\mathbb{R}^3$. In our notation, ρ_{TF} is the $T - F$ density for particles of a fixed spin; while V_{TF} arises from the Coulomb forces of the nucleus and of all the electrons, of all spins. Thus, ρ_{TF} and V_{TF} satisfy

$$(3) \qquad V_{TF}(x) = -\frac{Z}{|x|} + q \int_{\mathbb{R}^3} \frac{\rho_{TF}(y)dy}{|x-y|} \quad \text{and}$$

$$(4) \qquad \rho_{TF}(x) = \frac{1}{6\pi^2}|V_{TF}(x)|^{3/2}.$$

With $\mathcal{S}(x) = \min(Z|x|^{-1}, |x|^{-4})$, we have

$$(5) \qquad c\mathcal{S}(x) < -V_{TF}(x) < C\mathcal{S}(x) \quad \text{and}$$

$$(6) \qquad |\nabla V_{TF}(x)| \leq C\mathcal{S}(x)|x|^{-1} \quad \text{(See [L2])}$$

In this chapter c, C, etc. denote constants depending only on q. We assume that Z exceeds a large constant.

In terms of ρ_{TF}, the Thomas-Fermi approximation to the ground-state energy of the atom is

$$E_{TF}(Z,q) = qc_{TF}\int_{\mathbb{R}^3}\rho_{TF}^{5/3}dx - q\int_{\mathbb{R}^3}\frac{Z}{|x|}\rho_{TF}(x)dx + \frac{q^2}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|}. \tag{7}$$

We will be proving (1) and (2) for wave functions Ψ whose energy is bounded above by $E_{TF}(Z,q)+o(Z^{7/3})$. Our first result concerns $\mathrm{sneg}(-\Delta+V)$ = sum of the negative eigenvalues of $-\Delta+V$ for potentials V that behave like V_{TF}.

Lemma 1: *If* $c\mathcal{S}(x)\le -V(x)\le C\mathcal{S}(x)$ *and* $|\nabla V(x)|\le C\mathcal{S}(x)|x|^{-1}$, *then*

$$\mathit{sneg}(-\Delta+V) = -\frac{1}{15\pi^2}\int_{\mathbb{R}^3}|V(x)|^{5/2}dx + O(Z^{13/6}).$$

Sketch of Proof: If Q is a cube in $\mathbb{R}^3$ and W is a negative number, then define

$\mathrm{sneg}_D(Q,W)$ = sum of the negative eigenvalues of $-\Delta+W$ on Q, with Dirichlet boundary conditions; and

$\mathrm{sneg}_N(Q,W)$ = sum of the negative eigenvalues of $-\Delta+W$ on Q, with Neumann boundary conditions.

These quantities are readily expressed as sums over the lattice points in a ball, since the Dirichlet and Neumann Laplacians on Q are explicitly diagonalized. The lemmas on lattice points in the section on Free Particles in a Box imply the following estimates.

If $|W|(\mathrm{diam}\,Q)^2 > C$, then

$$\mathrm{sneg}_D(Q,W), \mathrm{sneg}_N(Q,W) = -\frac{1}{15\pi^2}|W|^{5/2}|Q| + O(|W|^2(\mathrm{diam}\,Q)^2). \tag{8}$$

If instead $|W|(\mathrm{diam}\,Q)^2\le C$, then trivially

$$-C'(\mathrm{diam}\,Q)^{-2}\le \mathrm{sneg}_N(Q,W)\le \mathrm{sneg}_D(Q,W)\le 0. \tag{9}$$

We need also a variant of (9) for potentials with a Coulomb singularity. Suppose $-\frac{CZ}{|x|}\le W(x)\le 0$, and let $\bar{Q}$ be a cube centered at the origin, with $cZ^{-1}<\mathrm{diam}\,\bar{Q}<CZ^{-1}$. Let

$\mathrm{sneg}_D(\bar{Q},W(x))$ = sum of the negative eigenvalues of $-\Delta+W(x)$ on $\bar{Q}$, with Dirichlet boundary conditions; and

$\mathrm{sneg}_N(\bar{Q},W(x))$ = sum of the negative eigenvalues of $-\Delta+W(x)$ on $\bar{Q}$, with Neumann boundary conditions.

Then

$$-C'Z^2 \le \text{sneg}_N(\bar{Q}, W(x)) \le \text{sneg}_D(\bar{Q}, W(x)) \le 0. \tag{10}$$

In fact, a simple scaling reduces (10) to the trivial case $Z = 1$.

Now subdivide $\mathbb{R}^3$ into pairwise disjoint cubes $\bar{Q}$, Q_ν, Q'_ν with the following geometrical properties:

(11)

$\bar{Q}$ is contained at the origin and has diameter $\bar{C}_1 Z^{-1}$ for a large const. $\bar{C}_1$.

(12)

Q_ν is contained in $\{CZ^{-1} < |x| < c\}$, and

$(\text{diam}\, Q_\nu) \sim \mathcal{S}^{-1/4}(x_\nu) \cdot |x_\nu|^{1/2}$, where x_ν is the center of Q_ν.

In particular, $(\text{diam}\, Q_\nu) < \frac{1}{2}|x_\nu|$.

(13)

Q'_ν is contained in $\{|x| > c'\}$, and $(\text{diam}\, Q'_\nu) \sim |x'_\nu|$,

where x'_ν is the center of Q'_ν.

The construction of the cubes $\bar{Q}$, Q_ν, Q'_ν may be left to the reader.

The minimax principle shows that

$$\text{sneg}(-\Delta + V) \ge \text{sneg}_N(\bar{Q}, V(x)) + \sum_\nu \text{sneg}_N(Q_\nu, \min_{Q_\nu} V) + \sum_\nu \text{sneg}_N(Q'_\nu, \min_{Q'_\nu} V)$$

and

$$\text{sneg}(-\Delta + V) \le \text{sneg}_D(\bar{Q}, V(x)) + \sum_\nu \text{sneg}_D(Q_\nu, \max_{Q_\nu} V) + \sum_\nu \text{sneg}_D(Q'_\nu, \max_{Q'_\nu} V).$$

We apply (8) to the Q_ν, (9) to the Q'_ν, and (10) to $\bar{Q}$. Thus,

(14)

$$\begin{aligned}\text{sneg}(-\Delta + V) \ge -C'Z^2 - \frac{1}{15\pi^2} \sum_\nu |\min_{Q_\nu} V|^{5/2} |Q_\nu| - C \sum_\nu |\min_{Q_\nu} V|^2 (\text{diam}\, Q_\nu)^2 \\ - C \sum_\nu (\text{diam}\, Q'_\nu)^{-2}, \quad \text{and}\end{aligned}$$

$$\text{sneg}(-\Delta + V) \le -\frac{1}{15\pi^2} \sum_\nu |\max_{Q_\nu} V|^{5/2} |Q_\nu| + C \sum_\nu |\max_{Q_\nu} V|^2 (\text{diam}\, Q_\nu)^2. \tag{15}$$

We have $\sum_\nu (\operatorname{diam} Q'_\nu)^{-2} < C$, and $|\min_{Q_\nu} V| \sim |\max_{Q_\nu} V| \sim \mathcal{S}(x_\nu)$, $(\operatorname{diam} Q_\nu)^2 \sim \mathcal{S}^{+1/4}(x_\nu)|x_\nu|^{-1/2}|Q_\nu|$, so that

$$|\min_{Q_\nu} V|^2 (\operatorname{diam} Q_\nu)^2 \sim |\max_{Q_\nu} V|^2 (\operatorname{diam} Q_\nu)^2 \sim \mathcal{S}^{9/4}(x_\nu)|x_\nu|^{-1/2}|Q_\nu| \sim \int_{x\in Q_\nu} \mathcal{S}^{9/4}(x)|x|^{-1/2}dx.$$

Hence, with $\Omega = \cup_\nu Q_\nu$, we get

$$\operatorname{sneg}(-\Delta + V) \geq -C''Z^2 - C\int_\Omega \mathcal{S}^{9/4}(x)|x|^{-1/2}dx - \frac{1}{15\pi^2}\sum_\nu |\min_{Q_\nu} V|^{5/2}|Q_\nu| \quad \text{and} \tag{16}$$

$$\operatorname{sneg}(-\Delta + V) \leq +C\int_\Omega \mathcal{S}^{9/4}(x)|x|^{-1/2}dx - \frac{1}{15\pi^2}\sum_\nu |\max_{Q_\nu} V|^{5/2}|Q_\nu|, \tag{17}$$

as consequences of (14) and (15). With $V_\nu = \min_{Q_\nu} V$ or $\max_{Q_\nu} V$, we have $|V(x)| \leq C|V_\nu|$ in Q_ν, and therefore

$$\Big||V(x)|^{5/2} - |V_\nu|^{5/2}\Big| \leq C|V_\nu|^{3/2}|V(x) - V_\nu| \leq C|V_\nu|^{3/2}\cdot(\operatorname{diam} Q_\nu)\cdot \max_{Q_\nu}|\nabla V| \leq C\mathcal{S}^{3/2}(x_\nu)\cdot[\mathcal{S}^{-1/4}(x_\nu)|x_\nu|^{1/2}]\cdot[\mathcal{S}(x_\nu)|x_\nu|^{-1}] = C\mathcal{S}^{9/4}(x_\nu)|x_\nu|^{-1/2}.$$

Hence,

$$\left||V_\nu|^{5/2}|Q_\nu| - \int_{Q_\nu}|V(x)|^{5/2}dx\right| \leq C\mathcal{S}^{9/4}(x_\nu)|x_\nu|^{-1/2}|Q_\nu| \leq C'\int_{x\in Q_\nu}\mathcal{S}^{9/4}(x)|x|^{-1/2}dx.$$

Putting this into (16) and (17), and again using $\Omega = \cup_\nu Q_\nu$, we see that

$$|\operatorname{sneg}(-\Delta + V) + \frac{1}{15\pi^2}\int_\Omega |V(x)|^{5/2}dx| \leq CZ^2 + C\int_\Omega \mathcal{S}^{9/4}(x)|x|^{-1/2}dx,$$

which implies

$$|\operatorname{sneg}(-\Delta + V) + \frac{1}{15\pi^2}\int_{\mathbb{R}^3}|V(x)|^{5/2}dx| \leq CZ^2 + C\int_\Omega \mathcal{S}^{9/4}(x)|x|^{-1/2}dx + C\int_{\mathbb{R}^3\setminus\Omega}|V(x)|^{5/2}dx. \tag{18}$$

By definition of $\mathcal{S}(x)$, we have

$$\int_{\Omega} \mathcal{S}^{9/4}(x)|x|^{-1/2}dx \leq \int_{\mathbb{R}^3} \mathcal{S}^{9/4}(x)|x|^{-1/2}dx = \tag{19}$$

$$= \int_{|x|<Z^{-1/3}} \left(\frac{Z}{|x|}\right)^{9/4} |x|^{-1/2}dx + \int_{|x|>Z^{-1/3}} (|x|^{-4})^{9/4}|x|^{-1/2}dx$$

$$= Z^{9/4} \int_{|x|<Z^{-1/3}} |x|^{-11/4}dx + \int_{|x|>Z^{-1/3}} |x|^{-19/2}dx$$

$$\leq CZ^{9/4} \cdot Z^{-1/12} + C(Z^{-1/3})^{-13/2} = C'Z^{13/6}.$$

Also, since $\mathbb{R}^3 \setminus \Omega \subset \{|x| < C'Z^{-1}\} \cup \{|x| > c\}$, we have

$$\int_{\mathbb{R}^3 \setminus \Omega} |V(x)|^{5/2}dx \leq C \int_{|x|<c'Z^{-1}} \mathcal{S}^{5/2}(x)dx + C \int_{|x|>c} \mathcal{S}^{5/2}(x)dx \tag{20}$$

$$= C \int_{|x|<C'Z^{-1}} \left(\frac{Z}{|x|}\right)^{5/2} dx + C \int_{|x|>c} (|x|^{-4})^{5/2}dx$$

$$= C''Z^{5/2}(C'Z^{-1})^{1/2} + C'' \leq C'''Z^2.$$

Putting (19) and (20) into (18), we obtain the conclusion of Lemma 1. □

Next, let spin: $\{1 \dots N\} \to \{1 \dots q\}$ and $\Psi(x_1 \dots x_N) \in L^2(\mathbb{R}^{3N})$ be given, with $\|\Psi\| = 1$, and with $\Psi(x_{\sigma 1} \dots x_{\sigma N}) = (\operatorname{sgn} \sigma)\Psi(x_1 \dots x_N)$ for spin-preserving permutations σ. Trivially, we have

$$\left\langle \sum_{k=1}^{N} (-\Delta_{x_k} + V(x_k))\Psi, \Psi \right\rangle \geq q \operatorname{sneg}(-\Delta + V), \tag{21}$$

and if $V(x)$ is as in the preceding Lemma, then by that Lemma, the right-hand side of (21) has the order of magnitude $Z^{7/3}$.

Lemma 2: *Let V be as in Lemma 1, and suppose Ψ satisfies*

$$\left\langle \sum_{k=1}^{N} (-\Delta_{x_k} + V(x_k))\Psi, \Psi \right\rangle \leq q \, sneg(-\Delta + V) + \eta Z^{7/3}, \tag{22}$$

with $0 < \eta < 1$.

Then

$$\left\langle \sum_{k=1}^{N} (-\Delta_{x_k})\Psi, \Psi \right\rangle = \frac{q}{10\pi^2} \int_{\mathbb{R}^3} |V(x)|^{5/2}dx + O(\eta^{1/2} + Z^{-1/12})Z^{7/3}. \tag{23}$$

Moreover, if $|W(x)| \le C\mathcal{S}(x)$ *and* $|\nabla W(x)| \le C\mathcal{S}(x)|x|^{-1}$, *then*

$$\left\langle \sum_{k=1}^{N} W(x_k)\Psi, \Psi \right\rangle = \frac{q}{6\pi^2}\int_{\mathbb{R}^3} W(x)|V(x)|^{3/2}dx + O(\eta^{1/2} + Z^{-1/12})Z^{7/3}. \tag{24}$$

Proof: We begin with (24). For $|\tau| \ll 1$, the potential $V_\tau = V + \tau W$ satisfies the hypotheses of Lemma 1. Hence,

$$\operatorname{sneg}(-\Delta + V_\tau) = O(Z^{13/6}) - \frac{1}{15\pi^2}\int_{\mathbb{R}^3}(-V_\tau(x))^{5/2}dx. \tag{25}$$

Since $-V(x) \sim \mathcal{S}(x)$ and $|W(x)| < C\mathcal{S}(x)$, we have

$$(-V_\tau(x))^{5/2} = (-V(x))^{5/2}\left(1 + \tau\frac{W(x)}{V(x)}\right)^{5/2} = (-V(x))^{5/2}\left(1 + \frac{5}{2}\tau\frac{W(x)}{V(x)} + O(\tau^2)\right),$$

so that

$$\int_{\mathbb{R}^3}(-V_\tau(x))^{5/2}dx = \int_{\mathbb{R}^3}(-V(x))^{5/2}dx - \frac{5}{2}\tau\int_{\mathbb{R}^3} W(x)(-V(x))^{3/2}dx + O(\tau^2 Z^{7/3}),$$

and (25) becomes

$$\begin{aligned}\operatorname{sneg}(-\Delta + V_\tau) = -\frac{1}{15\pi^2}\int_{\mathbb{R}^3}|V(x)|^{5/2}dx + \frac{1}{6\pi^2}\tau\int_{\mathbb{R}^3} W(x)|V(x)|^{3/2}dx \\ + O(\tau^2 + Z^{-1/6})Z^{7/3}.\end{aligned} \tag{26}$$

On the other hand, (21) applied to V_τ shows that

$$\begin{aligned} q\operatorname{sneg}(-\Delta + V_\tau) &\le \left\langle \sum_{k=1}^{N}(-\Delta_{x_k} + V_\tau(x_k))\Psi, \Psi \right\rangle \\ &= \left\langle \sum_{k=1}^{N}(-\Delta_{x_k} + V(x_k))\Psi, \Psi \right\rangle + \left\langle \sum_{k=1}^{N}\tau W(x_k)\Psi, \Psi \right\rangle \\ &\le q\operatorname{sneg}(-\Delta + V) + \eta Z^{7/3} + \tau\left\langle \sum_{k=1}^{N} W(x_k)\Psi, \Psi \right\rangle \text{ (by (22))} \\ &\le -\frac{q}{15\pi^2}\int_{\mathbb{R}^3}|V(x)|^{5/2}dx + O(Z^{-1/6} + \eta)Z^{7/3} + \tau\left\langle \sum_{k=1}^{N} W(x_k)\Psi, \Psi \right\rangle, \end{aligned} \tag{27}$$

by Lemma 1. Substituting (26) into the left-hand side of (27), we find that

$$\frac{\tau q}{6\pi^2}\int_{\mathbb{R}^3} W(x)|V(x)|^{3/2}dx \leq \tau\left\langle\sum_{k=1}^{N} W(x_k)\Psi, \Psi\right\rangle + C(\tau^2+\eta+Z^{-1/6})Z^{7/3}. \tag{28}$$

Taking $\tau = \pm(\eta + Z^{-1/6})^{1/2}$ in (28), we obtain conclusion (24).

To prove (23), we take $W = V$ in (24), to get

$$\left\langle\sum_{k=1}^{N} V(x_k)\Psi, \Psi\right\rangle = -\frac{q}{6\pi^2}\int_{\mathbb{R}^3} |V(x)|^{5/2}dx + O(\eta^{1/2}+Z^{-1/12})Z^{7/3}.$$

Also from (21), (22) and Lemma 1, we get

$$\left\langle\sum_{k=1}^{N}(-\Delta_{x_k}+V(x_k))\Psi, \Psi\right\rangle = -\frac{q}{15\pi^2}\int_{\mathbb{R}^3} |V(x)|^{5/2}dx + O(\eta+Z^{-1/6})Z^{7/3}.$$

Subtracting the last two equations, we obtain conclusion (23). □

Next, we make a rigorous comparison of the two Hamiltonians

$$H = \sum_{k=1}^{N}\left(-\Delta_{x_k} - \frac{Z}{|x_k|}\right) + \sum_{i<j}|x_i - x_j|^{-1} \quad \text{and}$$

$$H_{hf} = \sum_{k=1}^{N}(-\Delta_{x_k} + V_{TF}(x_k)).$$

Lemma 3: *Let $\varphi(x)$ be a non-negative radial, C_0^∞ function on $\mathbb{R}^3$, supported in $B(0, Z^{-2/3})$, dominated by CZ^2, and having integral 1 on $\mathbb{R}^3$. Set*

$$\widetilde{V}_{TF}(x) = -\frac{Z}{|x|} + q\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi(x-x')\rho_{TF}(y)dx'dy}{|x'-y|}.$$

Then for arbitrary points $x_1 \dots x_N \in \mathbb{R}^3$, we have

$$\sum_{k=1}^{N} -\frac{Z}{|x_k|} + \sum_{i<j}|x_i - x_j|^{-1} \geq \sum_{k=1}^{N}\widetilde{V}_{TF}(x_k) - \frac{q^2}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|} - CZ^{2/3}N.$$

Proof: We use the fact that

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{f(x)\overline{f(y)}}{|x-y|}dxdy = (\text{const})\int_{\mathbb{R}^3} |\hat{f}(\xi)|^2|\xi|^{-2}d\xi \geq 0 \tag{29}$$

for any f on $\mathbb{R}^3$.

Given $x_1 \dots x_N \in \mathbb{R}^3$, we set $\rho(x) = \sum_{k=1}^{N} \varphi(x - x_k)$. The mean-value properties of $\frac{1}{|x|}$ show that

$$\frac{1}{2}\sum_{i\neq j} |x_i - x_j|^{-1} \geq \frac{1}{2}\sum_{i\neq j} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi(x_i - x')\varphi(x_j - y')}{|x' - y'|} dx'dy'$$

$$= \frac{1}{2}\sum_{i,j} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi(x' - x_i)\varphi(y' - x_j)}{|x' - y'|} dx'dy' - \frac{1}{2}\sum_{i} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi(x' - x_i)\varphi(y' - x_i)}{|x' - y'|} dx'dy'$$

$$= \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho(x')\rho(y')}{|x' - y'|} dx'dy' - \frac{1}{2}\sum_{i=1}^{N} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi(x' - x_i)\varphi(y' - y_i)}{|x' - y'|} dx'dy'$$

$$\geq \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho(x')\rho(y')}{|x' - y'|} dx'dy' - CZ^{2/3}N$$

$$= \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{[\rho(x') - q\rho_{TF}(x')][\rho(y') - q\rho_{TF}(y')]}{|x' - y'|} dx'dy'$$

$$+ \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho(x')\cdot q\rho_{TF}(y')}{|x' - y'|} dx'dy' - \frac{q^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x')\rho_{TF}(y')}{|x' - y'|} dx'dy'$$

$$- CZ^{2/3}N.$$

The first term on the right is non-negative by (29), so we get

$$\sum_{i<j} |x_i - x_j|^{-1} \geq \iint_{\mathbb{R}^3\times\mathbb{R}^3} \rho(x')\cdot q\rho_{TF}(y') \frac{dx'dy'}{|x' - y'|} - \frac{q^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \rho_{TF}(x')\rho_{TF}(y') \frac{dx'dy'}{|x' - y'|}$$

$$- CZ^{2/3}N$$

$$= \sum_{k=1}^{N} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \varphi(x_k - x')\cdot q\rho_{TF}(y') \frac{dx'dy'}{|x' - y'|}$$

$$- \frac{q^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \rho_{TF}(x')\rho_{TF}(y') \frac{dx'dy'}{|x' - y'|} - CZ^{2/3}N.$$

Adding $\sum_{k=1}^{N} \left(-\frac{Z}{|x_k|}\right)$ to both sides and recalling the definition of $\widetilde{V}_{TF}$, we obtain the conclusion of Lemma 3. □

Lemma 4: *With $\widetilde{V}_{TF}$ as in the previous lemma, we have $\widetilde{V}_{TF}(x) \geq (1 + CZ^{-1/2})V_{TF}(x)$.*

Proof: By (3) and the definition of $\widetilde{V}_{TF}$, we have

$$\widetilde{V}_{TF}(x) - V_{TF}(x) = q \int_{\mathbb{R}^3} \rho_{TF}(y) \left[\int_{\mathbb{R}^3} \frac{\varphi(x - x')}{|x' - y|} dx' - \frac{1}{|x - y|}\right] dy.$$

The quantity in brackets is equal to zero when $|x-y| > Z^{-2/3}$, and is dominated by $\frac{1}{|x-y|}$ in absolute value when $|x-y| \leq Z^{-2/3}$. (That follows at once from the defining properties of φ and the mean-value property of $\frac{1}{|x|}$.) Hence,

$$(30) \qquad |\widetilde{V}_{TF}(x) - V_{TF}(x)| \leq C \int\limits_{|y-x|<Z^{-2/3}} \frac{\rho_{TF}(y)}{|x-y|} dy.$$

We estimate the right-hand side of (30). Note that $\rho_{TF}(y) \sim \mathcal{S}^{3/2}(y)$, by (4) and (5). If $|x| > 2Z^{-2/3}$, then $|y| \sim |x|$ for $|x-y| < Z^{-2/3}$, and therefore

$$\int\limits_{|y-x|<Z^{-2/3}} \frac{\rho_{TF}(y)dy}{|x-y|} \sim \mathcal{S}^{3/2}(x) \int\limits_{|y-x|<Z^{-2/3}} \frac{dy}{|x-y|} \sim Z^{-4/3}\mathcal{S}^{3/2}(x).$$

That is,

(31)
$$2Z^{-2/3} < |x| \leq Z^{-1/3} \text{ implies } \int\limits_{|y-x|<Z^{-2/3}} \frac{\rho_{TF}(y)dy}{|x-y|} \leq CZ^{-4/3} \cdot Z^{3/2}|x|^{-3/2} = CZ^{1/6}|x|^{-3/2}, \text{ and}$$

$$(32) \qquad Z^{-1/3} \leq |x| \text{ implies } \int\limits_{|y-x|<Z^{-2/3}} \frac{\rho_{TF}(y)dy}{|x-y|} \leq CZ^{-4/3}|x|^{-6}.$$

On the other hand, suppose $|x| \leq 2Z^{-2/3}$. Then

(33)
$$\int\limits_{|y-x|<Z^{-2/3}} \frac{\rho_{TF}(y)dy}{|x-y|} \leq \int\limits_{|y|<3Z^{-2/3}} \frac{\rho_{TF}(y)dy}{|x-y|}$$
$$\leq \int\limits_{|y-x|<\frac{1}{2}|x|} \frac{\rho_{TF}(y)dy}{|x-y|} + \int\limits_{\substack{|y-x|>\frac{1}{2}|x| \\ |y|<3Z^{-2/3}}} \frac{\rho_{TF}(y)dy}{|x-y|} \equiv \text{I} + \text{II}$$

We have $\rho_{TF}(y) \sim \mathcal{S}^{3/2}(y) \sim \mathcal{S}^{3/2}(x) = Z^{3/2}|x|^{-3/2}$ in the support of the integrand in I; while in the support of the integrand in II, we have $|x-y| \geq c|y|$. Therefore, for

$|x| \le 2Z^{-2/3}$, we get

$$\int\limits_{|y-x|<Z^{-2/3}} \frac{\rho_{TF}(y)dy}{|x-y|} \le CZ^{3/2}|x|^{-3/2} \int\limits_{|y-x|<\frac{1}{2}|x|} \frac{dy}{|x-y|} + C \int\limits_{|y|<3Z^{-2/3}} \frac{\rho_{TF}(y)dy}{|y|}$$

$$\le CZ^{3/2}|x|^{-3/2} \cdot |x|^2 + C \int\limits_{|y|<3Z^{-2/3}} \frac{\mathcal{S}^{3/2}(y)dy}{|y|}$$

$$= CZ^{3/2}|x|^{1/2} + CZ^{3/2} \int\limits_{|y|<3Z^{-2/3}} \frac{dy}{|y|^{5/2}}$$

$$\le CZ^{3/2}|x|^{1/2} + C'Z^{3/2}(3Z^{-2/3})^{1/2} = CZ^{3/2}|x|^{1/2} + C''Z^{7/6} \le C'''Z^{7/6}.$$

That is,

$$\int\limits_{|y-x|<Z^{-2/3}} \frac{\rho_{TF}(y)dy}{|x-y|} \le CZ^{7/6} \quad \text{for} \quad |x| < 2Z^{-2/3} \tag{34}$$

From (30), (31), (32), (34), we get:

$$|\widetilde{V}_{TF}(x) - V_{TF}(x)| \le \begin{cases} CZ^{7/6} & \text{for} \quad |x| \le 2Z^{-2/3} \\ CZ^{1/6}|x|^{-3/2} & \text{for} \quad 2Z^{-2/3} < |x| \le Z^{-1/3} \\ CZ^{-4/3}|x|^{-6} & \text{for} \quad Z^{-1/3} \le |x|. \end{cases}$$

On the other hand, $|V_{TF}(x)| \sim \mathcal{S}(x) = \begin{cases} Z|x|^{-1} \text{ for } |x| \le Z^{-1/3} \\ |x|^{-4} \text{ for } |x| \ge Z^{-1/3} \end{cases}$ Hence, for $|x| \le 2Z^{-2/3}$ we have

$$|\widetilde{V}_{TF}(x) - V_{TF}(x)|/|V_{TF}(x)| \le \frac{CZ^{7/6}}{cZ|x|^{-1}} = C'Z^{1/6}|x| \le C''Z^{-1/2}.$$

For $2Z^{-2/3} \le |x| \le Z^{-1/3}$ we have

$$|\widetilde{V}_{TF}(x) - V_{TF}(x)|/|V_{TF}(x)| \le \frac{CZ^{1/6}|x|^{-3/2}}{cZ|x|^{-1}} = C'Z^{-\frac{5}{6}}|x|^{-1/2}$$
$$\le C'Z^{-5/6}(2Z^{-2/3})^{-1/2} = C''Z^{-1/2}.$$

For $Z^{-1/3} \le |x|$ we have

$$|\widetilde{V}_{TF}(x) - V_{TF}(x)|/|V_{TF}(x)| \le \frac{CZ^{-4/3}|x|^{-6}}{c|x|^{-4}} = C'Z^{-4/3}|x|^{-2}$$
$$\le C'Z^{-\frac{2}{3}}.$$

So in all cases,

$$|\widetilde{V}_{TF}(x) - V_{TF}(x)| \leq CZ^{-1/2}|V_{TF}(x)|.$$

Since $V_{TF}(x) < 0$, the conclusion of Lemma 4 follows at once. □

Recall that H is the Hamiltonian for N quantized electrons and a fixed nucleus of charge Z.

