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

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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]2[1][1][2][1]2[1]2In the introduction, we neglect electron

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spin to simplify notation. When we prove our main results, we will take spin into account. as the infimum of the spectrum of the Hamiltonian

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

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

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

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

$$E(Z) \approx -c_0 Z^{7/3} + 18Z^2 - c_1 Z^{5/3}, 3$$

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

$$E(Z) = -c_0 Z^{7/3} + 18Z^2 + O(Z^\gamma) \quad with \quad \gamma < 2.4$$

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

Theorem: $E(Z) = -c_0 Z^{7/3} + 18Z^2 - c_1 Z^{5/3} + O(Z^{5/3-\varepsilon_0})$ *with* $\varepsilon_0 = 12835$.

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 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 $Q \subset R^3$, the minimum possible kinetic energy $KE(N,Q)$ is equal to the lowest eigenvalue of $-\Delta$ acting on antisymmetric $\Psi(x_1, , x_N) \in L^2(Q^N)$ with appropriate boundary conditions. One computes $KE(N,Q)$ trivially, by separation of variables. For large N, the answer is

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

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 $\Psi(x_1 \ldots x_N)$ in terms of the electron density

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

In fact, we set

$$\varepsilon_{TF}(\rho) = c_{TF} \int\limits_{R^3} \rho^{5/3}(x)dx - \int\limits_{R^3} Z|x|\rho(x)dx + 12_{R^3 \times R^3}\rho(x)\rho(y)|x-y|dxdy.7$$

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 $\Psi(x_1 \ldots x_N)$ for $N \gg 1$, while Thomas-Fermi theory deals merely with a function on 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

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

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.*[1]2[1][1][1][3][1]2[1]2This is not exactly the same as the usual Hartree-Fock approximation. The idea is that since the electron density is approximately ρ_{TF}, each electron behaves as if it were moving in a potential

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

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

$$H_{hf} = \sum_{k=1}^{N} \left(-\Delta_{x_k} + V_{TF}(x_k)\right), \ actingonantisymmetric$$

$\Psi(x_1 \ldots x_N)$. 10

$Unliketheoriginal Hamiltonian, (10) canbediagonalized using separation of variables, and the state of lowest energy can be written explicitly in terms of the eigenfunctions of$

[1]2

-$\Delta + V_{TF}$. 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

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

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

$$E_{hf}(Z) = sneg(-\Delta+V_{TF}) - 12_{R^3\times R^3}\rho_{TF}(x)\rho_{TF}(y)|x-y|dxdy - 12_{R^3\times R^3}|\mathrm{S}(x,y)|^2|x-y|dxdy12 + 12_{R^3\times R^3}[\rho_{hf}(x)-\rho_{TF}(x)][\rho_{hf}(y)-\rho_{TF}(y)]dxdy|x-y|,$$

with

$$sneg(-\Delta + V_{TF}) = \sum_k E_k, 13\rho_{hf}(x) = \sum_k |\varphi_k(x)|^2, 14\mathrm{S}(x,y) = \sum_k \varphi_k(x)\overline{\varphi_k(y)}.15$$

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

$$sneg(-\Delta+V_{TF}) \approx -115\pi^2 \int\limits_{R^3} |V_{TF}(x)|^{5/2}dx, 16\rho_{hf}(x) \approx 16\pi^2|V_{TF}(x)|^{3/2}, 1712_{R^3\times R^3}|\mathrm{S}(x,y)|^2dxdy|x-y| \approx c_D \int\limits_{R^3} \rho_{TF}^{4/3}(x)dx, \quad foruniversalconstant$$

c$_D$.18

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 $-c_0Z^{7/3}$. 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

$$E_{hf}(Z) \approx -c_0Z^{7/3} - c_1'Z^{5/3}.19$$

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

$$sneg(-\Delta + V) \approx -115\pi^2 \int\limits_{V<0} |V|^{5/2} + 18Z^2 + 148\pi^2 \int\limits_{V<0} |V|^{1/2}\Delta V.20$$

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

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

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

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

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 $V_{Coulomb}(x_1 \ldots x_N) = -\sum_{k=1}^{N} Z|x_k|^{-1} + \sum_{1\leq j<k\leq N} |x_j - x_k|^{-1}$, Lieb's inequality is

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

with $W(x)$ close to $V_{TF}(x)$, and E_0 close to $12_{R^3\times R^3}\rho_{TF}(x)\rho_{TF}(y)dxdy|x-y|$. We explain how to use (23), and then explain how to prove it. Assuming (23), we see at once that