From Lemmas 3 and 4 we get $H \geq \sum_{k=1}^{N}(-\Delta_{x_k} + [1 + CZ^{-1/2}]V_{TF}(x)) - \text{const}$, and from Lemma 2 we know the kinetic energy and particle density for a wave function with

$$\left\langle \sum_{k=1}^{N}(-\Delta_{x_k} + [1 + CZ^{-1/2}]V_{TF}(x_k))\Psi, \Psi \right\rangle$$

close to its least possible value. Combining these results, we will prove the following, which controls wave functions for an atom near the ground-state energy.

Lemma 5: *Suppose $N \leq CZ$ and $\langle H\Psi, \Psi\rangle \leq E_{TF}(Z,q) + \eta Z^{7/3}$ with $0 \leq \eta \leq 1$. Then*

$$\left\langle \sum_{k=1}^{N}(-\Delta_{x_k})\Psi, \Psi \right\rangle = qc_{TF} \int_{\mathbb{R}^3} \rho_{TF}^{5/3} dx + O(\eta^{1/2} + Z^{-1/12})Z^{7/3}. \tag{35}$$

Moreover, if $|W(x)| \leq C\mathcal{S}(x)$ and $|\nabla W(x)| \leq C\mathcal{S}(x)|x|^{-1}$, then

$$\left\langle \sum_{k=1}^{N} W(x_k)\Psi, \Psi \right\rangle = q \int_{\mathbb{R}^3} W\rho_{TF} dx + O(\eta^{1/2} + Z^{-1/12})Z^{7/3}. \tag{36}$$

Proof: Hypothesis and Lemmas 3, 4 yield

$$\begin{aligned}
(37)\quad & E_{TF}(Z,q) + \eta Z^{7/3} \geq \langle H\Psi, \Psi\rangle \geq \\
& \left\langle \sum_{k=1}^{N}(-\Delta_{x_k} + [1 + CZ^{-1/2}]V_{TF}(x_k))\Psi, \Psi \right\rangle - \frac{q^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \rho_{TF}(x)\rho_{TF}(y)\frac{dxdy}{|x-y|} - CZ^{5/3} = \\
& \left[\left\langle \sum_{k=1}^{N}(-\Delta_{x_k} + [1 + CZ^{-1/2}]V_{TF}(x_k))\Psi, \Psi \right\rangle - q\,\mathrm{sneg}(-\Delta_x + [1 + CZ^{-1/2}]V_{TF}(x))\right] \\
& \qquad + q\,\mathrm{sneg}(-\Delta + [1 + CZ^{-1/2}]V_{TF}) - \frac{q^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|} - CZ^{5/3} \\
& \geq \left[\left\langle \sum_{k=1}^{N}(-\Delta_{x_k} + [1 + CZ^{-1/2}]V_{TF}(x_k))\Psi, \Psi \right\rangle - q\,\mathrm{sneg}(-\Delta + [1 + CZ^{-1/2}]V_{TF})\right]
\end{aligned}$$

$$- \frac{q}{15\pi^2} \int_{\mathbb{R}^3} |[1 + CZ^{-1/2}]V_{TF}(x)|^{5/2} dx - CZ^{13/6}$$

$$- \frac{q^2}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y) dx dy}{|x-y|} - CZ^{5/3}$$

(by Lemma 1)

$$\geq \left[\left\langle \sum_{k=1}^{N} (-\Delta_{x_k} + [1 + CZ^{-1/2}]V_{TF}(x_k))\Psi, \Psi \right\rangle - q \operatorname{sneg}(-\Delta + [1 + CZ^{-1/2}]V_{TF}) \right]$$

$$+ \left\{ -\frac{q}{15\pi^2} \int_{\mathbb{R}^3} |V_{TF}|^{5/2} dx - \frac{q^2}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y) dx dy}{|x-y|} \right\} - CZ^{13/6}.$$

The expression in curly brackets is equal to the Thomas-Fermi energy $E_{TF}(Z, q)$. In fact, (3) and (4) show that

$$E_{TF}(Z,q) = q c_{TF} \int_{\mathbb{R}^3} \rho_{TF}^{5/3} dx - q \int_{\mathbb{R}^3} \frac{Z}{|x|} \rho_{TF}(x) dx + \frac{q^2}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y) dx dy}{|x-y|} \tag{38}$$

$$= q c_{TF} \int_{\mathbb{R}^3} \left(\frac{1}{6\pi^2} |V_{TF}(x)|^{3/2} \right)^{5/3} dx$$

$$+ q \int_{\mathbb{R}^3} \rho_{TF}(x) \left[-\frac{Z}{|x|} + q \int_{\mathbb{R}^3} \frac{\rho_{TF}(y) dy}{|x-y|} \right] dx - \frac{q^2}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y) dx dy}{|x-y|}$$

$$= q c_{TF} (6\pi^2)^{-5/3} \int_{\mathbb{R}^3} |V_{TF}(x)|^{5/2} dx + q \int_{\mathbb{R}^3} \rho_{TF}(x) V_{TF}(x) dx$$

$$- \frac{q^2}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_{TF}(x)\rho_{TF}(y) \frac{dx dy}{|x-y|}.$$

Since $c_{TF} = \frac{(6\pi^2)^{5/3}}{10\pi^2}$ and $\rho_{TF} V_{TF} = -\rho_{TF}|V_{TF}| = -\frac{1}{6\pi^2}|V_{TF}|^{5/2}$, (38) implies that

$$E_{TF}(Z,q) = \frac{q}{10\pi^2} \int_{\mathbb{R}^3} |V_{TF}(x)|^{5/2} dx - \frac{q}{6\pi^2} \int_{\mathbb{R}^3} |V_{TF}(x)|^{5/2} dx \tag{38 bis}$$

$$- \frac{q^2}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_{TF}(x)\rho_{TF}(y) \frac{dx dy}{|x-y|},$$

which is obviously equal to the expresion in curly brackets in (37). Thus, (37) becomes

$$E_{TF}(Z,q) + \eta Z^{7/3} \geq$$

$$E_{TF}(Z,q) - CZ^{13/6} +$$

$$\left[\left\langle \sum_{k=1}^{N} (-\Delta_{x_k} + [1 + CZ^{-1/2}]V_{TF}(x_k))\Psi, \Psi \right\rangle - q \operatorname{sneg}(-\Delta + [1 + CZ^{-1/2}]V_{TF}) \right].$$

That is,

$$\left\langle \sum_{k=1}^{N} (-\Delta_{x_k} + [1 + CZ^{-1/2}] V_{TF}(x_k)) \Psi, \Psi \right\rangle \leq q \operatorname{sneg}(-\Delta + [1 + CZ^{-1/2}] V_{TF}) + C(\eta + Z^{-1/6}) Z^{7/3}.$$

This is the hypothesis of Lemma 2, with $V = [1 + CZ^{-1/2}]V_{TF}$, and with $\eta + Z^{-1/6}$ in place of η. Hence, Lemma 2 implies

$$\left\langle \sum_{k=1}^{N} (-\Delta_{x_k}) \Psi, \Psi \right\rangle = \frac{q}{10\pi^2} \int_{\mathbb{R}^3} |V_{TF}(x) \cdot [1 + CZ^{-1/2}]|^{5/2} dx + O(\eta^{1/2} + Z^{-1/12}) Z^{7/3}$$

and

$$\left\langle \sum_{k=1}^{N} W(x_k) \Psi, \Psi \right\rangle = \frac{q}{6\pi^2} \int_{\mathbb{R}^3} W(x) |V_{TF}(x) \cdot [1 + CZ^{-1/2}]|^{3/2} dx + O(\eta^{1/2} + Z^{-1/12}) Z^{7/3},$$

provided $|W(x)| \leq C\mathcal{S}(x)$ and $|\nabla W(x)| \leq C\mathcal{S}(x)|x|^{-1}$. These equations are equivalent to

(39)
$$\left\langle \sum_{k=1}^{N} (-\Delta_{x_k}) \Psi, \Psi \right\rangle = \frac{q}{10\pi^2} \int_{\mathbb{R}^3} |V_{TF}(x)|^{5/2} dx + O(\eta^{1/2} + Z^{-1/12}) Z^{7/3}$$

and

(40)
$$\left\langle \sum_{k=1}^{N} W(x_k) \Psi, \Psi \right\rangle = \frac{q}{6\pi^2} \int_{\mathbb{R}^3} W(x) |V_{TF}(x)|^{3/2} dx + O(\eta^{1/2} + Z^{-1/12}) Z^{7/3}.$$

Since

$$\rho_{TF} = \frac{1}{6\pi^2} |V_{TF}|^{3/2}, \quad \text{and since}$$
$$c_{TF} \rho_{TF}^{5/3} = \left[\frac{(6\pi^2)^{5/3}}{10\pi^2} \right] \cdot \left[\frac{1}{6\pi^2} |V_{TF}|^{3/2} \right]^{5/3} = \frac{1}{10\pi^2} |V_{TF}|^{5/2},$$

equations (39) and (40) are equivalent to the conclusions of Lemma 5. □

At last we are ready to control $\mathcal{E}(\widehat{Q} + x, \rho_{TF}(x), \Psi)$, as explained at the start of this section. Recall that $\widehat{Q}$ is a cube centered at 0, with $Z^{-2/3} \ll \operatorname{diam} \widehat{Q} \ll Z^{-1/3}$, and that the definition of $\mathcal{E}(Q, \rho, \Psi)$ is given in the Main Theorem on Free Particles. In fact,

(41)
$$\mathcal{E}(Q, \rho, \Psi) = KE(Q, \Psi) - \frac{5}{3} c_{TF} \rho^{2/3} \langle \mathcal{N}_Q \Psi, \Psi \rangle + \frac{2}{3} q c_{TF} \rho^{5/3} |Q| + C_1 q \rho^{4/3} |Q|^{2/3},$$

with a slightly changed constant C_1.

Lemma 6: *Suppose $N \le CZ$ and $\langle H\Psi, \Psi\rangle \le E_{TF}(Z,q) + \eta Z^{7/3}$ with $0 \le \eta \le 1$. Set $A = \{x \in \mathbb{R}^3 \mid 10\,\mathrm{diam}\,\widehat{Q} < |x| < c(\mathrm{diam}\,\widehat{Q})^{1/2}\}$. Then $\mathcal{E}(\widehat{Q}+x, \rho_{TF}(x), \Psi) \ge 0$ for $x \in A$, and*

$$\int_A \mathcal{E}(\widehat{Q}+x, \rho_{TF}(x), \Psi)\frac{dx}{|\widehat{Q}|} \le$$
$$C(\eta^{1/2} + Z^{-1/12})Z^{7/3} + CZ^{5/3}(\mathrm{diam}\,\widehat{Q})^{-1} + CZ^{5/2}(\mathrm{diam}\,\widehat{Q})^{1/2}.$$

Proof: *The Main Theorem on Free Particles implies that*

$$\mathcal{E}(\widehat{Q}+x, \rho_{TF}(x), \Psi) \ge 0 \quad \text{provided} \quad \rho_{TF}(x)|\widehat{Q}| > C'.$$

Since $\rho_{TF}(x) \sim \mathcal{S}^{3/2}(x) \ge [(2c(diam\,\widehat{Q})^{1/2})^{-4}]^{3/2} = (2c)^{-6}(\mathrm{diam}\,\widehat{Q})^{-3}$ for $x \in A^* = \{(\mathrm{diam}\,\widehat{Q}) < |x| < 2c(\mathrm{diam}\,\widehat{Q})^{1/2}\}$, we have $\rho_{TF}(x)|\widehat{Q}| > C'$ for $x \in A^*$. Thus,

$$\mathcal{E}(\widehat{Q}+x, \rho_{TF}(x), \Psi) \ge 0 \quad \text{for} \quad x \in A^*, \tag{42}$$

in particular for $x \in A$. To estimate the integral in Lemma 6, we introduce $\theta(x)$ on $\mathbb{R}^3$, satisfying $0 \le \theta(x) \le 1$, $|\nabla\theta(x)| \le C|x|^{-1}$, $\theta(x) = 1$ for $x \in A$, $supp\,\theta \subset \{x \mid 5\,\mathrm{diam}\,\widehat{Q} < |x| < \frac{3}{2}c(\mathrm{diam}\,\widehat{Q})^{1/2}\} \subset A^*$. By (41) and (42) we have

$$\begin{aligned}
\int_{x\in A} \mathcal{E}(\widehat{Q}+x, \rho_{TF}(x), \Psi)\frac{dx}{|\widehat{Q}|} &\le \int_{\mathbb{R}^3} \theta(x)\mathcal{E}(\widehat{Q}+x, \rho_{TF}(x), \Psi)\frac{dx}{|\widehat{Q}|} \\
&= \int_{\mathbb{R}^3} KE(\widehat{Q}+x, \Psi)\frac{\theta(x)dx}{|\widehat{Q}|} - \frac{5}{3}c_{TF}\int_{\mathbb{R}^3} \rho_{TF}^{2/3}(x)\left\langle \mathcal{N}_{\widehat{Q}+x}\Psi, \Psi\right\rangle \frac{\theta(x)dx}{|\widehat{Q}|} \\
&\quad + \frac{2}{3}qc_{TF}\int_{\mathbb{R}^3} \rho_{TF}^{5/3}(x)\theta(x)dx + C_1 q|\widehat{Q}|^{-1/3}\int_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)\theta(x)dx.
\end{aligned} \tag{43}$$

We estimate separately each of the terms on the right in (43). By definition of $KE(Q,\Psi)$ and the fact that $KE(Q,\Psi) \ge 0$, we have

$$\begin{aligned}
\int_{\mathbb{R}^3} KE(\widehat{Q}+x, \Psi)\frac{\theta(x)dx}{|\widehat{Q}|} &\le \int_{\mathbb{R}^3} KE(\widehat{Q}+x, \Psi)\frac{dx}{|\widehat{Q}|} \\
&= \int_{\mathbb{R}^{3N+3}} \sum_{k=1}^N |\nabla_{x_k}\Psi(x_1 \dots x_N)|^2 \chi_{\widehat{Q}+x}(x_k)dx_1\dots dx_N\frac{dx}{|\widehat{Q}|} \\
&= \int_{\mathbb{R}^{3N}} \sum_{k=1}^N |\nabla_{x_k}\Psi(x_1 \dots x_N)|^2 \left[\int_{\mathbb{R}^3} \chi_{\widehat{Q}+x}(x_k)\frac{dx}{|\widehat{Q}|}\right]dx_1\dots dx_N
\end{aligned}$$

$$= \int_{\mathbb{R}^{3N}} \sum_{k=1}^{N} |\nabla_{x_k} \Psi(x_1 \dots x_N)|^2 dx_1 \dots dx_N$$

$$= \Big\langle \sum_{k=1}^{N} (-\Delta_{x_k}) \Psi, \Psi \Big\rangle.$$

Therefore, Lemma 5 implies

$$\int_{\mathbb{R}^3} KE(\widehat{Q} + x, \Psi) \frac{\theta(x) dx}{|\widehat{Q}|} \le q c_{TF} \int_{\mathbb{R}^3} \rho_{TF}^{5/3} dx + C Z^{7/3} (\eta^{1/2} + Z^{-1/12}). \tag{44}$$

The next term on the right in (43) is

$$\int_{\mathbb{R}^3} \rho_{TF}^{2/3}(x) \left\langle \mathcal{N}_{\widehat{Q}+x} \Psi, \Psi \right\rangle \theta(x) \frac{dx}{|\widehat{Q}|} = \tag{45}$$

$$\int_{\mathbb{R}^3} \rho_{TF}^{2/3}(x) \Big\langle \sum_{k=1}^{N} \chi_{\widehat{Q}+x}(x_k) \Psi, \Psi \Big\rangle \theta(x) \frac{dx}{|\widehat{Q}|} = \Big\langle \sum_{k=1}^{N} W(x_k) \Psi, \Psi \Big\rangle$$

with

$$W(x) = \int_{\mathbb{R}^3} \theta(y) \rho_{TF}^{2/3}(y) \chi_{\widehat{Q}+y}(x) \frac{dy}{|\widehat{Q}|}, \quad \textit{i.e.}$$

$$W(x) = \int_{y \in \widehat{Q}} \theta \rho_{TF}^{2/3}(x+y) \frac{dy}{|\widehat{Q}|}. \tag{46}$$

Since $\theta \rho_{TF}^{2/3} = -(const) \theta V_{TF}$*, we have*

$$|\theta \rho_{TF}^{2/3}(x)| \le C \mathcal{S}(x), \quad |\nabla(\theta \rho_{TF}^{2/3})(x)| \le C \mathcal{S}(x) |x|^{-1}.$$

Also, $\operatorname{supp} \theta \rho_{TF}^{2/3}(x) \subset \{|x| > 5 \operatorname{diam} \widehat{Q}\}$ *by definition of* θ*. Therefore, (46) implies*

$$|W(x)| \le C' \mathcal{S}(x), \ |\nabla W(x)| \le C' \mathcal{S}(x) |x|^{-1}, \ \operatorname{supp} W(x) \subset \{|x| > 4 \operatorname{diam} \widehat{Q}\}. \tag{47}$$

In particular, W *satisfies the hypotheses of Lemma 5, which therefore tells us that*

$$\Big\langle \sum_{k=1}^{N} W(x_k) \Psi, \Psi \Big\rangle = q \int_{\mathbb{R}^3} W(x) \rho_{TF}(x) dx + O(\eta^{1/2} + Z^{-1/12}) Z^{7/3} \tag{48}$$

$$= q \int_{\mathbb{R}^3} \theta(x) \rho_{TF}^{5/3}(x) dx + q \int_{\mathbb{R}^3} [W(x) - \theta(x) \rho_{TF}^{2/3}(x)] \rho_{TF}(x) dx$$

$$+ O(\eta^{1/2} + Z^{-1/12}) Z^{7/3}.$$

By (47) and the definition of θ, we have $\operatorname{supp}[W(x)-\theta(x)\rho_{TF}^{2/3}(x)] \subset \{|x| > 4\,\mathrm{diam}\,\widehat{Q}\}$. *Moreover, for $|x| > 4\,\mathrm{diam}\,\widehat{Q}$, we see from (46) that*

$$|W(x)-\theta(x)\rho_{TF}^{2/3}(x)| = \left| \int_{y\in\widehat{Q}} [\theta(x+y)\rho_{TF}^{2/3}(x+y) - \theta(x)\rho_{TF}^{2/3}(x)] \frac{dy}{|\widehat{Q}|} \right|$$
$$\leq (\mathrm{diam}\,\widehat{Q}) \max_{y\in\widehat{Q}} |\nabla(\theta\rho_{TF}^{2/3})(x+y)| \leq C(\mathrm{diam}\,\widehat{Q})\mathcal{S}(x)|x|^{-1}.$$

Hence,

$$(49)\quad \left|\int_{\mathbb{R}^3} [W(x)-\theta(x)\rho_{TF}^{2/3}(x)]\rho_{TF}(x)dx\right| \leq C \int_{|x|>4\,\mathrm{diam}\,\widehat{Q}} \left[(\mathrm{diam}\,\widehat{Q})\frac{\mathcal{S}(x)}{|x|}\right]\mathcal{S}^{3/2}(x)dx$$
$$= C(\mathrm{diam}\,\widehat{Q}) \int_{|x|>4\,\mathrm{diam}\,\widehat{Q}} \mathcal{S}^{5/2}(x)\frac{dx}{|x|}$$
$$= C(\mathrm{diam}\,\widehat{Q})\left[\int_{4\,\mathrm{diam}\,\widehat{Q}<|x|<Z^{-1/3}} Z^{5/2}\frac{dx}{|x|^{7/2}} + \int_{|x|>Z^{-1/3}} \frac{dx}{|x|^{11}}\right]$$
$$= C(\mathrm{diam}\,\widehat{Q})[Z^{5/2}(\mathrm{diam}\,\widehat{Q})^{-1/2} + Z^{\frac{8}{3}}].$$

We have $Z^{5/2}(\mathrm{diam}\,\widehat{Q})^{-1/2} \geq Z^{5/2}(Z^{-1/3})^{-1/2} = Z^{8/3}$, *so (49) is equivalent to*

$$\left|\int_{\mathbb{R}^3} [W(x)-\theta(x)\rho_{TF}^{2/3}(x)]\rho_{TF}(x)dx\right| \leq CZ^{5/2}(\mathrm{diam}\,\widehat{Q})^{+1/2}.$$

Putting this into (48), we see that

$$(50)\quad \left\langle \sum_{k=1}^{N} W(x_k)\Psi,\Psi\right\rangle = q\int_{\mathbb{R}^3} \theta(x)\rho_{TF}^{5/3}(x)dx + O(Z^{5/2}(\mathrm{diam}\,\widehat{Q})^{1/2} + Z^{7/3}(\eta^{1/2}+Z^{-1/12}))$$

Since $\theta = 1$ in A, we have also

$$(51)\quad \left|\int_{\mathbb{R}^3} (1-\theta(x))\rho_{TF}^{5/3}(x)dx\right| \leq \int_{\mathbb{R}^3\setminus A} C\mathcal{S}^{5/2}(x)dx \leq$$
$$C\int_{|x|<10\,\mathrm{diam}\,\widehat{Q}} Z^{5/2}\frac{dx}{|x|^{5/2}} + C\int_{|x|>c(\mathrm{diam}\,\widehat{Q})^{1/2}} |x|^{-10}dx$$
$$\leq C'Z^{5/2}(\mathrm{diam}\,\widehat{Q})^{1/2} + C''(\mathrm{diam}\,\widehat{Q})^{-7/2}.$$

Hence, (50) yields

$$\left\langle \sum_{k=1}^{N} W(x_k)\Psi, \Psi \right\rangle =$$
$$q \int_{\mathbb{R}^3} \rho_{TF}^{5/3}(x)dx + O(Z^{5/2}(\operatorname{diam}\widehat{Q})^{1/2} + (\operatorname{diam}\widehat{Q})^{-7/2} + Z^{7/3}(\eta^{1/2} + Z^{-1/12})).$$

This and (45) together yield

(52) $$-\frac{5}{3}c_{TF} \int_{\mathbb{R}^3} \rho_{TF}^{2/3}(x) \left\langle \mathcal{N}_{\widehat{Q}+x}\Psi, \Psi \right\rangle \theta(x) \frac{dx}{|\widehat{Q}|} \leq$$
$$-\frac{5}{3}qc_{TF} \int_{\mathbb{R}^3} \rho_{TF}^{5/3}dx + C[Z^{5/2}(\operatorname{diam}\widehat{Q})^{1/2} + (\operatorname{diam}\widehat{Q})^{-7/2} + Z^{7/3}(\eta^{1/2} + Z^{-1/12})].$$

The final terms on the right in (43) may be estimated trivially. We have

(53) $$\frac{2}{3}qc_{TF} \int_{\mathbb{R}^3} \rho_{TF}^{5/3}(x)\theta(x)dx \leq \frac{2}{3}qc_{TF} \int_{\mathbb{R}^3} \rho_{TF}^{5/3}dx,$$

and

(54) $$C_1 q|\widehat{Q}|^{-1/3} \int_{\mathbb{R}^3} \theta(x)\rho_{TF}^{4/3}(x)dx \leq C_1 q|\widehat{Q}|^{-1/3} \int_{\mathbb{R}^3} \rho_{TF}^{4/3}dx \leq C'(\operatorname{diam}\widehat{Q})^{-1}Z^{5/3}.$$

Putting (44), (52), (53), (54) into the right-hand side of (43), we get

$$\int_{x\in A} \mathcal{E}(\widehat{Q}+x, \rho_{TF}(x), \Psi) \frac{dx}{|\widehat{Q}|} \leq$$
$$\left[qc_{TF} \int_{\mathbb{R}^3} \rho_{TF}^{5/3}dx + CZ^{7/3}(\eta^{1/2} + Z^{-1/12})\right] +$$
$$\left[-\frac{5}{3}qc_{TF} \int_{\mathbb{R}^3} \rho_{TF}^{5/3}dx + CZ^{5/2}(\operatorname{diam}\widehat{Q})^{1/2} + C(\operatorname{diam}\widehat{Q})^{-7/2} + CZ^{7/3}(\eta^{1/2} + Z^{-1/12})\right]$$
$$+\left[\frac{2}{3}qc_{TF} \int_{\mathbb{R}^3} \rho_{TF}^{5/3}dx\right] + [C'(\operatorname{diam}\widehat{Q})^{-1}Z^{5/3}].$$

This is equivalent to

(55)
$$\int\limits_{x\in A} \mathcal{E}(\widehat{Q}+x,\rho_{TF}(x),\Psi)\frac{dx}{|\widehat{Q}|} \le CZ^{7/3}(\eta^{1/2}+Z^{-1/12})+CZ^{5/2}(\operatorname{diam}\widehat{Q})^{1/2}$$
$$+C(\operatorname{diam}\widehat{Q})^{-7/2}+C(\operatorname{diam}\widehat{Q})^{-1}Z^{5/3}$$

Since $Z^{-2/3} \le \operatorname{diam}\widehat{Q}$, *we have* $Z^{-5/3} \le (\operatorname{diam}\widehat{Q})^{5/2}$, *i.e.* $(\operatorname{diam}\widehat{Q})^{-7/2} \le Z^{5/3}$ $(\operatorname{diam}\widehat{Q})^{-1}$. *Hence the term* $(\operatorname{diam}\widehat{Q})^{-7/2}$ *may be dropped from the right-hand side of (55), so that*

$$\int\limits_{x\in A} \mathcal{E}(\widehat{Q}+x,\rho_{TF}(x),\Psi)\frac{dx}{|\widehat{Q}|} \le$$
$$CZ^{7/3}(\eta^{1/2}+Z^{-1/12})+CZ^{5/2}(\operatorname{diam}\widehat{Q})^{1/2}+CZ^{5/3}(\operatorname{diam}\widehat{Q})^{-1}.$$

This is the conclusion of Lemma 6. □

Corollary: *Let* Ψ, A *be as in Lemma 6. Given* $0<\delta<1$, *there is a set* $F\subset A$ *with the following properties.*

(56) $\mathcal{E}(\widehat{Q}+\mathfrak{z},\rho_{TF}(\mathfrak{z}),\Psi) < \delta\rho_{TF}^{5/3}(\mathfrak{z})|\widehat{Q}|$ *for* $\mathfrak{z}\in A\setminus F$.

(57) $\int\limits_F \rho_{TF}^{5/3}(\mathfrak{z})d\mathfrak{z} \le C\beta Z^{7/3}$, *with*

(58) $\beta=\delta^{-1}(\eta^{1/2}+Z^{-1/12}+Z^{-2/3}(\operatorname{diam}\widehat{Q})^{-1}+Z^{+1/6}(\operatorname{diam}\widehat{Q})^{\frac{1}{2}})$

(59) $\int\limits_F \rho_{TF}^{4/3}(\mathfrak{z})d\mathfrak{z} \le C\beta^{5/7}Z^{5/3}$.

Proof: Set $F=\{\mathfrak{z}\in A \mid \mathcal{E}(\widehat{Q}+\mathfrak{z},\rho_{TF}(\mathfrak{z}),\Psi)\ge\delta\rho_{TF}^{5/3}(\mathfrak{z})|\widehat{Q}|\}$. Property (56) is immediate from the definition of F. To check (57), we use lemma 6 and the definition of F to write

$$\int\limits_F \delta\rho_{TF}^{5/3}(\mathfrak{z})d\mathfrak{z} \le \int\limits_F \mathcal{E}(\widehat{Q}+\mathfrak{z},\rho_{TF}(\mathfrak{z}),\Psi)\frac{d\mathfrak{z}}{|\widehat{Q}|} \le$$
$$\int\limits_A \mathcal{E}(\widehat{Q}+\mathfrak{z},\rho_{TF}(\mathfrak{z}),\Psi)\frac{d\mathfrak{z}}{|\widehat{Q}|} \le C(\eta^{1/2}+Z^{-1/12})Z^{7/3}+CZ^{5/3}(\operatorname{diam}\widehat{Q})^{-1}$$
$$+CZ^{5/2}(\operatorname{diam}\widehat{Q})^{1/2}.$$

From these inequalities, (57) follows at once.

To check (59), we may assume β is less than a small constant c. (Otherwise, (59) would follow trivially, since $\int_{\mathbb{R}^3} \rho_{TF}^{4/3}(\mathfrak{z})d\mathfrak{z} \leq CZ^{5/3}$.) We set $t = \beta^{6/7}Z^2 \ll Z^2$, and note that $\rho_{TF}^{4/3} \leq t^{-1/3}\rho_{TF}^{5/3} + t^{1/3}\rho_{TF}\chi_{\rho_{TF}\leq t}$, which implies

(60) $$\int_F \rho_{TF}^{4/3}d\mathfrak{z} \leq t^{-1/3}\int_F \rho_{TF}^{5/3}d\mathfrak{z} + t^{1/3}\int_{\{\rho_{TF}\leq t\}} \rho_{TF}d\mathfrak{z}.$$

Since $t \ll Z^2$, we have

$$\rho_{TF}(\mathfrak{z})\chi_{\rho_{TF}(\mathfrak{z})\leq t} \leq C|\mathfrak{z}|^{-6}\chi_{|\mathfrak{z}|>ct^{-1/6}},$$

so that

$$t^{1/3}\int_{\{\rho_{TF}\leq t\}} \rho_{TF}d\mathfrak{z} \leq Ct^{1/3}\cdot(ct^{-1/6})^{-3} = C't^{5/6},$$

and (60) becomes

$$\int_F \rho_{TF}^{4/3}d\mathfrak{z} \leq t^{-1/3}\int_F \rho_{TF}^{5/3}d\mathfrak{z} + C't^{5/6} \leq Ct^{-1/3}\beta Z^{7/3} + C't^{5/6},$$

by (57). By definition of t, the right-hand side here is dominated by $C\beta^{5/7}Z^{5/3}$, which proves (59). □

We apply the above Corollary to study $\left\langle \sum_{i<j} K(x_i,x_j)\Psi,\Psi \right\rangle$ for short-range interactions $K(x,y)$.

Lemma 7: *Suppose we are given D, m, δ satisfying*

(61) $CZ^{-2/3} < D < cZ^{-1/3}$

(62) $m > C$

(63) $0 < \delta < cm^{-42/5}$

(64) $m^{63}D^{-3} < cZ^2$.

Suppose $K(x,y)$ satisfies

(65) $0 \leq K(x,y) = K(y,x) \leq |x-y|^{-1}$

(66) *$\mathrm{supp}\, K(x,y) \subset (A_m \times A_m) \cap U_m$, where*

(67) $A_m = \{x \in \mathbb{R}^3 \mid 20D \leq |x| \leq cm^{-21/2}D^{+1/2}\}$ *and*

(68) $U_m = \{(x,y) \in \mathbb{R}^3 \times \mathbb{R}^3 \mid \rho_{TF}(x) \cdot |x-y|^3 < cm\}$.

Assume the wave function Ψ *satisfies* $\langle H\Psi, \Psi\rangle \leq E_{TF}(Z,q) + \eta Z^{7/3}$ *with* $0 < \eta < c$. *Finally, assume* $N \leq CZ$. *Then*

(69)
$$\left\langle \sum_{i<j} K(x_i,x_j)\Psi, \Psi \right\rangle \geq$$
$$\frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy$$
$$- Cm^{2/3}\left[\frac{m^{1/3}Z}{D} + \delta^{1/63}Z^{5/3} + (Z^2D^3)^{-\frac{2}{15\cdot 63}}Z^{5/3} + \beta^{5/7}Z^{5/3} + DZ^2\ell nZ\right]$$

with

(70)
$$\beta = \delta^{-1}[\eta^{1/2} + Z^{-1/12} + Z^{1/6}D^{1/2} + Z^{-2/3}D^{-1}]$$

Remarks: The hypothesis supp $K \subset U_m$ suggests that a typical electron will interact with about m of its nearest neighbors. So if $m \leq C$, then we are dealing with a short-range interaction. Later, we will take m to be a small, positive power of Z.

We will not make a final choice of η, D, δ, m here. However, we note that these parameters can be picked satisfying (61)...(64), so that the error terms in (69) are $o(Z^{5/3})$. First we take $\eta = Z^{-a_0}$ for small, fixed a_0. Then we take $D = Z^{-a}$, $\delta = [\eta^{1/2} + Z^{-1/12} + Z^{1/6}D^{1/2} + Z^{-2/3}D^{-1}]^b$, $m = Z^\varepsilon$, with $1/3 < a < 2/3$, $0 < b < 1$, and $0 < \varepsilon \ll 1$ depending on a_0, a, b. The reader can easily verify that (61)...(64) hold, and that the error terms in (69) are $O(Z^\gamma)$, with $\gamma < 5/3$ depending on a_0, a, b, ε.

Proof of Lemma 7: Set $A_m^+ = \{x \in \mathbb{R}^3 \mid 10D \leq |x| \leq 2cm^{-21/2}D^{1/2}\}$, and let $\widehat{Q}$ be a cube centered at 0, with diameter D. Then with A as in Lemma 6, we have $A_m \subset A_m^+ \subset A$. Moreover, if $x \in \widehat{Q} + \mathfrak{z}$ and $x \in A_m$, then $\mathfrak{z} \in A_m^+$. Note that $m^{-21/2}D^{1/2} > Z^{-1/3}$ by (64). Let Q_0 be the middle half of $\widehat{Q}$.

Note that our two definitions (58), (70) of β are consistent. Define $K_\mathfrak{z}(x,y) = K(x,y)\chi_{x,y\in Q_0+\mathfrak{z}}$, and let F be as in the Corollary to Lemma 6. (Observe that Ψ satisfies the hypotheses of Lemma 6, so (56)...(59) hold.)

If $\mathfrak{z} \in A_m^+ \setminus F$, then the hypotheses of the Main Theorem on Free Particles (I) are satisfied, with: $\rho_{TF}(\mathfrak{z})$ in place of ρ_0; $\widehat{Q} + \mathfrak{z}$ in place of Q; $K_\mathfrak{z}(x,y)$ in place of $K(x,y)$; and $(m\rho_{TF}^{-1}(\mathfrak{z}))^{1/3}$ in place of $r_{\max}$. In fact, $\underline{N} = \rho_{TF}(\mathfrak{z})|\widehat{Q}| = \rho_{TF}(\mathfrak{z})D^3 \geq c_0[2cm^{-21/2}D^{1/2}]^{-6}D^3$ (since $\mathfrak{z} \in A_m^+$) $= Cm^{63} = C(\rho_{TF}(\mathfrak{z})r_{\max}^3)^{63}$. Also $\delta < cm^{-42/5} = c(\rho_{TF}(\mathfrak{z})r_{\max}^3)^{-42/5}$, and $\rho_{TF}(\mathfrak{z})r_{\max}^3 = m \geq 1$. So the hypotheses in (I) on the parameters ρ_0, $r_{\max}$, δ, $\underline{N}$ are satisfied. The hypotheses on $K(x,y)$ in (I) hold for $K_\mathfrak{z}(x,y)$, thanks to (65), (66), (68) and our choice of $r_{\max}$. The crucial hypothesis $\mathcal{E}(\widehat{Q} + \mathfrak{z}, \rho_{TF}(\mathfrak{z}), \Psi) \leq$

$\delta\rho_{TF}^{5/3}(\mathfrak{z})|\widehat{Q}|$ follows from (56), since we are taking $\mathfrak{z} \in A_m^+ \setminus F \subset A \setminus F$. So we have verified all the hypotheses of the Main Theorem on Free Particles (I). Applying that result, we get:

(71)

$$\left\langle \sum_{i<j} K_{\mathfrak{z}}(x_i, x_j)\Psi, \Psi \right\rangle \geq \frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_{\mathfrak{z}}(x,y)\{q^2\rho_{TF}^2(\mathfrak{z}) - q|\mathcal{S}_{\rho_{TF}(\mathfrak{z})}(x-y)|^2\}dxdy$$
$$- C\left(\delta + \left[\rho_{TF}(\mathfrak{z})|\widehat{Q}|\right]^{-\frac{2}{15}}\right)^{\frac{1}{63}} m^{2/3}\rho_{TF}^{4/3}(\mathfrak{z})|\widehat{Q}|$$

for $\mathfrak{z} \in A_m^+ \setminus F$.

On the other hand, suppose $\mathfrak{z} \in A_m^+ \cap F$. Then at least the left-hand side of (71) is non-negative, while the integral on the right is dominated by

$$\frac{1}{2} \iint\limits_{\substack{x\in Q_0+\mathfrak{z} \\ |y-x|<(m\rho_{TF}^{-1}(\mathfrak{z}))^{1/3}}} |x-y|^{-1}q^2\rho_{TF}^2(\mathfrak{z})dxdy \leq C\rho_{TF}^2(\mathfrak{z})|\widehat{Q}| \cdot (m\rho_{TF}^{-1}(\mathfrak{z}))^{2/3}$$
$$= Cm^{2/3}\rho_{TF}^{4/3}(\mathfrak{z})|\widehat{Q}|.$$

Hence,

$$(72) \quad \left\langle \sum_{i<j} \frac{K_{\mathfrak{z}}(x_i,x_j)}{|Q_0|}\Psi, \Psi \right\rangle \geq$$
$$\frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{K_{\mathfrak{z}}(x,y)}{|Q_0|}\{q^2\rho_{TF}^2(\mathfrak{z}) - q|\mathcal{S}_{\rho_{TF}(\mathfrak{z})}(x-y)|^2\}dxdy$$
$$- C\left[\delta^{1/63}m^{2/3}\rho_{TF}^{4/3}(\mathfrak{z}) + m^{2/3}\rho_{TF}^{4/3}(\mathfrak{z})\chi_{\mathfrak{z}\in F} + [\rho_{TF}(\mathfrak{z})|\widehat{Q}|]^{-\frac{2}{15\cdot 63}}m^{2/3}\rho_{TF}^{4/3}(\mathfrak{z})\right]$$

for $\mathfrak{z} \in A_m^+ \cap F$. Estimate (71) shows that (72) holds also for $\mathfrak{z} \in A_m^+ \setminus F$. Therefore, (72) holds for all $\mathfrak{z} \in A_m^+$.

The next step is to integrate (72) over all $\mathfrak{z} \in A_m^+$. Note that

$$\int\limits_{\mathfrak{z}\in A_m^+} \frac{K_{\mathfrak{z}}(x_i,x_j)}{|Q_0|}d\mathfrak{z} \leq \int\limits_{\mathfrak{z}\in\mathbb{R}^3} K_{\mathfrak{z}}(x_i,x_j)\frac{d\mathfrak{z}}{|Q_0|} = \int\limits_{\mathfrak{z}\in\mathbb{R}^3} K(x_i,x_j)\chi_{x_i,x_j\in Q_0+\mathfrak{z}}\frac{d\mathfrak{z}}{|Q_0|}$$
$$\leq \int\limits_{\mathfrak{z}\in\mathbb{R}^3} K(x_i,x_j)\chi_{x_i\in Q_0+\mathfrak{z}}\frac{d\mathfrak{z}}{|Q_0|} = K(x_i,x_j).$$

Therefore, integrating (72), we get

$$(73) \quad \left\langle \sum_{i<j} K(x_i,x_j)\Psi, \Psi \right\rangle \geq \int\limits_{\mathfrak{z}\in A_m^+} \left\langle \sum_{i<j} \frac{K_{\mathfrak{z}}(x_i,x_j)}{|Q_0|}\Psi, \Psi \right\rangle d\mathfrak{z} \geq$$

$$\frac{1}{2}\int\limits_{\mathfrak{z}\in A_m^+}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}\frac{K_{\mathfrak{z}}(x,y)}{|Q_0|}\{q^2\rho_{TF}^2(\mathfrak{z})-q|\mathcal{S}_{\rho_{TF}(\mathfrak{z})}(x-y)|^2\}dxdyd\mathfrak{z}$$
$$-C\delta^{1/63}m^{2/3}\int\limits_{\mathbb{R}^3}\rho_{TF}^{4/3}d\mathfrak{z}-Cm^{2/3}\int\limits_{F}\rho_{TF}^{4/3}d\mathfrak{z}$$
$$-Cm^{2/3}\int\limits_{\mathbb{R}^3}[\rho_{TF}(\mathfrak{z})|\widehat{Q}|]^{-\frac{2}{15\cdot 63}}\rho_{TF}^{4/3}(\mathfrak{z})d\mathfrak{z}.$$

We have $\int_{\mathbb{R}^3}\rho_{TF}^{4/3}d\mathfrak{z}\le CZ^{5/3}$, and $\int_F\rho_{TF}^{4/3}d\mathfrak{z}\le C\beta^{5/7}Z^{5/3}$ by (59). Also,

$$\int\limits_{\mathbb{R}^3}[\rho_{TF}(\mathfrak{z})|\widehat{Q}|]^{-\frac{2}{15\cdot 63}}\rho_{TF}^{4/3}(\mathfrak{z})d\mathfrak{z}\le$$
$$C\int\limits_{|\mathfrak{z}|<Z^{-1/3}}[Z^{3/2}|\mathfrak{z}|^{-3/2}|\widehat{Q}|]^{-\frac{2}{15\cdot 63}}\cdot Z^2|\mathfrak{z}|^{-2}d\mathfrak{z}$$
$$+C\int\limits_{|\mathfrak{z}|>Z^{-1/3}}\left[|\mathfrak{z}|^{-6}|\widehat{Q}|\right]^{-\frac{2}{15\cdot 63}}\cdot|\mathfrak{z}|^{-8}d\mathfrak{z}\le C'[Z^2|\widehat{Q}|]^{-\frac{2}{15\cdot 63}}Z^{5/3}.$$

Using these facts to bound the error terms in the right-hand side of (73), we obtain

$$(74)\quad \left\langle\sum_{i<j}K(x_i,x_j)\Psi,\Psi\right\rangle\ge$$
$$\frac{1}{2}\int\limits_{\mathfrak{z}\in A_m^+}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}\frac{K_{\mathfrak{z}}(x,y)}{|Q_0|}\{q^2\rho_{TF}^2(\mathfrak{z})-q|\mathcal{S}_{\rho_{TF}(\mathfrak{z})}(x-y)|^2\}dxdyd\mathfrak{z}$$
$$-C\left[\delta^{1/63}m^{2/3}Z^{5/3}+m^{2/3}(Z^2D^3)^{-\frac{2}{15\cdot 63}}Z^{5/3}+m^{2/3}\beta^{5/7}Z^{5/3}\right].$$

We want to replace $\{q^2\rho_{TF}^2(\mathfrak{z})-q|\mathcal{S}_{\rho_{TF}(\mathfrak{z})}(x-y)|^2\}$ by $\{q^2\rho_{TF}(x)\rho_{TF}(y)-q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}$ in (74). For $(x,y)\in\operatorname{supp}K_{\mathfrak{z}}$, we have $x,y\in Q_0+\mathfrak{z}$, so $|x-\mathfrak{z}|$, $|y-\mathfrak{z}|<\operatorname{diam}\widehat{Q}=D$. Since $|\mathfrak{z}|\ge 10D$ for $\mathfrak{z}\in A_m^+$, it follows that

$$|\rho_{TF}(x)-\rho_{TF}(\mathfrak{z})|,|\rho_{TF}(y)-\rho_{TF}(\mathfrak{z})|\le CD\max_{w\in Q_0+\mathfrak{z}}|\nabla\rho_{TF}(w)|$$
$$\le C'\frac{D}{|\mathfrak{z}|}\rho_{TF}(\mathfrak{z}).$$

These estimates imply $|\rho_{TF}^2(\mathfrak{z})-\rho_{TF}(x)\rho_{TF}(y)|\le\frac{CD}{|\mathfrak{z}|}\rho_{TF}^2(\mathfrak{z})$. Also, the Fermi radii $r_F(\mathfrak{z})=(\text{const})\rho_{TF}^{1/3}(\mathfrak{z})$ and $r_F(x)=(\text{const})\rho_{TF}^{1/3}(x)$ satisfy $|r_F(\mathfrak{z})-r_F(x)|<\frac{CD}{|\mathfrak{z}|}r_F(\mathfrak{z})$.

Since $\mathcal{S}_{\rho_{TF}(\mathfrak{z})}(w) = (\text{const}) \int_{|\xi|<r_F(\mathfrak{z})} e^{i\xi\cdot w} d\xi$ and $\mathcal{S}_{\rho_{TF}(x)}(w) = (\text{const}) \int_{|\xi|<r_F(x)} e^{i\xi\cdot w} d\xi$, it follows that

$$\begin{aligned} |\mathcal{S}_{\rho_{TF}(\mathfrak{z})}(w) - \mathcal{S}_{\rho_{TF}(x)}(w)| &\leq C|\mathrm{Vol}\, B(0, r_F(\mathfrak{z})) - \mathrm{Vol}\, B(0, r_F(x))| \\ &\leq C' r_F^2(\mathfrak{z}) \cdot |r_F(\mathfrak{z}) - r_F(x)| \leq C'' r_F^3(\mathfrak{z}) \cdot \frac{D}{|\mathfrak{z}|} = C''' \rho_{TF}(\mathfrak{z}) D/|\mathfrak{z}|. \end{aligned}$$

Since $|\mathcal{S}_{\rho_{TF}(\mathfrak{z})}(w)| \leq \rho_{TF}(\mathfrak{z})$, it follows also that

$$\Big| |\mathcal{S}_{\rho_{TF}(\mathfrak{z})}(w)|^2 - |\mathcal{S}_{\rho_{TF}(x)}(w)|^2 \Big| \leq C \rho_{TF}^2(\mathfrak{z}) \cdot \frac{D}{|\mathfrak{z}|}.$$

Consequently,

$$\begin{aligned} |\{q^2 \rho_{TF}^2(\mathfrak{z}) - q |\mathcal{S}_{\rho_{TF}(\mathfrak{z})}(x-y)|^2\} - \{q^2 \rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}| \\ \leq C\rho_{TF}^2(\mathfrak{z}) \cdot \frac{D}{|\mathfrak{z}|}. \end{aligned}$$

This in turn implies

$$\begin{aligned} (75) \quad & \Bigg| \int\limits_{\mathfrak{z}\in A_m^+} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{K_{\mathfrak{z}}(x,y)}{|Q_0|} \{q^2 \rho_{TF}^2(\mathfrak{z}) - q|\mathcal{S}_{\rho_{TF}(\mathfrak{z})}(x-y)|^2\} dx dy d\mathfrak{z} \\ & \quad - \int\limits_{\mathfrak{z}\in A_m^+} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{K_{\mathfrak{z}}(x,y)}{|Q_0|} \{q^2 \rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\} dx dy d\mathfrak{z} \Bigg| \\ & \leq \int\limits_{\mathfrak{z}\in A_m^+} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{K_{\mathfrak{z}}(x,y)}{|Q_0|} \cdot C\rho_{TF}^2(\mathfrak{z}) \frac{D}{|\mathfrak{z}|} dx dy d\mathfrak{z} \\ & \leq \int\limits_{\mathfrak{z}\in A_m^+} \left[\int_{\substack{x\in Q_0+\mathfrak{z} \\ |y-x|<(m\rho_{TF}^{-1}(x))^{1/3}}} \frac{|x-y|^{-1}}{|Q_0|} dx dy \right] \cdot \rho_{TF}^2(\mathfrak{z}) \frac{D}{|\mathfrak{z}|} d\mathfrak{z} \\ & \leq C' \int\limits_{\mathfrak{z}\in A_m^+} (m\rho_{TF}^{-1}(\mathfrak{z}))^{2/3} \rho_{TF}^2(\mathfrak{z}) \frac{D}{|\mathfrak{z}|} d\mathfrak{z} \\ & = C' m^{2/3} D \cdot \int\limits_{\mathfrak{z}\in A_m^+} \rho_{TF}^{4/3}(\mathfrak{z}) \frac{d\mathfrak{z}}{|\mathfrak{z}|} \\ & \leq C'' m^{2/3} D \cdot \left[\int\limits_{10D\leq|\mathfrak{z}|\leq Z^{-1/3}} Z^2 |\mathfrak{z}|^{-2} \frac{d\mathfrak{z}}{|\mathfrak{z}|} + \int\limits_{Z^{-1/3}<|\mathfrak{z}|} |\mathfrak{z}|^{-8} \frac{d\mathfrak{z}}{|\mathfrak{z}|} \right] \\ & \leq C''' m^{2/3} D \cdot Z^2 \ell n Z, \text{ since } D > Z^{-2/3}. \end{aligned}$$

From (74) and (75) we obtain

$$(76) \quad \left\langle \sum_{i<j} K(x_i, x_j)\Psi, \Psi \right\rangle \geq$$

$$\frac{1}{2}\int\limits_{\mathfrak{z}\in A_m^+}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}\frac{K_{\mathfrak{z}}(x,y)}{|Q_0|}\{q^2\rho_{TF}(x)\rho_{TF}(y)-q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdyd\mathfrak{z}$$
$$-C[\delta^{1/63}m^{2/3}Z^{5/3}+m^{2/3}(Z^2D^3)^{-\frac{2}{15\cdot 63}}Z^{5/3}+m^{2/3}\beta^{5/7}Z^{5/3}+m^{2/3}DZ^2\ell nZ].$$

We can replace $\mathfrak{z}\in A_m^+$ in the integral here by $\mathfrak{z}\in\mathbb{R}^3$, since $K_{\mathfrak{z}}(x,y)\equiv 0$ for $\mathfrak{z}\notin A_m^+$. To see this, recall that $\operatorname{supp} K_{\mathfrak{z}}(x,y)\subset\{x\in\widehat{Q}+\mathfrak{z}, x\in A_m\}$. We noted earlier that $\mathfrak{z}\in A_m^+$ whenever this set is non-empty. Therefore, by definition of $K_{\mathfrak{z}}(x,y)$ we have

(77) $$\frac{1}{2}\int\limits_{\mathfrak{z}\in A_m^+}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}\frac{K_{\mathfrak{z}}(x,y)}{|Q_0|}\{q^2\rho_{TF}(x)\rho_{TF}(y)-q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdyd\mathfrak{z}$$
$$=\frac{1}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}K(x,y)\left[\int\limits_{\mathbb{R}^3}\chi_{x,y\in Q_0+\mathfrak{z}}\frac{d\mathfrak{z}}{|Q_0|}\right]\{q^2\rho_{TF}(x)\rho_{TF}(y)-q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy$$
$$\geq\frac{1}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}K(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y)-q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy$$
$$-\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}K(x,y)\cdot\frac{C|x-y|}{\operatorname{diam}Q_0}\rho_{TF}^2(x)dxdy,$$

since $\left|1-\int_{\mathbb{R}^3}\chi_{x,y\in Q_0+\mathfrak{z}}\frac{d\mathfrak{z}}{|Q_0|}\right|\leq\frac{C|x-y|}{\operatorname{diam}Q_0}$ and $|q^2\rho_{TF}(x)\rho_{TF}(y)-q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2|\leq C\rho_{TF}^2(x)$ in $\operatorname{supp}K(x,y)$.