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

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

$$E(Z) \geq sneg(-\Delta + W) - E_0.24$$

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

$$sneg(-\Delta + V_{TF}) - 12_{R^3\times R^3}\rho_{TF}(x)\rho_{TF}(y)|x-y|dxdy.$$

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

$$|x-x'|^{-1} = 1\pi y \in R^3 R > 0 \chi_{x,x' \in B(y,R)} dy dR R^5 \quad for \quad x, x' \in R^3 .25$$

Except for the value of the constant 1π, 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

$$\sum_{j<k} |x_j - x_k|^{-1} = 1\pi y \in R^3 R > 0 N_{yR}(N_{yR}-1)2 dy dR R^5, 26$$

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

$$V(x_1 \ldots x_N) = y \in R^3 R > 0 F(N_{yR}, y, R) dy dR 27$$

has the form $\sum_{k=1}^{N} W(x_k)$ if $F = f(y,R) \cdot N_{yR}$. If instead $F = f(y,R) \cdot N_{yR}(N_{yR}-1)2$ 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

$$12 N_{yR}(N_{yR}-1) = 12(N_{yR} - \bar{N}_{yR})^2 + f(y,R) N_{yR} + g(y,R).28$$

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 $12(N_{yR} - \bar{N}_{yR})^2$ 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

$$12 N_{yR}(N_{yR}-1) \geq f(y,R) N_{yR} + g(y,R), 28a$$

which is useful when $\bar{N}_{yR} > 1$ (say). When $\bar{N}_{yR} \leq 1$, we use instead the trivial lower bound $12 N_{yR}(N_{yR}-1) \geq 0$. Therefore, (26) implies that

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

which has the form

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

Adding $-\sum_k Z|x_k|$ 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

$$12\pi_{\{\bar{N}_{yR}>1\}}(N_{yR}-\bar{N}_{yR})^2 dydRR^5 30$$

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

$$12\pi_{\{\bar{N}_{yR}>1\}} Variance(N_{yR}) dydRR^5.31$$

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)

$$E(Z)\geq sneg(-\Delta+V_{TF})-12_{R^3\times R^3}\rho_{TF}(x)\rho_{TF}(y)|x-y|dxdy-c_D\int_{R^3}\rho_{TF}^{4/3}(x)dx-CZ^{5/3-\varepsilon_0}$$

(B) (Density)

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

(C) (Correlation Function)

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

(D) (Eigenvalue Sum)

$$sneg(-\Delta+V_{TF})=-115\pi^2\int_{R^3}|V_{TF}(x)|^{5/2}dx+18Z^2+148\pi^2\int_{R^3}|V_{TF}(x)|^{1/2}\Delta V_{TF}(x)dx+O(Z^{5/3-\varepsilon_0}).$$

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

$$12_{R^3\times R^3}[\rho_{hf}(x)-\rho_{TF}(x)][\rho_{hf}(y)-\rho_{TF}(y)]dxdy|x-y|+\left\{c_D\int\limits_{R^3}\rho_{TF}^{4/3}(x)dx-12_{R^3\times R^3}|\mathrm{S}(x,y)|^2dxdy|x-y|\right\}+CZ^{5/3-\varepsilon_0}.$$

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

$$E(Z)==sneg(-\Delta+V_{TF})-12_{R^3\times R^3}\rho_{TF}(x)\rho_{TF}(y)dxdy|x-y|-c_D\int\limits_{R^3}\rho_{TF}^{4/3}(x)dx+O(Z^{5/3-\varepsilon_0}),$$

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

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

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

$$V_{Coulomb}=V_{Long-range}+V_{Short-range},with33V_{Long-range}=1\pi_{\bar{N}_{yR}\geq Z^{\varepsilon_0}}N_{yR}(N_{yr}-1)2dydRR^5and34V_{Short-range}=1\pi_{\bar{N}_{yR}<Z^{\varepsilon_0}}N_{yR}(N_{yR}-1)2dydRR^5.35$$

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

$$V_{Long-range}\geq\sum_{k=1}^N W(x_k)-E_0.36On the other hand,V_{Short-range}=\sum_{j<k}K(x_j,x_k),with37K(x,x')=1\pi_{\bar{N}_{yR}<Z^{\varepsilon_0}}\chi_{x,x'\in B(y,R)}dydRR^5.38$$

Moreover, (38) shows that $K(x,x')$ is short-range in the following sense. If the particles $x_1\ldots x_N$ 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 $H_{lowerbound}$ in which the interaction between particles may be treated as a small perturbation. In fact, (32) yields at once

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

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

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

for the lowest eigenvalue of $H_{lowerbound}$, 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

$$(lowesteigenvalueof$$

$\mathrm{H}_{lowerbound}) \approx sneg(-\Delta{+}W){-}E_0{+}12_{R^3\times R^3} K(x,y)\{\rho_{TF}(x)\rho_{TF}(y){-}|\mathrm{S}_{\rho_{TF}(x)}(x{-}y)|^2\}dxdy, where \mathrm{S}_\rho(y)$ is an elementary function (the correlation for an ideal gas).