Also,

$$\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}K(x,y)\cdot\frac{C|x-y|}{\operatorname{diam}Q_0}\rho_{TF}^2(x)dxdy$$
$$\leq\int\limits_{\substack{x\in\mathbb{R}^3\\|y-x|<(m\rho_{TF}^{-1}(x))^{1/3}}}|x-y|^{-1}\cdot\frac{C'|x-y|}{D}\rho_{TF}^2(x)dxdy$$
$$=\frac{C''}{D}\int\limits_{\mathbb{R}^3}[m\rho_{TF}^{-1}(x)]\cdot\rho_{TF}^2(x)dx=\frac{C''m}{D}\int\limits_{\mathbb{R}^3}\rho_{TF}(x)dx$$
$$\leq\frac{CmZ}{D}.$$

Hence, (76) and (77) imply

$$\left\langle\sum_{i<j}K(x_i,x_j)\Psi,\Psi\right\rangle\geq$$

$$\frac{1}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y) - q|\mathbb{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy$$

$$- C\left[\frac{mZ}{D} + \delta^{1/63}m^{2/3}Z^{5/3} + m^{2/3}(Z^2D^3)^{-\frac{2}{15\cdot 63}}Z^{5/3} + m^{2/3}\beta^{5/7}Z^{5/3} + m^{2/3}DZ^2\ell nZ\right].$$

This estimate is the conclusion of Lemma 7. □

Computation of the Ground-State Energy

Let $E(Z,q)$ denote the ground-state energy of an atom of atomic number Z, in which the electrons are allowed to have q possible spins. In this section, we give upper and lower bounds for $E(Z,q)$ that differ by $o(Z^{5/3})$. The upper bound is proved by computing the energy of a Hartree-Fock trial wave function. To prove the lower bound, we break up the Coulomb repulsion $\sum\limits_{i<j}|x_i - x_j|^{-1}$ into a long-range part $\sum\limits_{i<j}K_L(x_i,x_j)$ and a short-range part $\sum\limits_{i<j}K_s(x_i,x_j)$. The Hamiltonian H thus breaks up as

$$H = \left[\sum_k\left(-\Delta_{x_k} - \frac{Z}{|x_k|}\right) + \sum_{i<j}K_L(x_i,x_j)\right] + \sum_{i<j}K_s(x_i,x_j).$$

The operator in square brackets can be bounded below by using standard ideas, as in Lemmas 3, 4, 5 of the preceding section. To give a lower bound for the difficult term $\sum\limits_{i<j}K_s(x_i,x_j)$, we invoke Lemma 7 from the preceding section.

In addition to our previous results, we need some precise information on the eigenvalues and eigenfunctions of the three-dimensional Schrödinger operator $-\Delta + V_{TF}(x)$. Let $E_1, E_2, \ldots, E_{N_*}$ be the non-positive eigenvalues of $-\Delta + V_{TF}$; and let $\varphi_1(x), \ldots, \varphi_{N_*}(x)$ be the corresponding normalized eigenfunctions. In our papers [FS2…7], we prove the following results.

WKB Theorems:

(A) *Form the density* $\rho_*(x) = \sum\limits_{k=1}^{N_*}|\varphi_k(x)|^2$. *Then we have*

$$\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}[\rho_*(x) - \rho_{TF}(x)][\rho_*(y) - \rho_{TF}(y)]\frac{dxdy}{|x-y|} < CZ^{5/3-\gamma_0}$$

with $\gamma_0 = 1/75$.

(B) *The eigenvalue sum* $sneg(-\Delta + V_{TF}) = E_1 + \cdots + E_{N_*}$ *is given by*

$$sneg(-\Delta + V_{TF}) = -\frac{1}{15\pi^2}\int\limits_{\mathbb{R}^3}|V_{TF}|^{5/2} + \frac{Z^2}{8} + \frac{1}{48\pi^2}\int\limits_{\mathbb{R}^3}|V_{TF}|^{1/2}\Delta V_{TF} + O(Z^{5/3-\gamma_0}).$$

The proof of these results is long and complicated. Here we will simply assume (A) and (B). We will use (A) to compare the ground-state energy with the energy of the Hartree-Fock trial wave function Ψ_{hf}. Then we will use (B) to compute the energy of Ψ_{hf}.

In this section, C, c, etc. denote constants depending only on q. We assume that Z is greater than a large constant C.

We begin with a careful definition of $E(Z,q)$. Given N and a map spin: $\{1\dots N\} \to \{1\dots q\}$, we introduce the Hilbert space $\mathcal{H}$ of all complex-valued functions $\Psi(x_1\dots x_N)$ that satisfy $\Psi(x_{\sigma 1}\dots x_{\sigma N}) = (\operatorname{sgn}\sigma)\Psi(x_1\dots x_N)$ for spin-preserving permutations σ. The Hamiltonian for N electrons is then defined as

$$H = \sum_{k=1}^{N}\left(-\Delta_{x_k} - \frac{Z}{|x_k|}\right) + \sum_{1\le i<j\le N} |x_i - x_j|^{-1}, \text{ acting on } \mathcal{H}. \tag{1}$$

We write $E(Z,q,N,\text{spin})$ for the infimum of the spectrum of H. The ground-state energy $E(Z,q)$ is the infimum of $E(Z,q,N,\text{spin})$ over all choices of N and spin. It is known (see e.g. Lieb [L3]) that the infimum is assumed for an $N \le CZ$.

Next we define the Hartree-Fock trial wave function Ψ_{hf} and compute its energy. We use the eigenfunctions $\varphi_1(x)\dots\varphi_{N_*}(x)$ of $-\Delta + V_{TF}$, and set

$$\Phi(x_1\dots x_{N_*}) = (N_*!)^{-1/2}\sum_{\sigma}(\operatorname{sgn}\sigma)\varphi_{\sigma 1}(x_1)\dots\varphi_{\sigma N_*}(x_{N_*}), \tag{2}$$

where σ runs over all permutations of $\{1\dots N_*\}$.

Then we take $N = qN_*$, and write $(x_1\dots x_N)$ in the form $(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_q)$ with

$$\vec{x}_1 = (x_1, x_2, \dots, x_{N_*}),\ \vec{x}_2 = (x_{N_*+1}, x_{N_*+2}, \dots, x_{2N_*}),\ \text{etc.}$$

The Hartree-Fock wave function is defined as

$$\Psi_{hf}(x_1\dots x_N) = \Phi(\vec{x}_1)\Phi(\vec{x}_2)\cdots\Phi(\vec{x}_q). \tag{3}$$

The map spin is given by

$$\begin{aligned} \text{spin}(j) &= 1 \quad \text{for} \quad j = 1, 2, \dots, N_* \\ \text{spin}(j) &= 2 \quad \text{for} \quad j = N_*+1, N_*+2, \dots, 2N_*, \end{aligned}$$

and so on.

This construction is of course standard, and the following elementary formulas are well-known:

$$\|\Psi_{hf}\| = 1 \quad \text{and} \quad \Psi_{hf} \in \mathcal{H}. \tag{4}$$

The correlation functions for Ψ_{hf} are given by

$$\mathcal{S}_s(x, y, \Psi_{hf}) = \sum_{k=1}^{N_*} \varphi_k(x)\overline{\varphi_k(y)}, \text{ for } s = 1, \ldots, q. \tag{5}$$

In particular, the density of electrons of spin s is equal to

$$\rho_*(x) = \sum_{k=1}^{N_*} |\varphi_k(x)|^2. \tag{6}$$

The energy of Ψ_{hf} is given by

$$\begin{aligned} \langle H\Psi_{hf}, \Psi_{hf}\rangle = q\sum_{k=1}^{N_*} \|\nabla\varphi_k\|^2 - q\int\limits_{\mathbb{R}^3} \frac{Z}{|x|}\rho_*(x)dx \\ + \frac{q^2}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_*(x)\rho_*(y)dxdy}{|x-y|} - \frac{q}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\sum_{k=1}^{N_*}\varphi_k(x)\overline{\varphi_k(y)}|^2 dxdy}{|x-y|} \end{aligned} \tag{7}$$

The last term in (7) is the "exchange term". Note also that

$$\begin{aligned} \operatorname{sneg}(-\Delta + V_{TF}) &= \sum_{k=1}^{N_*} \langle(-\Delta_x + V_{TF}(x))\varphi_k, \varphi_k\rangle \\ &= \sum_{k=1}^{N_*} \|\nabla\varphi_k\|^2 + \int\limits_{\mathbb{R}^3} V_{TF}(x)\cdot\sum_{k=1}^{N_*}|\varphi_k(x)|^2 dx \\ &= \sum_{k=1}^{N_*} \|\nabla\varphi_k\|^2 + \int\limits_{\mathbb{R}^3} V_{TF}(x)\rho_*(x)dx. \end{aligned}$$

This equation may be rewritten in the form

$$\begin{aligned} q\operatorname{sneg}(-\Delta + V_{TF}) = q\sum_{k=1}^{N_*} \|\nabla\varphi_k\|^2 - q\int\limits_{\mathbb{R}^3} \frac{Z}{|x|}\rho_*(x)dx \\ + q^2\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \rho_*(x)\frac{\rho_{TF}(y)dxdy}{|x-y|}, \end{aligned} \tag{8}$$

since $V_{TF}(x) = -\frac{Z}{|x|} + q\int_{\mathbb{R}^3} \frac{\rho_{TF}(y)dy}{|x-y|}$. Comparing (5), (7) and (8), we see that

$$(9) \quad \langle H\Psi_{hf}, \Psi_{hf}\rangle = q\,\mathrm{sneg}(-\Delta + V_{TF}) - \frac{q^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|}$$

$$+ \frac{q^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} [\rho_*(x) - \rho_{TF}(x)][\rho_*(y) - \rho_{TF}(y)]\frac{dxdy}{|x-y|}$$

$$- \frac{1}{2}\sum_{s=1}^{q} \iint_{\mathbb{R}^3\times\mathbb{R}^3} |\mathbb{S}_s(x,y,\Psi_{hf})|^2 \frac{dxdy}{|x-y|}.$$

From the WKB Theorem (A) above, we know that the term involving $[\rho_* - \rho_{TF}]$ in (9) is $O(Z^{5/3-\gamma_0})$. Hence, we can get a crude upper bound for $\langle H\Psi_{hf}, \Psi_{hf}\rangle$ by merely dropping the last term in (9). That is,

$$\langle H\Psi_{hf}, \Psi_{hf}\rangle \le q\,\mathrm{sneg}(-\Delta + V_{TF}) - \frac{q^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \rho_{TF}(x)\rho_{TF}(y)\frac{dxdy}{|x-y|} + CZ^{5/3-\gamma_0}.$$

Using Lemma 1 from the previous section to estimate $\mathrm{sneg}(-\Delta + V_{TF})$, we therefore have the crude bound

$$\langle H\Psi_{hf}, \Psi_{hf}\rangle \le \left\{ -\frac{q}{15\pi^2}\int_{\mathbb{R}^3} |V_{TF}|^{5/2}dx - \frac{q^2}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \rho_{TF}(x)\rho_{TF}(y)\frac{dxdy}{|x-y|}\right\} + CZ^{13/6}$$

As we have seen in the previous section (equation (38 bis)), the expression in curly brackets is equal to $E_{TF}(Z,q)$. Thus,

$$\langle H\Psi_{hf}, \Psi_{hf}\rangle \le E_{TF}(Z,q) + \eta Z^{7/3}, \quad \text{with} \quad \eta = CZ^{-1/6}.$$

Also, $N = qN_* \le CZ$, by Lemma 9 in the preceding section. Therefore, the hypotheses of Lemma 8 in that section are satisfied, with $\eta = CZ^{-1/6}$. That lemma tells us that

$$(10) \quad \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} |\mathbb{S}_s(x,y,\Psi_{hf})|^2 \frac{dxdy}{|x-y|} \ge c_D \int_{\mathbb{R}^3} \rho_{TF}^{4/3}dx - C\cdot\mathrm{ERROR},$$

with

$$(11) \quad \mathrm{ERROR} = [Z^2D + D^{-5/2} + \delta^{\frac{1}{96}}Z^{5/3} + (Z^2D^3)^{-\frac{1}{15\cdot 48}}Z^{5/3} + \beta^{5/7}Z^{5/3}],$$

$$(12) \quad \beta = \delta^{-1}[CZ^{-1/12} + Z^{1/6}D^{1/2} + Z^{-2/3}D^{-1}].$$

Here we are free to pick $0 < \delta < c$ and $CZ^{-2/3} < D < cZ^{-1/3}$. Let us take $D = Z^{-1/2}$, so that (11) and (12) become

$$\text{ERROR} = [Z^{3/2} + Z^{5/4} + \delta^{\frac{1}{96}} Z^{5/3} + Z^{-\frac{1}{30\cdot 48}} Z^{5/3} + \beta^{5/7} Z^{5/3}], \tag{13}$$

$$\beta = C\delta^{-1} Z^{-\frac{1}{12}}. \tag{14}$$

We pick δ so that $\beta^{5/7} \sim \delta^{\frac{1}{96}}$, i.e.

$$\delta^{-5/7} Z^{-\frac{1}{12}\cdot\frac{5}{7}} \sim \delta^{\frac{1}{96}}.$$

Thus, $\delta^{1/96+5/7} \sim Z^{-\frac{1}{12}\cdot\frac{5}{7}}$, i.e.

$$\delta \sim Z^{-\frac{1}{12}\cdot\frac{5}{7}\cdot\frac{96\cdot 7}{(7+96\cdot 5)}} = Z^{-\frac{5}{12}\cdot\frac{96}{(7+96\cdot 5)}} \ll 1.$$

Our choice of D, δ is not optimal, even for (11) and (12). With our D, δ, we get

$$\begin{aligned} \delta^{\frac{1}{96}} Z^{5/3} \sim \beta^{5/7} Z^{5/3} &\sim Z^{-\frac{5}{12\cdot(7+96\cdot 5)}} \cdot Z^{5/3} \\ &\ll Z^{-\frac{1}{30\cdot 48}} Z^{5/3} = Z^{-\frac{1}{1440}} Z^{5/3}. \end{aligned}$$

Thus, (13) becomes $\text{ERROR} = CZ^{-\frac{1}{1440}} Z^{5/3}$, and (10) gives

$$\frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} |\mathbb{S}_s(x, y, \Psi_{hf})|^2 \frac{dxdy}{|x-y|} \geq c_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3} dx - CZ^{-\frac{1}{1440}} \cdot Z^{5/3}.$$

Substituting this back into (9) and again invoking the WKB Theorem (A), we get the sharp upper bound

$$\begin{aligned} &\langle H\Psi_{hf}, \Psi_{hf}\rangle \leq \\ &q\,\text{sneg}(-\Delta + V_{TF}) - \frac{q^2}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|} - qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx \\ &\qquad + CZ^{-\gamma_1} Z^{5/3}, \end{aligned} \tag{15}$$

with

$$\gamma_1 = \frac{1}{1440}. \tag{16}$$

From (15) and the minimax principle, we obtain at once

(17)

$$\begin{aligned} E(Z, q) \leq q\,\text{sneg}(-\Delta + V_{TF}) - \frac{q^2}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|} - qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3} dx \\ + CZ^{-\gamma_1} Z^{5/3}. \end{aligned}$$

This is our basic upper bound for $E(Z,q)$.

We turn now to the task of proving lower bounds for $E(Z,q)$. This amounts to giving lower bounds for $\langle H\Psi,\Psi\rangle$ whenever $\Psi(x_1\dots x_N)$ has norm 1 and is antisymmetric under spin-preserving permutations. Let us call the wave function $\Psi(x_1\dots x_N)$ *viable* if it satisfies $N\le CZ$ and $\langle H\Psi,\Psi\rangle \le E_{TF}(Z,q)+\eta Z^{7/3}$ with $\eta = CZ^{-1/6}$. Since the inf defining $E(Z,q)$ is attained for an $N\le CZ$, and since Ψ_{hf} is viable as we have seen above, it follows that

$$E(Z,q)=\inf\{<H\Psi,\Psi>\big|\ \Psi\,\text{viable}\}. \tag{18}$$

The crucial Lemma 7 from the previous section applies to viable wave functions.

Next we decompose the Coulomb interaction into a long-range and a short-range part. The construction depends on a parameter $m>1$ to be picked later. We fix once and for all a function $r(x)$ on $\mathbb{R}^3$ with the following properties.

$$r(x)<c_1\min\{|x|,(m\rho_{TF}^{-1}(x))^{1/3}\}<2r(x)\quad\text{for a small const. } c_1. \tag{19}$$

$$|\nabla r(x)|\le Cr(x)|x|^{-1} \tag{20}$$

The reader may easily verify that such functions exist. Also, we fix once and for all a non-negative, smooth radial function $\varphi_0(x)$ on $\mathbb{R}^3$, supported in the unit ball and having integral 1. In terms of $\varphi_0(x)$ and $r(x)$ we define

$$\varphi_x(x')=(r(x))^{-3}\varphi_0\left(\frac{x'-x}{r(x)}\right)\quad\text{and} \tag{21}$$

$$K_L(x,y)=\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\varphi_x(x')\varphi_y(y')}{|x'-y'|}dx'dy'. \tag{22}$$

Thus, $K_L(x,y)$ is the Coulomb potential between a spherical charge distribution in a ball of radius $r(x)$ centered at x, and a similar charge distribution centered at y. $K_L(x,y)$ is the long-range part of $|x-y|^{-1}$. The short-range part is then

$$K_s(x,y)=|x-y|^{-1}-K_L(x,y). \tag{23}$$

We set down the basic properties of $K_s(x,y)$ and $K_L(x,y)$.

Lemma 1:

(24) $0\le K_L(x,y)=K_L(y,x)\le|x-y|^{-1}$.

(25) *If* $|x-y|\ge 9r(x)$ *then* $K_L(x,y)=|x-y|^{-1}$. *Equivalently,*

(26) $0\le K_s(x,y)=K_s(y,x)\le|x-y|^{-1}$

(27) *$K_s(x,y)$ is supported in $\{(x,y) \mid |y-x| < 9r(x)\}$.*

Moreover,

(28) *If $d\mu$ is a signed measure on $\mathbb{R}^3 \setminus \{0\}$ and if $\iint_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y)|d\mu(x)|\,|d\mu(y)| < \infty$, then $\iint_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y)d\mu(x)d\mu(y) \geq 0$.*

Proof: Immediately from the mean-value property of the Coulomb protential, we have $0 \leq K_L(x,y) \leq |x-y|^{-1}$, and $K_L(x,y) = |x-y|^{-1}$ if $|x-y| > r(x)+r(y)$. We will show that $|x-y| > 9r(x)$ implies $|x-y| > r(x)+r(y)$. In fact, suppose $|x-y| \leq r(x)+r(y)$. Then by (19) we have $|x-y| \leq c_1|x| + c_1|y|$. Since c_1 is small, this implies that $\min\{|x|, (m\rho_{TF}^{-1}(x))^{1/3}\}$ and $\min\{|y|, (m\rho_{TF}^{-1}(y))^{1/3}\}$ differ at most by a factor of 2. Again using (19), we see that $r(x)$ and $r(y)$ differ at most by a factor of 8. Hence our assumption $|x-y| \leq r(x)+r(y)$ implies that $|x-y| < 9r(x)$. That is, $|x-y| \leq r(x)+r(y)$ implies $|x-y| < 9r(x)$. Equivalently, $|x-y| \geq 9r(x)$ implies $|x-y| > r(x)+r(y)$, which in turn implies $K_L(x,y) = |x-y|^{-1}$. We have proven all of (24), (25) except for $K_L(x,y) = K_L(y,x)$, which is immediate from the definition (22).

Properties (26), (27) are equivalent to (24), (25) in view of (23). Thus it remains only to check (28). With $f(x') = \int_{\mathbb{R}^3} \varphi_x(x')d\mu(x)$, we have

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y)d\mu(x)d\mu(y) = \iiiint_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi_x(x')\varphi_y(y')}{|x'-y'|} dx'dy'd\mu(x)d\mu(y)$$

$$= \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\left[\int_{\mathbb{R}^3}\varphi_x(x')d\mu(x)\right]\left[\int_{\mathbb{R}^3}\varphi_y(y')d\mu(y)\right]}{|x'-y'|} dx'dy'$$

$$= \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{f(x')f(y')}{|x'-y'|} dx'dy' = \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{f(x')\overline{f(y')}}{|x'-y'|} dx'dy'$$

$$= (\text{const}) \int_{\mathbb{R}^3} \frac{|\hat{f}(\xi)|^2}{|\xi|^2} d\xi \geq 0.$$

The hypothesis on the size of μ in (28) ensures that these formal manipulations are justified. The proof of Lemma 1 is complete. □

Note that (27) and (19) imply

(29) $$\operatorname{supp} K_s(x,y) \subset \{(x,y) \in \mathbb{R}^3 \times \mathbb{R}^3 \mid |y-x| < 9c_1(m\rho_{TF}^{-1}(x))^{1/3}\},$$

which justifies calling $K_s(x,y)$ a short-range interaction, if m is not too big.

Note also that

(30) $$\frac{1}{2}K_L(x,x) = c_\#(r(x))^{-1},$$

where $c_{\#}$ is a constant determined by the choice of $\varphi_0(x)$ in (21), (22).

Using $|x-y|^{-1} = K_s(x,y) + K_L(x,y)$, we next decompose the many-body Coulomb potential $-\sum_{k=1}^{N} \frac{Z}{|x_k|} + \sum_{1\le i<j\le N} |x_i - x_j|^{-1}$ into a long-range and a short-range part.

We have

$$
\begin{aligned}
(31)\quad \sum_{i<j} |x_i - x_j|^{-1} &= \sum_{i<j} K_s(x_i,x_j) + \sum_{i<j} K_L(x_i,x_j) \\
&= \sum_{i<j} K_s(x_i,x_j) + \frac{1}{2}\sum_{i,j} K_L(x_i,x_j) - \frac{1}{2}\sum_{i=1}^{N} K_L(x_i,x_i) \\
&= \sum_{i<j} K_s(x_i,x_j) - c_{\#}\sum_{k=1}^{N} (r(x_k))^{-1} + \frac{1}{2}\sum_{i,j} K_L(x_i,x_j) \quad \text{(by (30))} \\
&= \sum_{i<j} K_s(x_i,x_j) - c_{\#}\sum_{k=1}^{N} (r(x_k))^{-1} + \\
&\Bigg[\frac{1}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y)\Big\{\sum_i \delta(x-x_i) - q\rho_{TF}(x)\Big\}\cdot\Big\{\sum_j \delta(y-x_j) - q\rho_{TF}(y)\Big\}dxdy \\
&+ q\sum_i \int\limits_{\mathbb{R}^3} K_L(x_i,y)\rho_{TF}(y)dy \\
&- \frac{q^2}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy\Bigg].
\end{aligned}
$$

Here, of course, $\delta(\,\cdot\,)$ denotes the Dirac delta-function.

Set

$$
\begin{aligned}
(32)\quad &\bar{Y} = \bar{Y}(x_1 \dots x_N) = \\
&= \frac{1}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y)\Big\{\sum_{i=1}^{N} \delta(x-x_i) - q\rho_{TF}(x)\Big\}\Big\{\sum_{j=1}^{N} \delta(y-x_j) - q\rho_{TF}(y)\Big\}dxdy,
\end{aligned}
$$

and note that $\bar{Y} \ge 0$ by (28).

Then we obtain from (31), by subtracting $\sum\limits_k \frac{Z}{|x_k|}$ from both sides, the identity

(33)

$$-\sum_{k=1}^{N} \frac{Z}{|x_k|} + \sum_{1\le i<j\le N} |x_i - x_j|^{-1} = \sum_{i<j} K_s(x_i, x_j) - c_{\#} \sum_{k=1}^{N} (r(x_k))^{-1} + \bar{Y}(x_1 \dots x_N)$$
$$+ \sum_{k=1}^{N} \left(\frac{-Z}{|x_k|} + q \int_{\mathbb{R}^3} K_L(x_k, y) \rho_{TF}(y) dy \right)$$
$$- \frac{q^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y) \rho_{TF}(x) \rho_{TF}(y) dx dy.$$

We rewrite this slightly by noting that

$$V_{TF}(x) = \frac{-Z}{|x|} + q \int_{\mathbb{R}^3} |x-y|^{-1} \rho_{TF}(y) dy$$
$$= \left(\frac{-Z}{|x|} + q \int_{\mathbb{R}^3} K_L(x,y) \rho_{TF}(y) dy \right) + q \int_{\mathbb{R}^3} K_s(x,y) \rho_{TF}(y) dy.$$

Hence, with

(34) $$W_{\text{extra}}(x) = \int_{\mathbb{R}^3} K_s(x,y) \rho_{TF}(y) dy,$$

we have

$$\frac{-Z}{|x|} + q \int_{\mathbb{R}^3} K_L(x,y) \rho_{TF}(y) dy = V_{TF}(x) - q W_{\text{extra}}(x).$$

Substituting this into the right side of (33), we obtain our basic decomposition of the many-body Coulomb potential, namely

(35) $$-\sum_{k=1}^{N} \frac{Z}{|x_k|} + \sum_{i<j} |x_i - x_j|^{-1} =$$
$$\sum_{k=1}^{N} V_{TF}(x_k) - q \sum_{k=1}^{N} W_{\text{extra}}(x_k) - c_{\#} \sum_{k=1}^{N} (r(x_k))^{-1} + \bar{Y}(x_1 \dots x_N)$$
$$- \frac{q^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y) \rho_{TF}(x) \rho_{TF}(y) dx dy + \sum_{i<j} K_s(x_i, x_j).$$

Adding the Laplacian to both sides of (35), and taking expectations, we obtain

(36) $$\langle H\Psi, \Psi \rangle = \left\langle \sum_{k=1}^{N} (-\Delta_{x_k} + V_{TF}(x_k)) \Psi, \Psi \right\rangle$$

$$- q\Big\langle \sum_{k=1}^{N} W_{\text{extra}}(x_k)\Psi, \Psi \Big\rangle - c_{\#}\Big\langle \sum_{k=1}^{N}(r(x_k))^{-1}\Psi, \Psi \Big\rangle$$

$$+ \big\langle \bar{Y}(x_1 \ldots x_N)\Psi, \Psi \big\rangle - \frac{q^2}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy$$

$$+ \Big\langle \sum_{i<j} K_s(x_i, x_j)\Psi, \Psi \Big\rangle$$

for any wave function of norm 1.

We will prove a lower bound for $\langle H\Psi, \Psi\rangle$ whenever Ψ is viable, by looking separately at each of the terms on the right in (36). For the first term we use

$$\Big\langle \sum_{k=1}^{N}(-\Delta_k + V_{TF}(x_k))\Psi, \Psi \Big\rangle \geq q\, \text{sneg}(-\Delta + V_{TF}) \tag{37}$$

To control the second term, we need to understand the potential $W_{\text{extra}}(x)$.

Lemma 2: *We have*

$$0 \leq W_{\text{extra}}(x) < C(r(x))^2\rho_{TF}(x), \quad \textit{and} \tag{38}$$

$$|\nabla W_{\text{extra}}(x)| \leq C\frac{(r(x))^2\rho_{TF}(x)}{|x|}. \tag{39}$$

Proof: Immediately from the definition (34) and the fact (26) that $K_s(x,y) \geq 0$, we see that $W_{\text{extra}}(x) \geq 0$. On the other hand, (26), (27) and (34) show that

$$W_{\text{extra}}(x) \leq \int_{|y-x|<9r(x)} |x-y|^{-1}\rho_{TF}(y)dy. \tag{40}$$

For $|y-x| < 9r(x)$ we have $|y-x| < 9c_1|x|$ by (19). Since c_1 is small, this implies $\rho_{TF}(y) \leq C\rho_{TF}(x)$, and therefore (40) yields

$$W_{\text{extra}}(x) \leq C\rho_{TF}(x) \int_{|y-x|<9r(x)} |x-y|^{-1}dy \leq C'\rho_{TF}(x)(r(x))^2.$$

Thus, we have proved (38).

To prove (39), we note that

$$\nabla_x\Big[\int_{\mathbb{R}^3} |x-y|^{-1}\rho_{TF}(y)dy\Big] = \int_{\mathbb{R}^3} |x-y|^{-1}\nabla_y\rho_{TF}(y)dy$$

and

$$\nabla_x \left[\int_{\mathbb{R}^3} K_L(x,y)\rho_{TF}(y)dy \right] =$$

$$\int_{\mathbb{R}^3} \{(\nabla_x + \nabla_y)K_L(x,y)\}\rho_{TF}(y)dy + \int_{\mathbb{R}^3} K_L(x,y)\nabla_y \rho_{TF}(y)dy,$$

by integration by parts. Subtracting these equations, and comparing the left-hand side with (34) and the definition (23), we get the identity

$$\nabla_x W_{\text{extra}}(x) = \int_{\mathbb{R}^3} K_s(x,y)\nabla_y \rho_{TF}(y)dy - \int_{\mathbb{R}^3} \{(\nabla_x + \nabla_y)K_L(x,y)\}\rho_{TF}(y)dy. \tag{41}$$

We look separately at each of the two terms on the right. As in the proof of (38), we have

$$\left| \int_{\mathbb{R}^3} K_s(x,y)\nabla_y \rho_{TF}(y)dy \right| \le \int_{|x-y|<9r(x)} |x-y|^{-1}|\nabla_y \rho_{TF}(y)|dy, \tag{42}$$

and $|y-x| < 9c_1|x|$ in the region of integration on the right, so that $|\nabla_y \rho_{TF}(y)| \le \frac{C}{|x|}\rho_{TF}(x)$. Hence, (42) yields

$$\left| \int_{\mathbb{R}^3} K_s(x,y)\nabla_y \rho_{TF}(y)dy \right| \le \frac{C}{|x|}\rho_{TF}(x) \int_{|y-x|<9r(x)} |x-y|^{-1}dy \tag{43}$$

$$\le C' \frac{\rho_{TF}(x)(r(x))^2}{|x|}.$$

Let us examine $(\nabla_x + \nabla_y)K_L(x,y)$. Since $(\nabla_x + \nabla_y)[|x-y|^{-1}] = 0$, (25) shows that $(\nabla_x + \nabla_y)K_L(x,y) = 0$ for $|x-y| > 9r(x)$.

On the other hand, suppose $|y-x| \le 9r(x)$. Then, as before, $|y-x| < 9c_1|x|$, so that $|x| \sim |y|$ and $r(x) \sim r(y)$. By definition (22) we have

$$(\nabla_x + \nabla_y)K_L(x,y) = \iint_{\mathbb{R}^3\times\mathbb{R}^3} (\nabla_x + \nabla_y) \left\{ \frac{\varphi_x(x')\varphi_y(y')}{|x'-y'|} \right\} dx'dy'.$$

Equivalently,

(45)

$$(\nabla_x + \nabla_y)K_L(x,y) = \iint_{\mathbb{R}^3\times\mathbb{R}^3} (\nabla_x + \nabla_y + \nabla_{x'} + \nabla_{y'}) \left\{ \frac{\varphi_x(x')\varphi_y(y')}{|x'-y'|} \right\} dx'dy'$$

$$= \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi_x(x')(\nabla_y + \nabla_{y'})\varphi_y(y')}{|x'-y'|} dx'dy'$$

$$+ \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\varphi_y(y')(\nabla_x + \nabla_{x'})\varphi_x(x')}{|x'-y'|} dx'dy'$$

Elementary calculus gives

$$(\nabla_x + \nabla_{x'})\varphi_x(x') = (\nabla_x + \nabla_{x'}) \left\{ (r(x))^{-3} \varphi_0 \left(\frac{x - x'}{r(x)} \right) \right\}$$
$$= (\text{coeff}_1)(r(x))^{-4} (\nabla_x r(x)) \varphi_0 \left(\frac{x - x'}{r(x)} \right)$$
$$+ (\text{coeff}_2)(r(x))^{-4} \left[\left(\frac{x - x'}{r(x)} \right) \cdot (\nabla \varphi)\Big|_{\frac{x-x'}{r(x)}} \right] \nabla_x r(x)$$

for universal constants (coeff_1) and (coeff_2).

Since φ_0 is smooth and supported in the unit ball, and since $|\nabla r(x)| \le C|x|^{-1} r(x)$ (see (20)), we can read off the estimate

$$|(\nabla_x + \nabla_{x'})\varphi_x(x')| \le C(r(x))^{-3} |x|^{-1} \chi_{|x'-x|<r(x)}. \tag{46}$$

Similarly,

$$|(\nabla_y + \nabla_{y'})\varphi_y(y')| \le C(r(y))^{-3} |y|^{-1} \chi_{|y'-y|<r(y)}. \tag{47}$$

Notice that $\nabla_x \varphi_x(x')$ and $\nabla_y \varphi_y(y')$ behave much worse than (46) and (47). We had to be careful to use $(\nabla_x + \nabla_{x'})\varphi_x(x')$ instead of $\nabla_x \varphi_x(x')$. In addition to (46), (47), we have

$$|\varphi_x(x')| \le C(r(x))^{-3} \chi_{|x'-x|<r(x)} \text{ and } |\varphi_y(y')| \le C(r(y))^{-3} \chi_{|y'-y|<r(y)},$$

immediately from (21). Hence,

$$\left| \iint\limits_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\varphi_y(y')(\nabla_x + \nabla_{x'})\varphi_x(x')}{|x' - y'|} dx' dy' \right| \le \tag{48}$$
$$C \iint\limits_{\substack{|x'-x|<r(x) \\ |y'-y|<r(y)}} \frac{(r(y))^{-3} |x|^{-1} (r(x))^{-3}}{|x' - y'|} dx' dy' \le C|x|^{-1} (r(x))^{-1},$$

and similarly

$$\left| \iint\limits_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\varphi_x(x')(\nabla_y + \nabla_{y'})\varphi_y(y')}{|x' - y'|} dx' dy' \right| \le C|y|^{-1} (r(y))^{-1}. \tag{49}$$

Putting (48), (49) into (45) and recalling that $|x| \sim |y|$, $r(x) \sim r(y)$, we conclude that

$$|(\nabla_x + \nabla_y) K_L(x, y)| \le C|x|^{-1} (r(x))^{-1} \text{ for } |y - x| \le 9r(x). \tag{50}$$

We saw that $(\nabla_x + \nabla_y)K_L(x,y) = 0$ for $|y-x| > 9r(x)$, so (50) implies

$$\left|\int_{\mathbb{R}^3} \{(\nabla_x + \nabla_y)K_L(x,y)\}\rho_{TF}(y)dy\right| \le C \int_{|y-x|<9r(x)} |x|^{-1}(r(x))^{-1}\rho_{TF}(y)dy.$$

In the region $|y-x| < 9r(x) < 9c_1|x|$, we have $\rho_{TF}(y) < C\rho_{TF}(x)$, so the integral on the right is dominated by

$$C|x|^{-1}(r(x))^{-1}\rho_{TF}(x)\mathrm{Vol}\{y \in \mathbb{R}^3 \mid |y-x| < 9r(x)\} = C'\frac{(r(x))^2\rho_{TF}(x)}{|x|}.$$

So we know that

$$\left|\int_{\mathbb{R}^3} \{(\nabla_x + \nabla_y)K_L(x,y)\}\rho_{TF}(y)dy\right| \le C'\frac{(r(x))^2\rho_{TF}(x)}{|x|}.$$

Putting this and (43) into (41), we get $|\nabla W_{\text{extra}}(x)| \le C\frac{(r(x))^2\rho_{TF}(x)}{|x|}$, which is the remaining conclusion (39) of Lemma 2. □

Now we are ready to control $\left\langle \sum_{k=1}^{N} W_{\text{extra}}(x_k)\Psi, \Psi\right\rangle$, by using Lemma 2 above, and Lemma 5 from the previous section. Let $\chi_{\text{extra}}(x)$ be a cutoff function on $\mathbb{R}^3$, with $0 \le \chi_{\text{extra}} \le 1$ everywhere, $\chi_{\text{extra}}(x) = 1$ for $|x| < Z^{-5/16}$, $\chi_{\text{extra}}(x) = 0$ for $|x| > 2Z^{-5/16}$, $|\nabla\chi_{\text{extra}}(x)| \le C|x|^{-1}$. Then define $\widetilde{W}(x) = m^{-2/3}Z^{5/8}W_{\text{extra}}(x)\cdot\chi_{\text{extra}}(x)$.

Using Lemma 2 above, we will check that $\widetilde{W}(x)$ satisfies the hypotheses imposed on the potential W in Lemma 5 of the preceding section. In fact, since $r(x) < (m\rho_{TF}^{-1}(x))^{1/3}$ by (19), Lemma 2 implies

$$|W_{\text{extra}}(x)| \le C(m\rho_{TF}^{-1}(x))^{2/3}\rho_{TF}(x) = Cm^{2/3}\rho_{TF}^{1/3}(x) = C'm^{2/3}|V_{TF}(x)|^{1/2} \tag{51}$$

and

$$|\nabla W_{\text{extra}}(x)| \le \frac{C}{|x|}(m\rho_{TF}^{-1}(x))^{2/3}\rho_{TF}(x) = \frac{C}{|x|}m^{2/3}\rho_{TF}^{1/3}(x) = \frac{C'm^{2/3}}{|x|}|V_{TF}(x)|^{1/2}.$$

For $|x| < 2Z^{-5/16}$ we have

$$|V_{TF}(x)| > c(Z^{-5/16})^{-4} = cZ^{5/4},$$

so that

$$|V_{TF}(x)|^{1/2} \le CZ^{-5/8}|V_{TF}(x)|.$$

Therefore,

$$|W_{\text{extra}}(x)| \le C''m^{2/3}Z^{-5/8}|V_{TF}(x)|$$

and

$$|\nabla W_{\text{extra}}(x)| \leq \frac{C'' m^{2/3} Z^{-5/8}}{|x|} |V_{TF}(x)|,$$

in $\operatorname{supp} \chi_{\text{extra}}$. Hence,

$$|\chi_{\text{extra}} W_{\text{extra}}(x)| \leq C''' m^{2/3} Z^{-5/8} |V_{TF}(x)|$$

and

$$|\nabla (\chi_{\text{extra}} W_{\text{extra}})(x)| \leq C''' m^{2/3} Z^{-5/8} \frac{|V_{TF}(x)|}{|x|}$$

everywhere. That means

$$|\widetilde{W}(x)| \leq C |V_{TF}(x)| \quad \text{and} \quad |\nabla \widetilde{W}(x)| \leq C \frac{|V_{TF}(x)|}{|x|},$$

which is equivalent to the hypotheses on $W(x)$ in Lemma 5 of the preceding section. (See equation (5) in the preceding section.) Applying that Lemma with $\eta = Z^{-1/6}$, we obtain for viable wave functions Ψ the equation

$$\left\langle \sum_{k=1}^{N} \widetilde{W}(x_k) \Psi, \Psi \right\rangle = q \int_{\mathbb{R}^3} \widetilde{W}(x) \rho_{TF}(x) dx + O(Z^{-\frac{1}{12}} \cdot Z^{7/3}),$$

which means that

$$\left\langle \sum_{k=1}^{N} \chi_{\text{extra}}(x_k) W_{\text{extra}}(x_k) \Psi, \Psi \right\rangle = q \int_{\mathbb{R}^3} \chi_{\text{extra}}(x) W_{\text{extra}}(x) \rho_{TF}(x) dx$$
$$+ O(m^{2/3} Z^{-\frac{5}{8}} Z^{-\frac{1}{12}} Z^{7/3}), \quad \text{i.e.}$$

(52) $$\left\langle \sum_{k=1}^{N} \chi_{\text{extra}}(x_k) W_{\text{extra}}(x_k) \Psi, \Psi \right\rangle =$$
$$q \int_{\mathbb{R}^3} \chi_{\text{extra}}(x) W_{\text{extra}}(x) \rho_{TF}(x) dx + O(m^{2/3} Z^{-\frac{1}{24}} Z^{5/3}).$$

On the other hand, in $\operatorname{supp}(1 - \chi_{\text{extra}})$ we have $|x| \geq Z^{-5/16}$, so

$$|W_{\text{extra}}(x)| \leq C m^{2/3} |V_{TF}(x)|^{1/2} \text{ (by (51)) } \leq C m^{2/3} [(Z^{-5/16})^{-4}]^{1/2} = C m^{2/3} Z^{\frac{5}{8}}.$$

Thus,

(53) $$|(1 - \chi_{\text{extra}}(x)) W_{\text{extra}}(x)| \leq C m^{2/3} Z^{5/8}$$

for all x, which trivially implies

$$\left|\sum_{k=1}^{N}(1-\chi_{\text{extra}}(x_k))W_{\text{extra}}(x_k)\right| \le Cm^{2/3}Z^{5/8}N \le C'm^{2/3}Z^{5/8}\cdot Z$$
$$= C'm^{2/3}Z^{-1/24}Z^{5/3},$$

and in turn

$$\left\langle\sum_{k=1}^{N}(1-\chi_{\text{extra}}(x_k))W_{\text{extra}}(x_k)\Psi,\Psi\right\rangle = O(m^{2/3}Z^{-1/24}Z^{5/3}).$$

Combining this with (52), we get

$$\left\langle\sum_{k=1}^{N}W_{\text{extra}}(x_k)\Psi,\Psi\right\rangle = q\int_{\mathbb{R}^3}\chi_{\text{extra}}(x)W_{\text{extra}}(x)\rho_{TF}(x)dx+ O(m^{2/3}Z^{-1/24}Z^{5/3}). \tag{54}$$

Again using (53), we note that

$$\left|\int_{\mathbb{R}^3}(1-\chi_{\text{extra}}(x))W_{\text{extra}}(x)\rho_{TF}(x)dx\right| \le Cm^{2/3}Z^{5/8}\int_{\mathbb{R}^3}\rho_{TF}(x)dx$$
$$= C'm^{2/3}Z^{5/8}\cdot Z = C'm^{2/3}Z^{-1/24}\cdot Z^{5/3}.$$

Therefore, (54) can be rewritten as

$$\left\langle\sum_{k=1}^{N}W_{\text{extra}}(x_k)\Psi,\Psi\right\rangle = q\int_{\mathbb{R}^3}W_{\text{extra}}(x)\rho_{TF}(x)dx + O(m^{2/3}Z^{-1/24}\cdot Z^{5/3}).$$

Recalling the definition (34) of $W_{\text{extra}}(x)$, we obtain

$$-q\left\langle\sum_{k=1}^{N}W_{\text{extra}}(x_k)\Psi,\Psi\right\rangle = -q^2\iint_{\mathbb{R}^3\times\mathbb{R}^3}K_s(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy + O(m^{2/3}Z^{-1/24}\cdot Z^{5/3}) \tag{55}$$

for viable wave functions. Equation (55) controls the second term on the right in (36).

The third term on the right in (36) is analogous to the second term, only easier. We use the same cutoff function $\chi_{\text{extra}}(x)$ as above, and check that $\widetilde{W}(x) = Z^{5/8}\chi_{\text{extra}}(x)(r(x))^{-1}$ satisfies the hypotheses imposed on the potential $W(x)$ in Lemma 5 of the previous section. In fact, (19) gives

$$(r(x))^{-1} \le C|x|^{-1} + Cm^{-1/3}\rho_{TF}^{1/3}(x) \quad \text{for all } x. \tag{56}$$

In support of $\chi_{\text{extra}}(x)$ we have $|x| \le 2Z^{-5/16}$, so that $|V_{TF}(x)| \ge c(Z^{-5/16})^{-4} = cZ^{+5/4}$, and consequently

$$m^{-1/3}\rho_{TF}^{1/3}(x) \le \rho_{TF}^{1/3} = c|V_{TF}(x)|^{1/2} \le CZ^{-5/8}|V_{TF}(x)| \tag{57}$$

in $\operatorname{supp}\chi_{\text{extra}}$. If $|x| \le Z^{-1/3}$, then

$$|x|^{-1} = Z^{-1}\cdot(Z|x|^{-1}) \le CZ^{-1}|V_{TF}(x)|.$$

If $Z^{-1/3} \le |x| \le 2Z^{-5/16}$, then

$$|x|^{-1} = |x|^{+3}|x|^{-4} \le C|x|^{+3}|V_{TF}(x)| \le C'Z^{-15/16}|V_{TF}(x)|.$$

Hence,

$$|x|^{-1} \le CZ^{-15/16}|V_{TF}(x)| \quad \text{for all } x \in \operatorname{supp}\chi_{\text{extra}}. \tag{58}$$

Estimates (56), (57), (58) together show that

$$(r(x))^{-1} \le CZ^{-5/8}|V_{TF}(x)| \quad \text{in } \operatorname{supp}\chi_{\text{extra}}. \tag{59}$$

Then, from (20) we get $|\nabla\{(r(x))^{-1}\}| \le \frac{C(r(x))^{-1}}{|x|}$, so (59) implies

$$|\nabla\{(r(x))^{-1}\}| \le CZ^{-5/8}|V_{TF}(x)||x|^{-1} \quad \text{in } \operatorname{supp}\chi_{\text{extra}}. \tag{60}$$

Estimates (59) and (60) show that $\widetilde{W}(x) = Z^{5/8}\chi_{\text{extra}}(x)(r(x))^{-1}$ satisfies

$$|\widetilde{W}(x)| \le C|V_{TF}(x)| \text{ and } |\nabla\widetilde{W}(x)| \le \frac{C}{|x|}|V_{TF}(x)|,$$

as required in the hypotheses of Lemma 5 of the preceding section. Applying that lemma with $\eta = Z^{-1/6}$, we obtain for viable wave functions the equation

$$\left\langle \sum_{k=1}^{N} Z^{5/8}\chi_{\text{extra}}(x_k)(r(x_k))^{-1}\Psi, \Psi \right\rangle = q\int_{\mathbb{R}^3} Z^{5/8}\chi_{\text{extra}}(x)(r(x))^{-1}\rho_{TF}(x)dx + O(Z^{-1/12}\cdot Z^{7/3}), \quad \text{i.e.}$$

$$\left\langle \sum_{k=1}^{N} \chi_{\text{extra}}(x_k)(r(x_k))^{-1}\Psi, \Psi \right\rangle = q\int_{\mathbb{R}^3} \chi_{\text{extra}}(x)(r(x))^{-1}\rho_{TF}(x)dx + O(Z^{-1/24}Z^{5/3}) \tag{61}$$

On the other hand, in $\operatorname{supp}(1-\chi_{\text{extra}})$, we have $|x| \geq Z^{-5/16}$, so that (56) implies

$$(r(x))^{-1} \leq C|x|^{-1} + C\rho_{TF}^{1/3}(x) \leq C|x|^{-1} + C'|x|^{-2} \leq C'' Z^{+5/8}.$$

Thus, $|(1-\chi_{\text{extra}}(x_k))(r(x_k))^{-1}| \leq C'' Z^{5/8}$, so that trivially,

$$(62) \qquad \left\langle \sum_{k=1}^{N} (1-\chi_{\text{extra}}(x_k))(r(x_k))^{-1}\Psi, \Psi \right\rangle = O(Z^{5/8}N) = O(Z^{+5/8}Z) = O(Z^{-1/24}Z^{5/3}).$$

Adding (61) and (62), we get

$$(63) \qquad \left\langle \sum_{k=1}^{N} (r(x_k))^{-1}\Psi, \Psi \right\rangle = q \int_{\mathbb{R}^3} \chi_{\text{extra}}(x)(r(x))^{-1}\rho_{TF}(x)dx + O(Z^{-1/24}Z^{5/3}).$$

Let us estimate the integral on the right. From (56) we have

$$\left| \int_{\mathbb{R}^3} \chi_{\text{extra}}(x)(r(x))^{-1}\rho_{TF}(x)dx \right| \leq \int_{\mathbb{R}^3} (r(x))^{-1}\rho_{TF}(x)dx \leq$$

$$C \int_{\mathbb{R}^3} |x|^{-1}\rho_{TF}(x)dx + Cm^{-1/3} \int_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx$$

$$\leq C' \int_{|x|<Z^{-1/3}} |x|^{-1}(Z^{3/2}|x|^{-3/2})dx + C' \int_{|x|>Z^{-1/3}} |x|^{-1}(|x|^{-6})dx + C'm^{-1/3}Z^{5/3}$$

$$= C_1''(Z^{-1/3})^{1/2}Z^{3/2} + C_2''(Z^{-1/3})^{-4} + C'm^{-1/3}Z^{5/3}$$

$$\leq CZ^{4/3} + C'm^{-1/3}Z^{5/3}.$$

Substituting this into (63), we see that

$$(64) \qquad -c_{\#}\left\langle \sum_{k=1}^{N} (r(x_k))^{-1}\Psi, \Psi \right\rangle = O(Z^{-\frac{1}{24}} \cdot Z^{5/3} + m^{-1/3} \cdot Z^{5/3})$$

for viable wave functions. Equation (64) controls the third term on the right in (36).