We will prove the rigorous inequality

$$\langle H_{lowerbound}\Psi, \Psi\rangle \geq sneg(-\Delta{+}W){-}E_0{+}12_{R^3\times R^3} K(x,y)\{\rho_{TF}(x)\rho_{TF}(y){-}|\mathrm{S}_{\rho_{TF}(x)}(x{-}y)|^2\}dxdy{-}CZ^{5/3-\varepsilon_0}41$$

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

¿From (39) and (41) follows immediately

$$E(Z) \geq sneg(-\Delta{+}W){-}E_0{+}12_{R^3\times R^3} K(x,y)\{\rho_{TF}(x)\rho_{TF}(y){-}|\mathrm{S}_{\rho_{TF}(x)}(x{-}y)|^2\}dxdy{-}CZ^{5/3-\varepsilon_0}$$

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

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

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

implies

$$\left\langle \sum_{j<k} K(x_j, x_k)\Psi, \Psi \right\rangle \geq 12_{R^3\times R^3} K(x,y)\{\rho_{TF}(x)\rho_{TF}(y){-}|\mathrm{S}_{\rho_{TF}(x)}(x{-}y)|^2\}dxdy{-}CZ^{5/3-\varepsilon_0}.43$$

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

$$\left\langle H_{lowerbound}\Psi, \Psi \right\rangle \geq sneg(-\Delta{+}W){-}E_0{+}\left\langle \sum_{j<k} K(x_j, x_k)\Psi, \Psi \right\rangle \geq sneg(-\Delta{+}W){-}E_0{+}{+} \quad 12_{R^3\times R^3} K(x,y)\{\rho_{TF}(x)\rho_{TF}(y){-}|\mathrm{S}_{\rho_{TF}(x)}(x{-}y)|^2\}dxdy \quad {-}CZ^{5/3-\varepsilon_0},$$

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

$$\left\langle H_{lowerbound}\Psi, \Psi \right\rangle \geq \left\langle \sum_{k=1}^N (-\Delta_{x_k} + W(x_k))\Psi, \Psi \right\rangle - E_0 \geq sneg(-\Delta + W) + Z^{7/3-\varepsilon_1} - E_0.$$

This implies (41), since the integral in (41) has order of magnitude $Z^{53+23\varepsilon_0} \ll Z^{73-\varepsilon_1}$. 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 $T = R^3/LZ^3$ 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

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

$$\left\langle \sum_{j<k} K(x_j, x_k)\Psi_0, \Psi_0 \right\rangle \approx 12_{T\times T}K(x, y)\{\rho^2 - |\mathrm{S}_\rho(x-y)|^2\}dxdy.$$

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

$$\left\langle \sum_{j<k} K(x_j, x_k)\Psi, \Psi \right\rangle \ge 12_{T\times T}K(x, y)\{\rho^2 - |\mathrm{S}_\rho(x-y)|^2\}dxdy - (\delta + N^{-1})^{\varepsilon_0}\rho^{4/3}L^3$$

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 $T = R^3/LZ^3$ as before, and define a Hamiltonian

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

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

$$E(\tau, \rho) = \lim N, L \to \infty NL^3 \to \rho \left\{ lowesteigenvalueof H^{\tau NL} N \right\} .44$$

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 $\tau \geq 0$, but not when $\tau < 0$. Our results show that $\partial\partial\tau E(\tau, \rho)$ 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 $sneg(-\Delta + V_{TF})$, which refines (D). The formula is as follows.

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

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

for $1 \leq \ell \leq \ell_{\max}$. Finally, set $\beta(t) = -112 + \min_{k \in Z} |t - k|^2$. Then we conjecture that

$$sneg(-\Delta + V_{TF}) \approx -115\pi^2 \int_{R^3} |V_{TF}(x)|^{5/2} dx + Z^2 8 + 148\pi^2 \int_{R^3} |V_{TF}(x)|^{1/2} \Delta V_{TF}(x) dx 45 + (const) \sum_{1 \leq \ell \leq \ell_{\max}} (2\ell+1) n_\ell \beta(\psi_\ell).$$