We leave the fourth and fifth terms in (36) alone, and turn our attention to the final term. It involves the short-range interaction $K_s(x,y)$, and we will control it by invoking Lemma 7 from the previous section, with $\eta = Z^{-1/6}$. In addition to m, that Lemma involves parameters D, δ which are assumed to satisfy

(65) $CZ^{-2/3} < D < cZ^{-1/3}$

(66) $m > C$

(67) $0 < \delta < cm^{-42/5}$

(68) $m^{63}D^{-3} < cZ^2$.

As in Lemma 7 of the previous section, let

$$A_m = \{x \in \mathbb{R}^3 \mid 20D < |x| < cm^{-21/2}D^{1/2}\}. \tag{69}$$

Then set $K(x,y) = \chi_{A_m}(x)\chi_{A_m}(y)K_s(x,y)$. We will check that $K(x,y)$ satisfies the hypotheses of Lemma 7 in the previous section. We need to check that

(70) $0 \le K(x,y) = K(y,x) \le |x-y|^{-1}$

(71) $\operatorname{supp} K(x,y) \subset A_m \times A_m$

(72) $\operatorname{supp} K(x,y) \subset \{\rho_{TF}(x) \cdot |x-y|^3 < cm\}$

Property (70) follows from (26), and property (71) is immediate from the definition of $K(x,y)$. To check property (72), we use (27) and (19) to see that any $(x,y) \in \operatorname{supp} K$ satisfies $\rho_{TF}(x) \cdot |x-y|^3 \le \rho_{TF}(x) \cdot (9r(x))^3 \le \rho_{TF}(x) \cdot (9c_1[m\rho_{TF}^{-1}(x)]^{1/3})^3 = (9c_1)^3 m$. Hence (72) holds if we pick c_1 small enough in (19).

Therefore, if (65)...(68) hold and Ψ is viable, then D, δ, m, $K(x,y)$ and Ψ satisfy all the hypotheses of Lemma 7 in the preceding section, with $\eta = Z^{-1/6}$. That Lemma tells us the following conclusion:

$$\left\langle \sum_{i<j} K(x_i,x_j)\Psi, \Psi \right\rangle \ge \frac{1}{2} \iint\limits_{\mathbb{R}^3 \times \mathbb{R}^3} K(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy - \text{Junk}, \tag{73}$$

where

$$\text{Junk} = Cm^{2/3}\left[\frac{m^{1/3}Z}{D} + \delta^{\frac{1}{63}}Z^{5/3} + (Z^2D^3)^{-\frac{2}{15\cdot 63}}Z^{5/3} + \beta^{5/7}Z^{5/3} + DZ^2\ell n Z\right] \tag{74}$$

with

$$\beta = \delta^{-1}[Z^{-1/12} + Z^{1/6}D^{1/2} + Z^{-2/3}D^{-1}]. \tag{75}$$

By definition of K we have trivially

$$\left\langle \sum_{i<j} K_s(x_i,x_j)\Psi, \Psi \right\rangle \ge \left\langle \sum_{i<j} K(x_i,x_j)\Psi, \Psi \right\rangle. \tag{76}$$

Also, by (70) and by equation (91) in the section on *Removing Periodic Boundary Conditions*, we have

$$(77) \qquad \frac{1}{2} \iint\limits_{\mathbb{R}^3 \times \mathbb{R}^3} K(x,y) q |\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2 dxdy \leq \frac{q}{2} \iint\limits_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2}{|x-y|} dxdy$$

$$= q \int\limits_{\mathbb{R}^3} \left[\frac{1}{2} \int\limits_{\mathbb{R}^3} \frac{|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2}{|x-y|} dy \right] dx = q c_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x) dx.$$

Putting (76) and (77) into (73), we learn that

$$\left\langle \sum_{i<j} K_s(x_i,x_j)\Psi, \Psi \right\rangle \geq$$

$$\frac{q^2}{2} \iint\limits_{\mathbb{R}^3 \times \mathbb{R}^3} K(x,y) \rho_{TF}(x) \rho_{TF}(y) dxdy - q c_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x) dx - \text{Junk},$$

with Junk given by (74), (75). That is,

$$(78) \qquad \left\langle \sum_{i<j} K_s(x_i,x_j)\Psi, \Psi \right\rangle \geq$$

$$\frac{q^2}{2} \iint\limits_{A_m \times A_m} K_s(x,y) \rho_{TF}(x) \rho_{TF}(y) dxdy - q c_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x) dx - \text{Junk}.$$

We want to replace $A_m \times A_m$ by $\mathbb{R}^3 \times \mathbb{R}^3$ on the right in (78). To do so, note that

$$\iint\limits_{\mathbb{R}^3 \setminus (A_m \times A_m)} K_s(x,y) \rho_{TF}(x) \rho_{TF}(y) dxdy \leq$$

$$\int\limits_{x \in \mathbb{R}^3 \setminus A_m} \left[\int\limits_{y \in \mathbb{R}^3} K_s(x,y) \rho_{TF}(y) dy \right] \rho_{TF}(x) dx +$$

$$\int\limits_{y \in \mathbb{R}^3 \setminus A_m} \left[\int\limits_{x \in \mathbb{R}^3} K_s(x,y) \rho_{TF}(x) dx \right] \rho_{TF}(y) dy.$$

The two terms on the right are obviously equal and the first expression in square brackets is equal to $W_{\text{extra}}(x)$. (See (34).) Therefore,

(79)

$$\iint\limits_{(\mathbb{R}^3\times\mathbb{R}^3)\smallsetminus(A_m\times A_m)} K_s(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy$$

$$\leq 2\int\limits_{\mathbb{R}^3\smallsetminus A_m} W_{\text{extra}}(x)\rho_{TF}(x)dx \leq C\int\limits_{\mathbb{R}^3\smallsetminus A_m}(r(x))^2(\rho_{TF}(x))^2dx$$

(by (38))

$$\leq Cm^{2/3}\int\limits_{\mathbb{R}^3\smallsetminus A_m}\rho_{TF}^{4/3}(x)dx \quad \text{(by (19))}.$$

Recalling the definition (69) of A_m, and noting that $20D < Z^{-1/3} < cm^{-21/2}D^{1/2}$ by (65) and (68), we can rewrite (79) in the form

$$\iint\limits_{(\mathbb{R}^3\times\mathbb{R}^3)\smallsetminus(A_m\times A_m)} K_s(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy$$

$$\leq Cm^{2/3}\int\limits_{|x|<20D}\frac{Z^2}{|x|^2}dx + Cm^{2/3}\int\limits_{|x|>cm^{-21/2}D^{1/2}}|x|^{-8}dx$$

$$= C'm^{2/3}Z^2D + C'm^{2/3}\cdot m^{+\frac{105}{2}}D^{-5/2}.$$

Combining this with (78), we see that

$$\text{(80)} \qquad \left\langle \sum_{i<j} K_s(x_i,x_j)\Psi,\Psi\right\rangle \geq$$

$$\frac{q^2}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_s(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy - qc_D\int\limits_{\mathbb{R}^3}\rho_{TF}^{4/3}(x)dx - \text{Junk}_*$$

for viable wave functions, with

$$\text{Junk}_* = \text{Junk} + C'm^{2/3}(Z^2D + m^{\frac{105}{2}}D^{-5/2}).$$

That is,

$$\text{(81)} \qquad \text{Junk}_* = Cm^{2/3}\left[\frac{m^{1/3}Z}{D} + \delta^{1/63}Z^{5/3} + (Z^2D^3)^{-\frac{2}{15\cdot 63}}Z^{5/3} + \beta^{5/7}Z^{5/3} + DZ^2\ell nZ + m^{\frac{105}{2}}D^{-5/2}\right]$$

with

$$\text{(82)} \qquad \beta = \delta^{-1}[Z^{-1/12} + Z^{1/6}D^{1/2} + Z^{-2/3}D^{-1}].$$

Estimates (80)...(82) control the final term in (36).

Now we combine our estimates for the various terms in (36). Substituting (37), (55), (64) and (80) into the right-hand side of (36), we obtain for viable wave functions the estimate

$$
\begin{aligned}
&< H\Psi, \Psi > \geq \\
&\quad [q\,\mathrm{sneg}(-\Delta + V_{TF})] + \Bigg[-q^2 \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_s(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy - Cm^{2/3}Z^{-\frac{1}{24}}Z^{5/3}\Bigg] \\
&\qquad + [-CZ^{-\frac{1}{24}}Z^{5/3} - Cm^{-1/3}Z^{5/3}] + \langle \bar{Y}(x_1 \ldots x_N)\Psi, \Psi\rangle \\
&\qquad - \frac{q^2}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy \\
&\qquad + \Bigg[\frac{q^2}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_s(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy - qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx - \mathrm{Junk}_*\Bigg].
\end{aligned}
$$

Since $K_s(x,y) + K_L(x,y) = |x-y|^{-1}$, the above estimate is equivalent to

(83)

$$
\begin{aligned}
\langle H\Psi, \Psi\rangle \geq &\left\{q\,\mathrm{sneg}(-\Delta + V_{TF}) - \frac{q^2}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|} - qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx\right\} \\
&+ \langle \bar{Y}(x_1 \ldots x_N)\Psi, \Psi\rangle - \mathrm{ERROR}
\end{aligned}
$$

with

$$\mathrm{ERROR} = Cm^{2/3}Z^{-\frac{1}{24}}Z^{5/3} + Cm^{-1/3}Z^{5/3} + \mathrm{Junk}_*.$$

In view of (81), (82), we have

(84) ERROR =

$$
\begin{aligned}
&Cm^{-1/3}Z^{5/3} + Cm^{2/3}\Bigg[Z^{-1/24}Z^{5/3} + \frac{m^{1/3}Z}{D} + \delta^{1/63}Z^{5/3} + (Z^2D^3)^{-\frac{2}{15\cdot 63}}Z^{5/3} \\
&\qquad\qquad + \beta^{5/7}Z^{5/3} + DZ^2\ell n Z + m^{\frac{105}{2}}D^{-5/2}\Bigg]
\end{aligned}
$$

with

(85) $$\beta = \delta^{-1}[Z^{-1/12} + Z^{1/6}D^{1/2} + Z^{-2/3}D^{-1}].$$

In (83), (84), (85) we may use any D, δ m that satisfy the constraints (65)...(68). Let us now pick D, δ, m. We arbitrarily pick $D = Z^{-1/2}$ so that (85) becomes

$$\beta \sim \delta^{-1}Z^{-1/12}.$$

Next we pick δ so that $\delta^{\frac{1}{63}} Z^{5/3} \sim \beta^{5/7} Z^{5/3}$, i.e.

$$\delta^{\frac{1}{63}} \sim \delta^{-\frac{5}{7}} Z^{-\frac{5}{7\cdot 12}}, \quad \text{i.e.} \quad \delta \sim Z^{-\frac{5\cdot 63}{12\cdot(7+5\cdot 63)}}.$$

With that δ we have

$$\beta^{5/7} Z^{5/3} \sim \delta^{\frac{1}{63}} Z^{5/3} \sim Z^{-\frac{5}{12\cdot(7+5\cdot 63)}} Z^{5/3}.$$

Hence, (84) becomes

$$\begin{aligned} \text{ERROR} = {} & Cm^{-1/3} Z^{5/3} + CmZ^{3/2} + Cm^{\frac{2}{3}+\frac{105}{2}} Z^{\frac{5}{4}} \\ & + Cm^{2/3} \Big[Z^{-\frac{1}{24}} Z^{5/3} + Z^{\frac{-5}{12\cdot(7+5\cdot 63)}} Z^{\frac{5}{3}} + Z^{-\frac{1}{15\cdot 63}} Z^{5/3} \\ & \qquad + Z^{\frac{3}{2}} \ell n Z \Big] \end{aligned}$$

or, equivalently,

$$\text{ERROR} \sim Cm^{-1/3} Z^{5/3} + CmZ^{3/2} + Cm^{\frac{2}{3}+\frac{105}{2}} Z^{\frac{5}{4}} + Cm^{2/3} \left[Z^{-\frac{1}{15\cdot 63}} Z^{5/3} \right] \tag{86}$$

From (86) we see that we ought to take $m = Z^{\frac{1}{15\cdot 63}}$, so that

$$\text{ERROR} \sim CZ^{-\frac{1}{3\cdot 15\cdot 63}} \cdot Z^{5/3} = CZ^{-\frac{1}{2835}} \cdot Z^{5/3}. \tag{87}$$

Note that our m, D, δ, namely

$$m = Z^{\frac{1}{15\cdot 63}},\ D = Z^{-\frac{1}{2}},\ \delta = Z^{-\frac{5\cdot 63}{12\cdot(7+5\cdot 63)}},$$

satisfy constraints (65)...(68). Therefore, estimate (83) holds for viable wave functions, with ERROR given by (87). That is,

$$\begin{aligned} (88) \quad & < H\Psi, \Psi > \geq \\ & q\,\text{sneg}(-\Delta + V_{TF}) - \frac{q^2}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|} - qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx \\ & \qquad + < \bar{Y}(x_1 \ldots x_N)\Psi, \Psi > - CZ^{-\frac{1}{2835}} Z^{5/3}, \quad \text{for viable } \Psi. \end{aligned}$$

Since $\bar{Y}(x_1 \ldots x_N) \geq 0$, we may drop the term $\langle \bar{Y}(x_1 \ldots x_N)\Psi, \Psi \rangle$ from the right-hand side of (88). Then taking the infimum over all viable Ψ in (88), and recalling (18), we see that

$$\begin{aligned} E(Z,q) \geq q\,\text{sneg}(-\Delta + V_{TF}) - \frac{q^2}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|} - qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx \\ - CZ^{-\frac{1}{2835}} Z^{5/3}. \end{aligned}$$

This equation and (16), (17) show that

(89)

$$E(Z,q) = q\,\mathrm{sneg}(-\Delta + V_{TF}) - \frac{q^2}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|} - qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx + O(Z^{5/3-\gamma_2})$$

with

(90)
$$\gamma_2 = \frac{1}{2835}.$$

Putting (89) and (90) into (88), we get

(91)
$$\langle H\Psi, \Psi\rangle \geq E(Z,q) + \langle \bar{Y}(x_1 \dots x_N)\Psi, \Psi\rangle - CZ^{5/3-\gamma_2} \quad \text{for viable } \Psi.$$

We shall return later to (91). Now, however, we substitute the WKB Theorem (B) into (89), to derive the formula for $E(Z,q)$. The result is

(92)

$$\begin{aligned} E(Z,q) = &-\frac{q}{15\pi^2} \int\limits_{\mathbb{R}^3} |V_{TF}(x)|^{5/2}dx + \frac{qZ^2}{8} + \frac{q}{48\pi^2} \int\limits_{\mathbb{R}^3} |V_{TF}(x)|^{1/2} \Delta V_{TF}(x)dx \\ &- \frac{q^2}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|} - qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx \\ &+ O(Z^{5/3-\gamma_2}). \end{aligned}$$

In view of equation (38 bis) from the section *Applications to Atoms*, we can rewrite (92) in the form

(93)
$$\begin{aligned} E(Z,q) = E_{TF}(Z,q) + \frac{qZ^2}{8} + \frac{q}{48\pi^2} \int\limits_{\mathbb{R}^3} |V_{TF}(x)|^{1/2} \Delta V_{TF}(x)dx \\ - qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx + O(Z^{5/3-\gamma_2}). \end{aligned}$$

Here we recognize the Scott, Schwinger and Dirac corrections to the Thomas-Fermi energy. We rewrite (93) by using the Thomas-Fermi equations,

$$-\Delta V_{TF} = 4\pi q \rho_{TF} \quad \text{and} \quad \frac{1}{6\pi^2}|V_{TF}|^{3/2} = \rho_{TF}.$$

These equations imply $|V_{TF}|^{1/2}\Delta V_{TF} = -4\pi q\cdot(6\pi^2)^{1/3}\rho_{TF}^{4/3}$, and hence

$$\frac{q}{48\pi^2}\int\limits_{\mathbb{R}^3}|V_{TF}|^{1/2}\Delta V_{TF}dx = -\frac{q^2}{2^{5/3}3^{2/3}\pi^{1/3}}\int\limits_{\mathbb{R}^3}\rho_{TF}^{4/3}dx.$$

On the other hand, one computes from the definition of c_D the formula $c_D = \frac{3^{4/3}}{2^{5/3}\pi^{1/3}}$, so that

$$qc_D\int\limits_{\mathbb{R}^3}\rho_{TF}^{4/3}dx = \frac{3^{4/3}q}{2^{5/3}\pi^{1/3}}\int\limits_{\mathbb{R}^3}\rho_{TF}^{4/3}dx.$$

Thus,

$$\frac{q}{48\pi^2}\int\limits_{\mathbb{R}^3}|V_{TF}|^{1/2}\Delta V_{TF}dx = -\frac{q}{9}\cdot qc_D\int\limits_{\mathbb{R}^3}\rho_{TF}^{4/3}dx,$$

so that (93) may be rewritten as

$$E(Z,q) = E_{TF}(Z,q) + \frac{qZ^2}{8} - \left(1+\frac{1}{9}q\right)\cdot qc_D\int\limits_{\mathbb{R}^3}\rho_{TF}^{4/3}dx + O(Z^{5/3-\gamma_2}). \tag{94}$$

Finally, for the reader's convenience, we recall how $E_{TF}(Z,q)$ and $\int_{\mathbb{R}^3}\rho_{TF}^{4/3}dx$ scale as functions of Z and q, and we rewrite (94) accordingly.

Let $V_1(x)$ and $\rho_1(x)$ solve the Thomas-Fermi equations

$$V_1(x) = -\frac{1}{|x|} + \int\limits_{\mathbb{R}^3}\frac{\rho_1(y)dy}{|x-y|} < 0 \tag{95}$$

$$\rho_1(x) = \frac{1}{6\pi^2}|V_1(x)|^{3/2} \tag{96}$$

on $\mathbb{R}^3$. These are universal functions, independent of Z and q. Then for each Z, q the solution to our usual Thomas-Fermi equations is given by

$$V_{TF}(x) = q^{2/3}Z^{4/3}V_1(q^{2/3}Z^{1/3}x)$$

and

$$\rho_{TF}(x) = qZ^2\rho_1(q^{2/3}Z^{1/3}x).$$

(Recall that in our notation, ρ_{TF} is the density of electrons *of a fixed spin.*) Consequently, $E_{TF}(Z,q) = -c_0q^{2/3}Z^{7/3}$, with

$$-c_0 = c_{TF}\int\limits_{\mathbb{R}^3}\rho_1^{5/3}dx - \int\limits_{\mathbb{R}^3}\frac{1}{|x|}\rho_1(x)dx + \frac{1}{2}\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\rho_1(x)\rho_1(y)}{|x-y|}dxdy,$$

and

$$qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3} dx = c_1 q^{1/3} Z^{5/3},$$

with

$$c_1 = c_D \int\limits_{\mathbb{R}^3} \rho_1^{4/3} dx.$$

Putting these formulas into (94), we obtain the following result.

Main Theorem: *Let $c_{TF} = \frac{(6\pi^2)}{10\pi^2}^{5/3}$ and $c_D = \left(\frac{81}{32\pi}\right)^{1/3}$. Let $V_1(x) < 0$ and $\rho_1(x) > 0$ be radial functions on $\mathbb{R}^3$, solving*

$$V_1(x) = -|x|^{-1} + \int\limits_{\mathbb{R}^3} \rho_1(y)|x-y|^{-1} dy \quad \text{and} \quad \rho_1(y) = \frac{1}{6\pi^2}|V_1(y)|^{3/2}.$$

Define c_0 and c_1 by

$$-c_0 = c_{TF} \int\limits_{\mathbb{R}^3} \rho_1^{5/3}(x)dx - \int\limits_{\mathbb{R}^3} |x|^{-1}\rho_1(x)dx + \frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_1(x)\rho_1(y)dxdy}{|x-y|}$$

and

$$c_1 = c_D \int\limits_{\mathbb{R}^3} \rho_1^{4/3}(x)dx.$$

Then the ground-state energy $E(Z,q)$ for atomic number Z and q spins is given by

$$E(Z,q) = -c_0 q^{2/3} Z^{7/3} + q\frac{Z^2}{8} - \left(1 + \frac{1}{9}q\right) q^{1/3} c_1 Z^{5/3} + ERROR(Z,q)$$

with $|ERROR(Z,q)| \leq C_q Z^{\frac{5}{3}-\frac{1}{2835}}$. The constant C_q depends only on q.

Additional Results

We keep the notation of the preceding section. Our goal is to understand the behavior of wave functions Ψ having energy very near the ground-state energy. More precisely, we assume

$$\langle H\Psi, \Psi\rangle \le E(Z,q) + \eta Z^{5/3} \quad \text{with} \quad 0 < \eta < C, \quad \text{and} \quad N \le CZ. \tag{1}$$

(This is of course much stronger than our previous assumption that Ψ is viable.)

We will see that (1) forces the electrons to distribute themselves in $\mathbb{R}^3$ with a charge density close to $q\rho_{TF}$. Also, we will study the number $\mathcal{N}_{(x_0 r_0)}$ of electrons in a ball $B(x_0, r_0) \subset \mathbb{R}^3$. We suppose $|x_0| \sim Z^{-1/3}$ and $r_0 \sim Z^{-2/3}$, so that $B(x_0, r_0)$ may be expected to contain ~ 1 electron. We will calculate the mean and variance of $\mathcal{N}_{(x_0 r_0)}$ modulo a small error.

Let us begin by recalling estimate (91) from the preceding section, which together with (1) above yields

$$\langle \bar{Y}(x_1 \dots x_N)\Psi, \Psi\rangle \le C(\eta + Z^{-\gamma_2})Z^{5/3}. \tag{2}$$

Recalling also the definition of $\bar{Y}(x_1 \dots x_N)$ and $K_L(x,y)$, we have for fixed $x_1 \dots x_N \in \mathbb{R}^3$ the formulas:

$$\bar{Y}(x_1 \dots x_N) = \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y)\,d\mu(x)\,d\mu(y) \quad \text{with}$$

$$d\mu(x) = \sum_{k=1}^{N} \delta(x - x_k)\,dx - q\rho_{TF}(x)\,dx; \quad \text{and}$$

$$\frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y)\,d\mu(x)\,d\mu(y) = \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{f(x)f(y)\,dx\,dy}{|x-y|}$$

with

$$f(x') = \int_{\mathbb{R}^3} \varphi_x(x')\,d\mu(x).$$

Hence,

$$\bar{Y}(x_1 \dots x_N) = \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{f(x)f(y)\,dx\,dy}{|x-y|} \tag{2 bis}$$

with

$$f(x') = \sum_{k=1}^{N} \varphi_{x_k}(x') - q \int_{\mathbb{R}^3} \varphi_x(x')\rho_{TF}(x)\,dx. \tag{3}$$

We would like to replace the integral in (3) by $\rho_{TF}(x')$. So we define

$$g(x') = -\rho_{TF}(x') + \int_{\mathbb{R}^3} \varphi_x(x')\rho_{TF}(x)dx$$

and estimate g. Recall that $\varphi_x(x') = (r(x))^{-3}\varphi_0\left(\frac{x-x'}{r(x)}\right)$, with φ_0 radial, smooth, and supported in the unit ball. Hence

$$g(x') = -\rho_{TF}(x') + \int_{\mathbb{R}^3} (r(x))^{-3}\varphi_0\left(\frac{x'-x}{r(x)}\right)\rho_{TF}(x)dx. \tag{4}$$

In the integral in (4), we want to replace $\rho_{TF}(x)$ by $\rho_{TF}(x')$ and $r(x)$ by $r(x')$. Taylor-expanding to second order, we have

$$\rho_{TF}(x) = \rho_{TF}(x') + \nabla\rho_{TF}(x')\cdot(x-x') + O\left(\frac{\rho_{TF}(x')}{|x'|^2}|x-x'|^2\right) \tag{5}$$

for $x \in B(x', 9r(x'))$. More crudely,

$$\rho_{TF}(x) = \rho_{TF}(x') + O\left(\frac{\rho_{TF}(x')}{|x'|}\cdot|x-x'|\right) \tag{6}$$

for $x \in B(x', 9r(x'))$. Still more crudely,

$$\rho_{TF}(x) = O(\rho_{TF}(x')) \tag{7}$$

for $x \in B(x', 9r(x'))$. To check (5), (6), (7) we recall that $|\partial^\alpha\rho_{TF}(x)| \le C_\alpha \frac{\rho_{TF}(x)}{|x|^\alpha}$ and $B(x', 9r(x')) \subset B\left(x', \frac{1}{2}|x'|\right)$.