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

¿From (45) we expect that

$$E(Z) \approx -c_0 Z^{7/3} + 18Z^2 - c_1 Z^{5/3} + (const) \sum_{1 \le \ell \le \ell_{\max}} (2\ell+1) n_\ell \beta(\psi_\ell).$$

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 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 $T = R^3/LZ^3$. 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

$$\Psi(x_{\sigma_1} \dots x_{\sigma_N}) = (sgn\,\sigma)\Psi(x_1 \dots x_N)\ 4.5truecmforpermutations$$

σ that preserve spin.1

$$Thekineticenergyof$$

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

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

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

j$\in$ $\{1 \dots N\}$ with $spin\ s$.3

$$We assume that$$

Ψ has low kinetic energy in the sense that

$$\|\nabla\Psi\|^2 \le (1+\delta) c_{TF} \sum_{1 \le s \le q} N_s^{5/3} L^{-2}, \quad 0 < \delta < 14$$

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

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

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 $\mathrm{S}_s(x_1, x_2, \Psi)$ is close to $\mathrm{S}_s(x_1, x_2, \Psi_0)$ 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 $\Lambda = 2\pi L Z^3 \subset R^3$. 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 $16\pi^2 R^3 L^3 \cdot (1 + Error)$, with $|Error| \leq C R^{-1} L^{-1}$.*

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

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

$$[Number of \xi \in \Lambda \cap \overline{B(0,R)}] \geq vol\left(\bigcup_{Q_\xi \subset \overline{B(0,R)}} Q_\xi\right) \Big/ ()2\pi L^3 \geq 4\pi 3 (R - 100L^{-1})^3 / ()2\pi L^3 \geq ()4\pi 3 (2\pi)^{-3} R^3 L^3 \cdot (1 - CR^{-1}L^{-1}) = 16\pi^2 R^3 L^3 \cdot (1 - CR^{-1}L^{-1}).$$

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

$$[Number of \xi \in \Lambda \cap \overline{B(0,R)}] \leq 16\pi^2 R^3 L^3 \cdot (1 + CR^{-1}L^{-1}).$$

Lemma 2: *For $RL \geq C$ and $\rho_0 = 16\pi^2 R^3$, we have*

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

with $|Error| \leq C R^{-1} L^{-1}$.

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

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

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

$$\left| \sum_{\xi \in S} |\xi|^2 - L^3 (2\pi)^3 \int_{\eta \in \bigcup_S Q_\xi} |\eta|^2 \right| \leq CRL^{-1} \cdot (Number of$$

$\xi \in S)6$ -12pt $\leq CRL^{-1} \cdot R^3 L^3 = CR^4 L^2, by Lemma 1. Now \bigcup_S Q_\xi \subset B(0,R)$, and $B(0,R) \bigcup_S Q_\xi \subset$ $B(0,R) B(0, R-100L^{-1})$. Therefore,

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

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

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

Therefore,

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

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

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

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

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

Since

$c_{TF} \rho_0^{5/3} = (6\pi^2) 10 \pi^{2\,5/3} \cdot \left(16\pi^2 R^3\right)^{5/3} = 110 \pi^2 R^5 = ()4\pi 5 (2\pi)^{-3} R^5 \ 2.0 in by (2) and the definition of$

$\rho_0,$

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

Lemma 3: *For $RL > C_1^2$ and $\rho_0 = 16\pi^2 R^3$, 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*

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

Proof: First we establish the weaker inequality

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

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 $\widetilde{\xi}$ with $|\widetilde{\xi}|^2 \geq 2 \sum_{\xi \in A_0} |\xi|^2$, 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 $\xi_2 \in \Lambda A$, then $|\xi_1| \leq |\xi_2|$, for otherwise we would have

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

With $R_1 = \max\{|\xi| : \xi \in A\}$ and $R_2 = \min\{|\xi| : \xi \in \Lambda A\}$, we have therefore $R_1 \leq R_2$. 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

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

and

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

Since $N \geq \rho_0 L^3 \cdot (1 - C_1 R^{-1} L^{-1}) \geq 12 \rho_0 L^3 (because \mathrm{RL¿C}_1^2) = 112\pi^2 R^3 L^3 \geq C_1^6 12\pi^2$, 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

$$\left| N - 16\pi^2 R_1^3 L^3 \right| \leq C R_1^2 L^2.$$

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

$$16\pi^2 R_1^3 L^3 (1 + C R_1^{-1} L^{-1}) \geq N \geq 16\pi^2 R^3 L^3 (1 - C R^{-1} L^{-1})$$

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

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

which is the desired estimate.