Next, we Taylor-expand $r^{-3}\varphi_0(y/r)$ in r. In general, if φ is smooth, radial, and supported in the unit ball, then

$$\frac{\partial}{\partial r}[r^{-m}\varphi(y/r)] = r^{-(m+1)}\tilde{\varphi}(y/r) \quad \text{with} \quad \tilde{\varphi}(y) = -m\varphi(y) - y\cdot\nabla\varphi(y)$$

again smooth, radial, and supported in the unit ball. Hence

$$\left(\frac{\partial}{\partial r}\right)^m \{r^{-3}\varphi_0(y/r)\} = r^{-3-m}\varphi_m(y/r)$$

with φ_m smooth, radial, and supported in the unit ball. So Taylor's theorem implies

(8)
$$\begin{aligned}(r(x))^{-3}\varphi_0(y/r(x)) &= (r(x'))^{-3}\varphi_0(y/r(x')) + (r(x'))^{-4}\varphi_1(y/r(x'))\cdot[r(x)-r(x')] \\ &\quad + O((r(x'))^{-5}|r(x)-r(x')|^2),\end{aligned}$$

uniformly in y, x, x' provided $c < r(x)/r(x') < C$. We recall that $r(x)$ was defined to satisfy (19), (20) from the previous section. Let us take $r(x)$ to satisfy also

$$|\nabla^2 r(x)| \le C r(x)|x|^{-2}. \tag{9}$$

(The reader can easily verify that such functions $r(x)$ exist.) Then

$$r(x) - r(x') = \nabla r(x') \cdot (x - x') + O\left(\frac{r(x')}{|x'|^2}|x - x'|^2\right)$$

for $x \in B(x', 9r(x'))$. More crudely,

$$|r(x) - r(x')| \le C\frac{r(x')}{|x'|} \cdot |x - x'|$$

for $x \in B(x', 9r(x'))$. Putting these estimates into (8), and setting $y = x - x'$, we get

$$\begin{aligned}(r(x))^{-3}\varphi_0\left(\frac{x-x'}{r(x)}\right) &= (r(x'))^{-3}\varphi_0\left(\frac{x-x'}{r(x')}\right) + \left[(r(x'))^{-4}\varphi_1\left(\frac{x-x'}{r(x')}\right)\nabla r(x')\cdot(x-x')\right.\\ &\quad \left. + O\left((r(x'))^{-4}\cdot\frac{r(x')}{|x'|^2}|x-x'|^2\right)\right] + O\left((r(x'))^{-5}\cdot\left\{\frac{r(x')}{|x'|}\cdot|x-x'|\right\}^2\right),\\ &\qquad \text{for} \quad x \in B(x', 9r(x')).\end{aligned}$$

That is

$$\begin{aligned}(r(x))^{-3}\varphi_0\left(\frac{x-x'}{r(x)}\right) &= (r(x'))^{-3}\varphi_0\left(\frac{x-x'}{r(x')}\right) + (r(x'))^{-4}\varphi_1\left(\frac{x-x'}{r(x')}\right)\nabla r(x')\cdot(x-x')\\ &\quad + O\left((r(x'))^{-3}\frac{|x-x'|^2}{|x'|^2}\right) \quad \text{for} \quad x \in B(x', 9r(x')).\end{aligned} \tag{10}$$

We multiply both sides of (10) by $\rho_{TF}(x)$. On the right-hand side, we use formula (5) for $\rho_{TF}(x)$ in the first term, formula (6) for $\rho_{TF}(x)$ in the second term, and formula (7) for $\rho_{TF}(x)$ in the third term. Thus,

$$\begin{aligned}&(r(x))^{-3}\varphi_0\left(\frac{x-x'}{r(x)}\right)\rho_{TF}(x) = \\ &\left[(r(x'))^{-3}\varphi_0\left(\frac{x-x'}{r(x')}\right)\rho_{TF}(x') + (r(x'))^{-3}\varphi_0\left(\frac{x-x'}{r(x')}\right)\nabla\rho_{TF}(x')\cdot(x-x')\right.\\ &\qquad \left. + O\left((r(x'))^{-3}\cdot\frac{\rho_{TF}(x')}{|x'|^2}|x-x'|^2\right)\right]\\ &\quad + \left[(r(x'))^{-4}\varphi_1\left(\frac{x-x'}{r(x')}\right)\nabla r(x')\cdot(x-x')\rho_{TF}(x')\right.\end{aligned} \tag{11}$$

$$+\,O\left((r(x'))^{-4}|\nabla r(x')|\cdot|x-x'|\cdot\frac{\rho_{TF}(x')}{|x'|}|x-x'|\right)\Bigg]$$
$$+\left[O\left((r(x'))^{-3}|x-x'|^2|x'|^{-2}\cdot\rho_{TF}(x')\right)\right]\quad\text{for}\quad x\in B(x',9r(x')).$$

Since $|\nabla r(x')|\le\frac{Cr(x')}{|x'|}$ by (20) of the previous section, and since $|x-x'|<9r(x')$ for $x\in B(x',9r(x'))$, (11) implies

$$\begin{aligned}(r(x))^{-3}\varphi_0\left(\frac{x-x'}{r(x)}\right)\rho_{TF}(x)&=(r(x'))^{-3}\varphi_0\left(\frac{x-x'}{r(x')}\right)\rho_{TF}(x')\\&\quad+(r(x'))^{-3}\varphi_0\left(\frac{x-x'}{r(x')}\right)\nabla\rho_{TF}(x')\cdot(x-x')\\&\quad+(r(x'))^{-4}\varphi_1\left(\frac{x-x'}{r(x')}\right)\nabla r(x')\cdot(x-x')\rho_{TF}(x')\\&\quad+O\left((r(x'))^{-3}\cdot\left(\frac{r(x')}{|x'|}\right)^2\rho_{TF}(x')\right)\quad\text{for}\quad x\in B(x',9r(x')).\end{aligned}$$

We integrate this equation over all $x\in B(x',9r(x'))$ for fixed x'.

The second and third integrals on the right-hand side will be zero, since the integrands are odd functions of $x-x'$. (Recall that φ_1, φ_0 are radial.) Hence, we obtain

$$\int\limits_{x\in B(x',9r(x'))}(r(x))^{-3}\varphi_0\left(\frac{x-x'}{r(x)}\right)\rho_{TF}(x)dx=$$
$$\int\limits_{x\in B(x',9r(x'))}(r(x'))^{-3}\varphi_0\left(\frac{x-x'}{r(x')}\right)\rho_{TF}(x')dx+O\left(\rho_{TF}(x')\left(\frac{r(x')}{|x'|}\right)^2\right).$$

We may replace $B(x',9r(x'))$ in these integrals by $\mathbb{R}^3$, since the integrands are supported in $B(x',9r(x'))$. Since φ_0 has integral 1, we obtain

$$\int\limits_{x\in\mathbb{R}^3}(r(x))^{-3}\varphi_0\left(\frac{x-x'}{r(x)}\right)\rho_{TF}(x)dx=\rho_{TF}(x')+O\left(\rho_{TF}(x')\cdot\left(\frac{r(x')}{|x'|}\right)^2\right).$$

In view of (4), this means

$$|g(x')|\le C\rho_{TF}(x')\cdot\left(\frac{r(x')}{|x'|}\right)^2\quad\text{for all}\quad x'\in\mathbb{R}^3.\tag{12}$$

Equation (19) from the previous section gives the order of magnitude of $r(x')$, which allows us to conclude from (12) that

$$|g(x')|\le C\min\{m^{2/3}\rho_{TF}^{1/3}(x')|x'|^{-2},\rho_{TF}(x')\}\quad\text{for all}\quad x'\in\mathbb{R}^3.$$

Thus,

$$|g(x)| \le Cm^{2/3}Z^{1/2}|x|^{-5/2} \quad \text{for} \quad |x| \le Z^{-1/3} \tag{13}$$

$$|g(x)| \le CZ^{3/2}|x|^{-3/2} \quad \text{for} \quad |x| \le Z^{-1/3} \tag{14}$$

$$|g(x)| \le Cm^{2/3}|x|^{-4} \quad \text{for} \quad |x| \ge Z^{-1/3}. \tag{15}$$

We apply (13), (14), (15) to estimate $\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{g(x)g(y)dxdy}{|x-y|}$. Since g is radial, we can invoke the formula

$$\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{g(x)g(y)dxdy}{|x-y|} = \int\limits_0^\infty \Big(\int\limits_{B(0,R)} g(x)dx \Big)^2 \frac{dR}{R^2}, \tag{16}$$

which follows from the fact that $\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{d\mu(x)d\nu(y)}{|x-y|} = \frac{\mu(\mathbb{R}^3)\nu(\mathbb{R}^3)}{\max(r,s)}$ where μ and ν denote uniform measure on spheres of radii r and s, respectively, centered at the origin.

If $0 < R < Z^{-10}$, then (14) gives $\int\limits_{B(0,R)} |g(x)|dx \le CZ^{3/2}R^{3/2}$. If $Z^{-10} \le R \le Z^{-1/3}$, then (13) gives $\int\limits_{B(0,R)} |g(x)|dx \le Cm^{2/3}Z^{1/2}R^{1/2}$. In particular, $\int\limits_{B(0,Z^{-1/3})} |g(x)|dx \le Cm^{2/3}Z^{1/3}$. From (15) we get $\int\limits_{\mathbb{R}^3\setminus B(0,Z^{-1/3})} |g(x)|dx \le Cm^{2/3}Z^{1/3}$, and so

$$\begin{aligned}\int\limits_{B(0,R)} |g(x)|dx \le \int\limits_{\mathbb{R}^3} |g(x)|dx &= \int\limits_{B(0,Z^{-1/3})} |g(x)|dx + \int\limits_{\mathbb{R}^3\setminus B(0,Z^{-1/3})} |g(x)|dx \\ &\le Cm^{2/3}Z^{1/3}, \quad \text{for all } R.\end{aligned}$$

The above estimates for $\int\limits_{B(0,R)} |g(x)|dx$ yield:

$$\begin{aligned}\int\limits_0^\infty \Big(\int\limits_{B(0,R)} g(x)dx \Big)^2 \frac{dR}{R^2} &\le \int\limits_0^{Z^{-10}} (CZ^3R^3)\frac{dR}{R^2} + \int\limits_{Z^{-10}}^{Z^{-1/3}} (Cm^{4/3}ZR)\frac{dR}{R^2} \\ &+ \int\limits_{Z^{-1/3}}^\infty (Cm^{2/3}Z^{1/3})^2 \frac{dR}{R^2} \\ &\le C'm^{4/3}Z\ell nZ.\end{aligned} \tag{17}$$

Recall from the previous section that $m = Z^{\frac{1}{15\cdot 63}}$, so

$$\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{g(x)g(y)dxdy}{|x-y|} \le CZ^{\frac{5}{3}-\gamma_2}. \tag{18}$$

Thus we have succeeded in estimating g.

Now from (3) and (4) we obtain

$$f(x') + qg(x') = \sum_{k=1}^{N} \varphi_{x_k}(x') - q\rho_{TF}(x'). \tag{19}$$

Since

$$u \longmapsto \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{u(x)\overline{u(y)}}{|x-y|} dxdy = (\text{const}) \int\limits_{\mathbb{R}^3} \frac{|\hat{u}(\xi)|^2}{|\xi|^2} d\xi$$

is a positive quadratic form, we know that

$$\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} (f(x)+qg(x))(f(y)+qg(y)) \frac{dxdy}{|x-y|} \leq$$

$$C \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} f(x)f(y)\frac{dxdy}{|x-y|} + C \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} q^2 g(x)g(y)\frac{dxdy}{|x-y|}.$$

Putting (2 bis), (18), (19) into this inequality, we learn that

$$\int\limits_{\mathbb{R}^3\times\mathbb{R}^3} \left[\sum_{k=1}^{N} \varphi_{x_k}(x) - q\rho_{TF}(x)\right] \left[\sum_{k=1}^{N} \varphi_{x_k}(y) - q\rho_{TF}(y)\right] \frac{dxdy}{|x-y|} \leq C\bar{Y}(x_1 \ldots x_N) + CZ^{5/3-\gamma_2}. \tag{20}$$

This holds for any $x_1 \ldots x_N \in \mathbb{R}^3$. From (2) and (20) we obtain at once

$$\left\langle \int\limits_{\mathbb{R}^3\times\mathbb{R}^3} \left[\sum_{k=1}^{N} \varphi_{x_k}(x) - q\rho_{TF}(x)\right] \left[\sum_{k=1}^{N} \varphi_{x_k}(y) - q\rho_{TF}(y)\right] \frac{dxdy}{|x-y|} \Psi, \Psi \right\rangle \leq C(\eta + Z^{-\gamma_2})Z^{5/3}. \tag{21}$$

This shows that a slightly smeared version of $\sum_{k=1}^{N} \delta(x-x_k)$ is very close to $q\rho_{TF}$. So, as promised, the particles are forced to distribute themselves according to the charge density $q\rho_{TF}$. Estimate (21) strengthens an inequality used in [FS8] to study the asymptotic neutrality of large ions, and in [SSS] to study the binding energy of the outermost electron. We expect that (21) will allow one to sharpen the results derived there.

Next we prepare to estimate the mean and variance of $\mathcal{N}_{x_0r_0} = \mathcal{N}_{x_0r_0}(x_1 \ldots x_N) =$ number of x_k belonging to $B(x_0, r_0)$.

The idea is to prove lower bounds for a perturbed Hamiltonian $H + \sum_{i<j} K_\#(x_i, x_j)$, by the methods of the previous section. Here, the interaction $K_\#(x,y)$ is assumed to

satisfy $K_\#(x,y) = K_\#(y,x)$ and $|K_\#(x,y)| \leq K_s(x,y)$, and to have support contained in $A_m \times A_m$. (See equation (69) from the preceding section.) Equation (36) from the preceding section gives

$$
\begin{aligned}
(22)\quad \langle H\Psi,\Psi\rangle + \Big\langle \sum_{i<j} K_\#(x_i,x_j)\Psi,\Psi\Big\rangle = \\
\Big\langle \sum_{k=1}^{N}(-\Delta_{x_k} + V_{TF}(x_k))\Psi,\Psi\Big\rangle - q\Big\langle \sum_{k=1}^{N} W_{\text{extra}}(x_k)\Psi,\Psi\Big\rangle \\
- c_\#\Big\langle \sum_{k=1}^{N}(r(x_k))^{-1}\Psi,\Psi\Big\rangle + \Big\langle \bar{Y}(x_1\dots x_N)\Psi,\Psi\Big\rangle \\
- \frac{q^2}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} K_L(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy \\
+ \Big\langle \sum_{i<j}(K_s + K_\#)(x_i,x_j)\Psi,\Psi\Big\rangle.
\end{aligned}
$$

On the right-hand side, only the last term differs from its analogue in equation (36) of the previous section. Hence, as in that section, we have

$$
(23)\qquad \Big\langle \sum_{k=1}^{N}(-\Delta_{x_k} + V_{TF}(x_k))\Psi,\Psi\Big\rangle \geq q\,\mathrm{sneg}(-\Delta + V_{TF})
$$

$$
\begin{aligned}
(24)\qquad -q\Big\langle \sum_{k=1}^{N} W_{\text{extra}}(x_k)\Psi,\Psi\Big\rangle \geq & - q^2 \iint_{\mathbb{R}^3\times\mathbb{R}^3} K_s(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy \\
& - Cm^{2/3}Z^{-1/24}Z^{5/3}
\end{aligned}
$$

$$
(25)\qquad -c_\#\Big\langle \sum_{k=1}^{N}(r(x_k))^{-1}\Psi,\Psi\Big\rangle \geq -CZ^{-\frac{1}{24}}\cdot Z^{5/3} - Cm^{-1/3}Z^{5/3},
$$

for viable wave functions. In view of (1), our wave function is viable. To estimate the last term on the right in (22), we set

$$
\widetilde{K}(x,y) \equiv \chi_{A_m}(x)\chi_{A_m}(y)K_s(x,y) + K_\#(x,y) \equiv K(x,y) + K_\#(x,y)
$$

Evidently, $K_s(x,y) + K_\#(x,y) \geq \widetilde{K}(x,y)$, so

$$
(26)\qquad \Big\langle \sum_{i<j}(K_s + K_\#)(x_i,x_j)\Psi,\Psi\Big\rangle \geq \Big\langle \sum_{i<j} \widetilde{K}(x_i,x_j)\Psi,\Psi\Big\rangle.
$$

As in the discussion of $K(x,y)$ in the previous section (see equations (70)...(73) there), we find here that $\frac{1}{2}\widetilde{K}(x,y)$ satisfies the hypotheses of Lemma 7 in the section *Applications to Atoms*. Applying Lemma 7, we obtain

$$\left\langle \sum_{i<j} \widetilde{K}(x_i,x_j)\Psi,\Psi \right\rangle \geq$$
$$\frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \widetilde{K}(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy$$
$$- \text{Junk},$$

with Junk given by equations (74), (75) in the previous section. Combining this with (26) and the definition of $\widetilde{K}$, we get

$$\text{(27)} \quad \left\langle \sum_{i<j}(K_s + K_{\#})(x_i,x_j)\Psi,\Psi \right\rangle \geq$$
$$\left[\frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy - \text{Junk}\right]$$
$$+ \frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_{\#}(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy$$

As in the derivation of equation (80) of the preceding section, the quantity in square brackets is greater than or equal to

$$\frac{q^2}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_s(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy - qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx$$
$$- \text{Junk}_*, \qquad \text{with}$$
$$\text{Junk}_* = \text{Junk} + C'm^{2/3}(Z^2D + m^{\frac{105}{2}}D^{-5/2}).$$

Therefore,

$$\text{(28)} \quad \left\langle \sum_{i<j}(K_s(x_i,x_j) + K_{\#}(x_i,x_j))\Psi,\Psi \right\rangle \geq$$
$$\frac{q^2}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_s(x,y)\rho_{TF}(x)\rho_{TF}(y)dxdy - qc_D \int\limits_{\mathbb{R}^3} \rho_{TF}^{4/3}(x)dx - \text{Junk}_*$$
$$+ \frac{1}{2} \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} K_{\#}(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy.$$

Next, we substitute (23), (24), (25), (28) into (22), to derive the inequality

$$\text{(29)} \quad \langle H\Psi,\Psi\rangle + \left\langle \sum_{i<j} K_{\#}(x_i,x_j)\Psi,\Psi \right\rangle \geq$$

$$q\,\mathrm{sneg}(-\Delta + V_{TF}) - \frac{q^2}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho_{TF}(x)\rho_{TF}(y)dxdy}{|x-y|} - qc_D\int_{\mathbb{R}^3}\rho_{TF}^{4/3}(x)dx$$

$$- \mathrm{ERROR} + \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} K_{\#}(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy$$

$$\text{with}\quad \mathrm{ERROR} = Cm^{2/3}Z^{-1/24}Z^{5/3} + Cm^{-1/3}Z^{5/3} + \mathrm{Junk}_*.$$

Picking parameters D, δ, m as in the previous section, and using equation (89) from that section, we obtain from (29) the estimate

$$\langle H\Psi,\Psi\rangle + \left\langle \sum_{i<j} K_{\#}(x_i,x_j)\Psi,\Psi\right\rangle \geq$$

$$E(Z,q) + \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} K_{\#}(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy - CZ^{\frac{5}{3}-\gamma_2}.$$

Combining this with (1), we find that

$$(30)\qquad \left\langle \sum_{i<j} K_{\#}(x_i,x_j)\Psi,\Psi\right\rangle \geq \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} K_{\#}(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy - C(\eta + Z^{-\gamma_2})Z^{5/3}.$$

We have proven (30) for Ψ satisfying (1), and for $K_{\#}(x,y)$ satisfying $K_{\#}(x,y) = K_{\#}(y,x)$, $|K_{\#}(x,y)| \leq K_s(x,y)$, $\mathrm{supp}\, K_{\#}(x,y) \subset A_m \times A_m$.

Note that $-K_{\#}(x,y)$ may be used in place of $K_{\#}(x,y)$ in (30), and therefore, (30) implies

$$(31)\qquad \left\langle \sum_{i<j} K_{\#}(x_i,x_j)\Psi,\Psi\right\rangle = \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} K_{\#}(x,y)\{q^2\rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\}dxdy + O(\eta + Z^{-\gamma_2})Z^{5/3}.$$

Equation (31) is closely related to the variance of $\mathcal{N}_{x_0r_0}$. To see the connection, let $G(x_0)$ be a real-valued function on $\mathbb{R}^3$, bounded by a small constant in absolute value, and supported in $\{|x_0| \sim Z^{-1/3}\}$. With $r_0 \sim Z^{-2/3}$, we set

$$(32)\qquad K_{\#}(x,y) = \int_{\mathbb{R}^3} r_0^{-4}\chi_{x,y\in B(x_0,r_0)}G(x_0)dx_0.$$

Note that $K_\#(x,y) = K_\#(y,x)$, and that

$$\text{supp}\, K_\#(x,y) \subset \{|x-y| < 2r_0, |x| \sim Z^{-1/3}, |y| \sim Z^{-1/3}\} \subset A_m \times A_m. \tag{33}$$

To check the hypotheses imposed above on $K_\#$, it remains only to show that $|K_\#(x,y)| \le K_s(x,y)$. In view of (33), we may assume $|x| \sim Z^{-1/3}$, $|y| \sim Z^{-1/3}$, $|x-y| < 2r_0$. By definition (32), we have

$$|K_\#(x,y)| \le \|G\|_{L^\infty} r_0^{-4} \int\limits_{x,y \in B(x_0,r_0)} dx_0 \le \frac{1}{100} r_0^{-1}. \tag{34}$$

For $|x| \sim Z^{-1/3}$, $|y| \sim Z^{-1/3}$, $|x-y| < 2r_0$, we have

$$K_s(x,y) = |x-y|^{-1} - K_L(x,y) \ge \frac{1}{2r_0} - K_L(x,y) \ge \frac{1}{4} r_0^{-1}. \tag{35}$$

To see the last inequality in (35), recall from (28) and (30) of the preceding section that the matrix $\begin{pmatrix} K_L(x,x) & K_L(y,x) \\ K_L(x,y) & K_L(y,y) \end{pmatrix}$ is positive semi-definite, and that $K_L(x,x) = c_\#(r(x))^{-1} \le Cm^{-1/3}Z^{2/3}$, $K_L(y,y) = c_\#(r(y))^{-1} \le Cm^{-1/3}Z^{2/3}$ for $|x|, |y| \sim Z^{-1/3}$. These facts imply $|K_L(x,y)|^2 \le K_L(x,x)K_L(y,y) \le Cm^{-2/3}Z^{4/3} \ll r_0^{-2}$, since $m \gg 1$. So the last inequality in (35) is correct.

Immediately from (34) and (35), we get the desired inequality $|K_\#(x,y)| \le K_s(x,y)$. Thus, $K_\#(x,y)$ satisfies all the hypotheses used in the derivation of (31). Consequently, (31) holds with $K_\#(x,y)$ given by (32). That is,

$$\begin{aligned} r_0^{-4} \int\limits_{x_0 \in \mathbb{R}^3} & G(x_0) \Big\langle \sum_{i<j} \chi_{x_i,x_j \in B(x_0,r_0)} \Psi, \Psi \Big\rangle dx_0 \\ &= \int\limits_{x_0 \in \mathbb{R}^3} r_0^{-4} G(x_0) \cdot \frac{1}{2} \iint\limits_{x,y \in B(x_0,r_0)} \{q^2 \rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\} dxdy\, dx_0 \\ &+ O(\eta + Z^{-\gamma_2})Z^{5/3}. \end{aligned}$$

This holds for all functions $G(x)$ supported in $\{|x| \sim Z^{-1/3}\}$ with $\|G\|_{L^\infty} < c$. Therefore,

$$\begin{aligned} r_0^{-4} \int\limits_{|x_0| \sim Z^{-1/3}} & \Bigg| \Big\langle \sum_{i<j} \chi_{x_i,x_j \in B(x_0,r_0)} \Psi, \Psi \Big\rangle - \\ & \frac{1}{2} \iint\limits_{x,y \in B(x_0,r_0)} \{q^2 \rho_{TF}(x)\rho_{TF}(y) - q|\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2\} dxdy \Bigg| dx_0 \\ & \le C(\eta + Z^{-\gamma_2})Z^{5/3}. \end{aligned} \tag{36}$$

Since $\mathcal{N}_{x_0 r_0} = [\text{number of } x_j \text{ in } B(x_0, r_0)]$, we have

$$\sum_{i<j} \chi_{x_i, x_j \in B(x_0, r_0)} = \frac{1}{2} \mathcal{N}_{x_0 r_0} (\mathcal{N}_{x_0 r_0} - 1).$$

Putting this identity into (36) and recalling that $r_0 \sim Z^{-2/3}$, we get

$$\text{(37)} \qquad \int\limits_{|x_0| \sim Z^{-1/3}} \Bigg| \big\langle (\mathcal{N}^2_{x_0 r_0} - \mathcal{N}_{x_0 r_0}) \Psi, \Psi \big\rangle - \iint\limits_{x,y \in B(x_0, r_0)} \{ q^2 \rho_{TF}(x) \rho_{TF}(y) - q |\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2 \} dx dy \Bigg| dx_0 \leq C(\eta + Z^{-\gamma_2}) \cdot Z^{-1}.$$

If we can understand $\langle \mathcal{N}_{x_0 r_0} \Psi, \Psi \rangle$, the mean of $\mathcal{N}_{x_0, r_0}$, then (37) will control the variance of $\mathcal{N}_{x_0 r_0}$. We will rewrite (37) in a slightly simpler form, and then begin to study the mean.

Recall that $|\nabla \rho_{TF}(x)| \leq C \frac{\rho_{TF}(x)}{|x|} \leq C Z^{7/3}$ for $|x| \sim Z^{-1/3}$. Therefore for $x, y \in B(x_0, r_0)$ and $|x_0| \sim Z^{-1/3}$ we have

$$\text{(38)} \qquad |\rho_{TF}(x) - \rho_{TF}(x_0)|, \quad |\rho_{TF}(y) - \rho_{TF}(x_0)| \leq C Z^{5/3}.$$

Also, since $\mathcal{S}_\rho(w) = (\text{const}) \int\limits_{|\xi| < (\text{const}) \rho^{1/3}} e^{i \xi \cdot w} d\xi$, we have

$$\text{(39)} \qquad \begin{aligned} |\mathcal{S}_{\rho_{TF}(x)}(w) - \mathcal{S}_{\rho_{TF}(x_0)}(w)| &\leq C |(\rho_{TF}(x))^{1/3} - (\rho_{TF}(x_0))^{1/3}| \cdot \rho^{2/3}_{TF}(x) \\ &\leq C' |\rho_{TF}(x) - \rho_{TF}(x_0)| \leq C'' Z^{5/3}, \quad \text{for} \quad w \in \mathbb{R}^3. \end{aligned}$$

Since $|\rho_{TF}(x)|$, $|\mathcal{S}_{\rho_{TF}(x_0)}(w)| \leq C Z^2$, (38) and (39) imply

$$\iint\limits_{x,y \in B(x_0, r_0)} |\rho_{TF}(x) \rho_{TF}(y) - \rho^2_{TF}(x_0)| dx dy \leq C Z^{-1/3} \ll Z^{-\gamma_2}$$

and

$$\iint\limits_{x,y \in B(x_0, r_0)} \Big| |\mathcal{S}_{\rho_{TF}(x)}(x-y)|^2 - |\mathcal{S}_{\rho_{TF}(x_0)}(x-y)|^2 \Big| dx dy \leq C Z^{-1/3} \ll Z^{-\gamma_2},$$

for $|x_0| \sim Z^{-1/3}$. Therefore, (37) is equivalent to the following:

$$\text{(40)} \qquad \int\limits_{|x_0| \sim Z^{-1/3}} \Big| \big\langle (\mathcal{N}^2_{x_0 r_0} - \mathcal{N}_{x_0 r_0}) \Psi, \Psi \big\rangle - \left(q \rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 \right)^2 + q \iint\limits_{x,y \in B(x_0, r_0)} |\mathcal{S}_{\rho_{TF}(x_0)}(x-y)|^2 dx dy \Big| dx_0 \leq C(\eta + Z^{-\gamma_2}) Z^{-1}.$$

Now we begin to study the mean $\langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle$. Equation (40) gives us some useful information on the mean. In fact, by the Cauchy-Schwartz inequality,

$$\langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle^2 \leq \left\langle \mathcal{N}^2_{x_0 r_0}\Psi, \Psi\right\rangle \leq \left\langle [2(\mathcal{N}^2_{x_0 r_0} - \mathcal{N}_{x_0 r_0}) + 1]\Psi, \Psi\right\rangle = 2\left\langle (\mathcal{N}^2_{x_0 r_0} - \mathcal{N}_{x_0 r_0})\Psi, \Psi\right\rangle + 1.$$

Hence, (40) implies for any $E \subset \{|x_0| \sim Z^{-1/3}\}$ the estimate

$$\int\limits_{x_0 \in E} \langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle^2 \, dx_0 \leq |E| + C(\eta + Z^{-\gamma_2})Z^{-1}$$
$$+ \int\limits_{x_0 \in E} \left\{ (q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3)^2 - q \iint\limits_{x,y \in B(x_0, r_0)} |\mathcal{S}_{\rho_{TF}(x_0)}(x-y)|^2 dx dy \right\} dx_0$$
$$\leq |E| + C(\eta + Z^{-\gamma_2})Z^{-1} + \int\limits_{x_0 \in E} (q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3)^2 dx_0.$$

The integrand on the right-hand side is bounded, so we get

$$\int\limits_{x_0 \in E} \langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle^2 \, dx_0 \leq C(\eta + Z^{-\gamma_2})Z^{-1} + C|E| \tag{41}$$

for measurable subsets $E \subset \{|x_0| \sim Z^{-1/3}\}$. We will use (41) for a suitable small subset E.

For most x_0 with $|x_0| \sim Z^{-1/3}$, we will control $\langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle$ using the Corollary to Lemma 6 from the section on *Applications to Atoms*, and part (B) of the *Main Theorem on Free Particles* with $h = 0$. Let $\widehat{Q}$ be a cube centered at the origin, of diameter $D = Z^{-1/2}$, as in the previous section. Since Ψ is viable, the Corollary to Lemma 6 produces a subset $F \subset A = \{x \in \mathbb{R}^3 \mid 10D \leq |x| \leq cD^{1/2}\}$, with the following properties:

(42) $\mathcal{E}(\widehat{Q} + \mathfrak{z}, \rho_{TF}(\mathfrak{z}), \Psi) < \delta\rho^{5/3}_{TF}(\mathfrak{z})|\widehat{Q}|$ for $\mathfrak{z} \in A \setminus F$.

(43) $\int\limits_F \rho^{5/3}_{TF}(\mathfrak{z})d\mathfrak{z} \leq C\beta Z^{7/3}$, with

(44) $\beta = \delta^{-1}(Z^{-1/12} + Z^{-2/3}D^{-1} + Z^{1/6}D^{1/2}) \sim \delta^{-1}Z^{-1/12}$.

Set $A_0 = \{x \in \mathbb{R}^3 \mid cZ^{-1/3} < |x| < CZ^{-1/3}\}$ and $F_0 = F \cap A_0$. Then, since $\rho_{TF}(\mathfrak{z}) \sim Z^2$ on A_0, (43) implies

$$cZ^{10/3}|F_0| \leq \int\limits_{F_0} \rho^{5/3}_{TF}(\mathfrak{z})d\mathfrak{z} \leq C\beta Z^{7/3}, \quad \text{i.e.}$$

$$(45) \qquad |F_0| \leq C\beta Z^{-1},$$

So F_0 is a small subset of A_0. For $\mathfrak{z} \in A_0 \setminus F_0$, (42) and part (B) of the *Main Theorem on Free Particles* with $h = 0$ together yield

$$(46) \qquad \int_{x \in Q_0 + \mathfrak{z}} |\mathcal{S}_s(x,x,\Psi) - \rho_{TF}(\mathfrak{z})| dx \leq C(\delta + \underline{\mathrm{N}}^{-2/15})^{\frac{1}{48}} \rho_{TF}(\mathfrak{z}) |\widehat{Q}|,$$

with Q_0 = middle half of $\widehat{Q}$ and $\underline{\mathrm{N}} = \rho_{TF}(\mathfrak{z})|\widehat{Q}| \sim \rho_{TF}(\mathfrak{z}) D^3$. Recall that $\delta = Z^{\frac{-5 \cdot 63}{12 \cdot (7 + 5 \cdot 63)}}$, $D = Z^{-1/2}$, and $\rho_{TF}(\mathfrak{z}) \sim Z^2$ for $\mathfrak{z} \in A_0$. Hence $\underline{\mathrm{N}} \sim \rho_{TF}(\mathfrak{z}) D^3 \sim Z^2 \cdot Z^{-3/2} = Z^{1/2}$, so $\underline{\mathrm{N}}^{-\frac{2}{15}} \sim Z^{-\frac{1}{15}} \gg \delta$, and thus $(\delta + \underline{\mathrm{N}}^{-2/15})^{\frac{1}{48}} \sim Z^{-\frac{1}{15 \cdot 48}}$. Estimate (46) is therefore equivalent to the following.

$$(47) \qquad \int_{x \in Q_0 + \mathfrak{z}} |\mathcal{S}_s(x,x,\Psi) - \rho_{TF}(\mathfrak{z})| dx \leq C Z^{-\frac{1}{15 \cdot 48}} Z^2 |Q_0| \quad \text{for} \quad \mathfrak{z} \in A_0 \setminus F_0.$$

Equation (47) controls $\langle \mathcal{N}_{x_0, r_0} \Psi, \Psi \rangle$ since $\mathcal{S}_s(x,x,\Psi)$ is the density of particles on spin s. In fact,

$$\langle \mathcal{N}_{x_0, r_0} \Psi, \Psi \rangle = \sum_{s=1}^{q} \int_{x \in B(x_0, r_0)} \mathcal{S}_s(x,x,\Psi) dx,$$

so

$$\begin{aligned} &\langle \mathcal{N}_{x_0 r_0} \Psi, \Psi \rangle - q \rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 = \\ &\qquad \sum_{s=1}^{q} \int_{x \in B(x_0, r_0)} [\mathcal{S}_s(x,x,\Psi) - \rho_{TF}(x_0)] dx = \\ &\qquad \sum_{s=1}^{q} \int_{x \in B(x_0, r_0)} [\mathcal{S}_s(x,x,\Psi) - \rho_{TF}(\mathfrak{z})] dx + q(\rho_{TF}(\mathfrak{z}) - \rho_{TF}(x_0)) \cdot \frac{4\pi}{3} r_0^3. \end{aligned}$$

If $\mathfrak{z} \in A_0$ and $x_0 \in \widehat{Q} + \mathfrak{z}$, then

$$\begin{aligned} |\rho_{TF}(\mathfrak{z}) - \rho_{TF}(x_0)| &\leq C Z^{7/3} |\mathfrak{z} - x_0| \\ &\leq C Z^{\frac{7}{3}} \cdot Z^{-1/2}, \end{aligned}$$

so that

$$|(\rho_{TF}(\mathfrak{z}) - \rho_{TF}(x_0)) r_0^3| \leq C Z^{7/3} Z^{-1/2} Z^{-2} = C Z^{-1/6}.$$

Hence we have

$$\begin{aligned} &| \langle \mathcal{N}_{x_0 r_0} \Psi, \Psi \rangle - q \rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 | \leq \\ &\qquad \sum_{s=1}^{q} \int_{x \in B(x_0, r_0)} |\mathcal{S}_s(x,x,\Psi) - \rho_{TF}(\mathfrak{z})| dx + C Z^{-1/6} \\ &\qquad\qquad \text{for } \mathfrak{z} \in A_0,\ x_0 \in \widehat{Q} + \mathfrak{z}. \end{aligned}$$

We integrate this inequality over all $x_0 \in Q_1 + \mathfrak{z}$, where Q_1 is the middle half of Q_0. Thus we obtain

(48)
$$\int\limits_{x_0 \in Q_1+\mathfrak{z}} \left| \langle \mathcal{N}_{x_0 r_0} \Psi, \Psi \rangle - q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 \right| dx_0 \leq$$

$$CZ^{-1/6}|Q_1| + \sum_{s=1}^{q} \iint\limits_{\substack{x_0 \in Q_1+\mathfrak{z} \\ x \in B(x_0, r_0)}} |\mathcal{S}_s(x,x,\Psi) - \rho_{TF}(\mathfrak{z})| \, dx \, dx_0$$

$$= CZ^{-1/6}|Q_1| + \sum_{s=1}^{q} \int\limits_{x \in \mathbb{R}^3} \left\{ \int\limits_{\substack{x_0 \in Q_1+\mathfrak{z} \\ x \in B(x_0, r_0)}} dx_0 \right\} |\mathcal{S}_s(x,x,\Psi) - \rho_{TF}(\mathfrak{z})| dx$$

for $\mathfrak{z} \in A_0$. The integral in curly brackets is dominated by $\frac{4\pi}{3} r_0^3 \chi_{x \in Q_0+\mathfrak{z}}$, so (48) implies

$$\int\limits_{x_0 \in Q_1+\mathfrak{z}} \left| \langle \mathcal{N}_{x_0 r_0} \Psi, \Psi \rangle - q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 \right| dx_0 \leq$$

$$CZ^{-1/6}|Q_1| + \sum_{s=1}^{q} CZ^{-2} \int\limits_{x \in Q_0+\mathfrak{z}} |\mathcal{S}_s(x,x,\Psi) - \rho_{TF}(\mathfrak{z})| dx$$

for $\mathfrak{z} \in A_0$. Applying (47) and noting that $|Q_0| \sim |Q_1|$, we conclude that

(49)
$$\int\limits_{x_0 \in Q_1+\mathfrak{z}} \left| \langle \mathcal{N}_{x_0 r_0} \Psi, \Psi \rangle - q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 \right| dx_0 \leq$$

$$CZ^{-1/6}|Q_1| + CZ^{-\frac{1}{15\cdot 48}}|Q_0| \leq C'Z^{-\frac{1}{15\cdot 48}}|Q_1| \text{ for } \mathfrak{z} \in A_0 \setminus F_0.$$

With a small $\sigma > 0$ to be picked later, define

(50)
$$F_\# = \left\{ x_0 \in A_0 \;\middle|\; \left| \langle \mathcal{N}_{x_0 r_0} \Psi, \Psi \rangle - q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 \right| > \sigma \right\}$$

Immediately from (49), we see that

(51)
$$|F_\# \cap (Q_1 + \mathfrak{z})| \leq \frac{C'Z^{-\frac{1}{15\cdot 48}}}{\sigma} |Q_1| \quad \text{for} \quad \mathfrak{z} \in A_0 \setminus F_0,$$

which allows us to estimate $|F_\#|$ as follows.

For $x \in A_0$ we have $1 \leq C \int\limits_{\mathfrak{z} \in A_0} \chi_{x \in Q_1+\mathfrak{z}} \frac{d\mathfrak{z}}{|Q_1|}$. Integrating this inequality over all $x \in F_\#$ yields

(52)
$$|F_\#| \leq C \iint\limits_{\substack{x \in F_\# \\ \mathfrak{z} \in A_0}} \chi_{x \in Q_1+\mathfrak{z}} \frac{dx d\mathfrak{z}}{|Q_1|} = C \int\limits_{\mathfrak{z} \in A_0} \left\{ \int\limits_{x \in F_\#} \chi_{x \in Q_1+\mathfrak{z}} \frac{dx}{|Q_1|} \right\} d\mathfrak{z}$$

$$= C \int\limits_{\mathfrak{z} \in A_0} \frac{|F_\# \cap (Q_1 + \mathfrak{z})|}{|Q_1|} d\mathfrak{z}.$$

The integrand on the right is dominated by $\frac{C'Z^{-\frac{1}{15\cdot 48}}}{\sigma}$ for $\mathfrak{z} \in A_0 \setminus F_0$ thanks to (51). For $\mathfrak{z} \in F_0$ we use simply $\frac{|F_{\#} \cap (Q_1+\mathfrak{z})|}{|Q_1|} \leq 1$. Hence from (45) and (52) we get

$$|F_{\#}| \leq \int\limits_{\mathfrak{z}\in A_0} \frac{C'Z^{-\frac{1}{15\cdot 48}}}{\sigma} d\mathfrak{z} + |F_0| \leq \frac{C''Z^{-\frac{1}{15\cdot 48}}}{\sigma} Z^{-1} + |F_0|$$

$$\leq \frac{CZ^{-\frac{1}{15\cdot 48}}}{\sigma} Z^{-1} + C\beta Z^{-1}.$$

In view of (44), this is equivalent to

$$|F_{\#}| \leq C(Z^{-\frac{1}{15\cdot 48}}\sigma^{-1} + \delta^{-1}Z^{-1/12})Z^{-1}. \tag{53}$$

Now we invoke (41) with $E = F_{\#}$ to get

$$\int\limits_{x_0\in F_{\#}} \langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle^2 \, dx_0 \leq C(\eta + Z^{-\gamma_2})Z^{-1} + C|F_{\#}|. \tag{54}$$

Since $|q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3| \leq C$ for $x_0 \in F_{\#} \subset A_0$, it follows that

$$\left| \langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle - q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 \right|^2 \leq C \langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle^2 + C,$$

so (53) and (54) imply

$$\begin{aligned} \int\limits_{x_0\in F_{\#}} \left| \langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle - q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 \right|^2 dx_0 \leq \\ C \int\limits_{x_0\in F_{\#}} \langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle^2 \, dx_0 + C|F_{\#}| \leq \\ C'(\eta + Z^{-\gamma_2})Z^{-1} + C'|F_{\#}| \leq \\ C(Z^{-\frac{1}{15\cdot 48}}\sigma^{-1} + \delta^{-1}Z^{-1/12} + \eta + Z^{-\gamma_2})Z^{-1}. \end{aligned} \tag{55}$$

On the other hand, the definition (50) shows at once that

$$\int\limits_{x_0\in A_0 \setminus F_{\#}} \left| \langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle - q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 \right|^2 dx_0 \leq$$

$$\sigma^2 |A_0 \setminus F_{\#}| \leq \sigma^2 |A_0| \leq C\sigma^2 Z^{-1}.$$

Combining this with (55), we conclude that

$$\begin{aligned} \int\limits_{x_0\in A_0} \left| \langle \mathcal{N}_{x_0 r_0}\Psi, \Psi\rangle - q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 \right|^2 dx_0 \leq \\ C(\sigma^2 + Z^{-\frac{1}{15\cdot 48}}\sigma^{-1} + \delta^{-1}Z^{-1/12} + \eta + Z^{-\gamma_2})Z^{-1}. \end{aligned} \tag{56}$$

Taking $\sigma = Z^{-\frac{1}{3\cdot 15\cdot 48}}$ and recalling that $\delta = Z^{-\frac{5\cdot 63}{12\cdot(7+5\cdot 63)}}$, we get

$$Z^{-\frac{1}{15\cdot 48}}\sigma^{-1} = \sigma^2 = Z^{-\frac{2}{3\cdot 15\cdot 48}}$$

and

$$\delta^{-1}Z^{-\frac{1}{12}} = Z^{\frac{5\cdot 63}{12(7+5\cdot 63)}}Z^{-\frac{(7+5\cdot 63)}{12\cdot(7+5\cdot 63)}} = Z^{-\frac{7}{12\cdot(7+5\cdot 63)}}.$$

Both these quantities are small compared to $Z^{-\gamma_2}$, so (56) simplifies to

$$\int\limits_{x_0\in A_0} \left|\langle \mathcal{N}_{x_0r_0}\Psi,\Psi\rangle - q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3\right|^2 dx_0 \leq C(\eta + Z^{-\gamma_2})Z^{-1}. \tag{57}$$

This controls the mean $\langle \mathcal{N}_{x_0r_0}\Psi,\Psi\rangle$. We derive some elementary consequences of (57) and then return to the variance of $\mathcal{N}_{x_0r_0}$. From (57) and Cauchy-Schwartz we have

$$\int\limits_{x_0\in A_0} \left|\langle \mathcal{N}_{x_0r_0}\Psi,\Psi\rangle - q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3\right| dx_0 \leq C(\eta + Z^{-\gamma_2})^{1/2}Z^{-1}. \tag{58}$$

Using the elementary identity $P^2 - Q^2 = (P-Q)^2 + 2Q(P-Q)$ with $P = \langle \mathcal{N}_{x_0r_0}\Psi,\Psi\rangle$ and $Q = q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3 = O(1)$, we get

$$\int\limits_{x_0\in A_0} \left|\langle \mathcal{N}_{x_0r_0}\Psi,\Psi\rangle^2 - \left(q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3\right)^2\right| dx \leq C(\eta + Z^{-\gamma_2})^{1/2}Z^{-1} \tag{59}$$

as a consequence of (57) and (58). Another use of (58) gives

(60)

$$\int\limits_{x_0\in A_0} \left|\left\{\langle \mathcal{N}_{x_0r_0}\Psi,\Psi\rangle - \langle \mathcal{N}_{x_0r_0}\Psi,\Psi\rangle^2\right\} - \left\{\left(q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3\right) - \left(q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3\right)^2\right\}\right| dx$$
$$\leq C(\eta + Z^{-\gamma_2})^{1/2}Z^{-1}.$$

Now we discuss the variance of $\mathcal{N}_{x_0r_0}$, which is given by the formula $\text{Var}(x_0,r_0) = \left\langle \mathcal{N}^2_{x_0r_0}\Psi,\Psi\right\rangle - \langle \mathcal{N}_{x_0r_0}\Psi,\Psi\rangle^2$. We rewrite this formula as

$$\begin{aligned}\text{(61)}\quad \text{Var}(x_0,r_0) &= \left\langle\left(\mathcal{N}^2_{x_0r_0} - \mathcal{N}_{x_0r_0}\right)\Psi,\Psi\right\rangle + \left\{\langle \mathcal{N}_{x_0r_0}\Psi,\Psi\rangle - \langle \mathcal{N}_{x_0r_0}\Psi,\Psi\rangle^2\right\}\\ &= \left[\left(q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3\right)^2 - q\iint\limits_{x,y\in B(x_0,r_0)} |\mathcal{S}_{\rho_{TF}(x_0)}(x-y)|^2 dxdy\right]\\ &+ \left[\left\langle\left(\mathcal{N}^2_{x_0r_0} - \mathcal{N}_{x_0r_0}\right)\Psi,\Psi\right\rangle - \left(q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3\right)^2 + q\iint\limits_{x,y\in B(x_0,r_0)} |\mathcal{S}_{\rho_{TF}(x_0)}(x-y)|^2 dxdy\right]\end{aligned}$$

$$+\left[\left(q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3\right)-\left(q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3\right)^2\right]$$

$$+\left[\left\{\langle\mathcal{N}_{x_0r_0}\Psi,\Psi\rangle-\langle\mathcal{N}_{x_0r_0}\Psi,\Psi\rangle^2\right\}-\right.$$

$$\left.\left\{\left(q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3\right)-\left(q\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3\right)^2\right\}\right]$$

$$\equiv \mathrm{Term}_1(x_0,r_0)+\mathrm{Term}_2(x_0,r_0)+\mathrm{Term}_3(x_0,r_0)+\mathrm{Term}_4(x_0,r_0).$$

Here, $\mathrm{Term}_1 \dots \mathrm{Term}_4$ denote the four expressions in square brackets in (61).

Comparing equation (40) with the definition of Term_2, we see that

$$\int_{x_0\in A_0}|\mathrm{Term}_2(x_0,r_0)|dx \le C(\eta+Z^{-\gamma_2})Z^{-1}. \tag{62}$$

Comparing (60) with the definition of Term_4, we get

$$\int_{x_0\in A_0}|\mathrm{Term}_4(x_0,r_0)|dx \le C(\eta+Z^{-\gamma_2})^{1/2}Z^{-1}. \tag{63}$$

Adding Terms 1 and 3 together, we get

$$\mathrm{Term}_1(x_0,r_0)+\mathrm{Term}_3(x_0,r_0)= q\left\{\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3-\iint_{x,y\in B(x_0,r_0)}|\mathcal{S}_{\rho_{TF}(x_0)}(x-y)|^2dxdy\right\}. \tag{64}$$

Putting (62), (63), (64) back into (61), we learn that

$$\int_{x_0\in A_0}\left|\mathrm{Var}(x_0,r_0)-q\left\{\rho_{TF}(x_0)\cdot\frac{4\pi}{3}r_0^3-\iint_{x,y\in B(x_0,r_0)}|\mathcal{S}_{\rho_{TF}(x_0)}(x-y)|^2dxdy\right\}\right|dx_0 \le C(\eta+Z^{-\gamma_2})^{1/2}Z^{-1}. \tag{65}$$

Our main results in this section are (21), (57), and (65). We restate them as theorems, for convenient reference. Our notation changes slightly in the statements of these results.

Theorem 1: *Let $r(x)$, $\varphi_0(x)$ be functions on $\mathbb{R}^3$, satisfying the following properties.*

(a) $r(x) < c\,\min\{|x|,(Z^{\gamma_2}\rho_{TF}^{-1/3}(x))\} < 2r(x)$ *with a small constant c.*

(b) $|\partial_x^\alpha r(x)| \le Cr(x)|x|^{-|\alpha|}$ *for* $0\le|\alpha|\le 2$.

(c) *$\varphi_0(x)$ is smooth, non-negative, radial, supported in the unit ball, and has integral* 1.

Given $x_1 \dots x_N \in \mathbb{R}^3$, we define a charge density $f(\cdot; x_1 \dots x_N)$ on $\mathbb{R}^3$ by

$$f(x; x_1 \dots x_N) = \sum_{k=1}^{N} (r(x_k))^{-3} \varphi_0 \left(\frac{x - x_k}{r(x_k)} \right) - q\rho_{TF}(x).$$

If $N \leq CZ$ and $\langle H\Psi, \Psi \rangle \leq E(Z, q) + \eta Z^{5/3}$ with $0 \leq \eta \leq C$, then

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \int_{\mathbb{R}^{3N}} \frac{f(x; x_1 \dots x_N) f(y; x_1 \dots x_N)}{|x - y|} |\Psi(x_1 \dots x_N)|^2 dx_1 \dots dx_N \, dxdy$$
$$\leq C'(\eta + Z^{-\gamma_2}) Z^{5/3}.$$

The constant C' depends only on c, C, q and on the C^∞ seminorms of the function $\varphi_0(x)$.

Theorem 2: *Suppose $N \leq CZ$ and $\langle H\Psi, \Psi \rangle \leq E(Z, q) + \eta Z^{5/3}$ with $0 \leq \eta < C$. Define*

$$\mathcal{N}_{x_0, r_0}(x_1 \dots x_N) = \sum_{k=1}^{N} \chi_{B(x_0, r_0)}(x_k)$$

$$\mathit{Mean}(x_0, r_0) = \int_{\mathbb{R}^{3N}} \mathcal{N}_{x_0, r_0}(x_1 \dots x_N) |\Psi(x_1 \dots x_N)|^2 dx_1 \dots dx_N$$

$$\mathit{Var}(x_0, r_0) = \int_{\mathbb{R}^{3N}} |\mathcal{N}_{x_0, r_0}(x_1 \dots x_N) - \mathit{Mean}(x_0, r_0)|^2 |\Psi(x_1 \dots x_N)|^2 dx_1 \dots dx_N,$$

and set

$$A = \left\{ x \in \mathbb{R}^3 \;\middle|\; cZ^{-1/3} < |x| < CZ^{-1/3} \right\}.$$

Then for $cZ^{-2/3} < r_0 < CZ^{-2/3}$, we have

$$\frac{1}{\mathit{Vol}\, A} \int_{x_0 \in A} \left| \mathit{Mean}(x_0, r_0) - q\rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 \right|^2 dx_0 \leq C'(\eta + Z^{-\gamma_2})$$

and

$$\frac{1}{\mathit{Vol}\, A} \int_{x_0 \in A} \left| \mathit{Var}(x_0, r_0) - q \left\{ \rho_{TF}(x_0) \cdot \frac{4\pi}{3} r_0^3 - \iint_{x, y \in B(x_0, r_0)} |\mathcal{S}_{\rho_{TF}(x_0)}(x - y)|^2 dxdy \right\} \right| dx$$
$$\leq C'(\eta + Z^{-\gamma_2})^{1/2}.$$

The constant C' depends only on c, C, q.

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