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

$$H(A) > C_2 R^2 L^2 14$$

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

$$L^3(2\pi)^3 vol\{B(0,R)B(0,R_1)\} = H(A)2.15$$

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

$$H(A) \leq [Number of points in \Lambda \cap \overline{B(0,R)}] < 32L^3(2\pi)^3 vol\, B(0,R).$$

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

$$L^3(2\pi)^3 vol\{B(0,R)B(0,R_1)\} + CR^2L^2 = 12H(A) + CR^2L^2.$$

The set $[\Lambda \cap \overline{B(0,R)}]A$ contains $H(A)$ points, at most $12H(A) + CR^2L^2$ of which belong to $\overline{B(0,R)B(0,R_1)}$. Therefore, $[\Lambda \cap \overline{B(0,R_1)}]A$ contains at least $12H(A) - CR^2L^2$ points.

We can also derive a lower bound for the number of points in $A\overline{B(0,R)}$. To see this, recall that A contains at least $\rho_0 L^3 \cdot (1 - C_1R^{-1}L^{-1})$ 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, $A\overline{B(0,R)}$ contains at least

$$\{\rho_0 L^3 \cdot (1 - C_1R^{-1}L^{-1})\} - \{\rho_0 L^3 \cdot (1 + CR^{-1}L^{-1}) - H(A)\} = H(A) - C'R^2L^2 \ points.$$

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

Hence we can define a new subset $\widetilde{A} \subset \Lambda$ by removing from A at least $14H(A)$ points lying outside $\overline{B(0,R)}$, and replacing them by an equal number of points of $\Lambda \cap \overline{B(0,R_1)}A$. Evidently, A and $\widetilde{A}$ contain the same number of points, so (11) applied to $\widetilde{A}$ yields

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

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

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

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

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

$R(R-R_1) \geq cH(A)RL^3$. Putting this into (17), we find that

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

which, together with (16), implies

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

This is the conclusion of the Lemma. However, to prove it, we assumed that $H(A) > C_2 R^2 L^2$.

It remains to prove the lemma assuming that $H(A) \leq C_2 R^2 L^2$. In this case, $(H(A))^2 RL^3 \leq C_3 R^3 L = C_3 R^5 L^3 R^2 L^2 = C_4 \rho_0^{5/3} L^3 R^2 L^2$. Thus, the conclusion of the lemma follows if we can show that $\sum\limits_{\xi \in A} |\xi|^2 \geq c_{TF}\rho_0^{5/3} L^3 \cdot \left(1 - C''LR + C_4 L^2 R^2\right)$. 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 $Q \subset R^3$ centered at 0. Assume $\rho|Q| > C_\varepsilon$ but $diam\, Q < 110L$. Then we can find smooth orthonormal functions $\varphi_1(x), \varphi_2(x), , \varphi_{\underline{N}}(x)$ supported in Q, with the following properties:*

(A) $|\underline{N} - \rho|Q|| \leq C_\varepsilon (\rho|Q|)^{89+3\varepsilon}$

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

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

and

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

m¿0),wherer$_F$ is the Fermi radius, given by

$$\rho = 16\pi^2 r_F^3 .18$$

(C) *For $x, y \in 34Q$ (= the middle 3/4 of Q), we have*

$$\left| \sum_{1 \leq \alpha \leq \underline{N}} \varphi_\alpha(x)\overline{\varphi_\alpha(y)} - \mathrm{S}_\rho(x-y) \right| \leq C_\varepsilon \rho \cdot \left(\underline{N}^{-19+3\varepsilon} + |x-y| diam\, Q\right),$$

with

$$\mathrm{S}_\rho(\mathrm{z}) = \int\limits_{B(0,r_F)} e^{i\eta\cdot z} d\eta (2\pi)^3 \quad and \quad r_F \quad given by (18).19$$

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

$\theta(t) = 1$ if $|t| \leq D \cdot \left(1 - (\rho|Q|)^{\varepsilon - 19}\right) \equiv D_1$.

$1 > \theta(t) > 0$ if $D \cdot \left(1 - (\rho|Q|)^{\varepsilon - 19}\right) < |t| < D$.

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

$|()ddt^\alpha \theta(t)| \leq C_\alpha \left[D \cdot (\rho|Q|)^{\varepsilon - 19}\right]^{-\alpha}$ 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 $\Phi\colon R^3 \to R^3$ 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 $\eta \in 2\pi 2 D_\# Z^3 \cap B(0, r_F \cdot \left(1 - (\rho|Q|)^{\varepsilon - 19}\right))$, we define

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

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

$$\int\limits_{R^3} \varphi_\eta(x) \overline{\varphi_{\eta'}(x)} dx = \int\limits_{Q} \varphi_\eta(x) \overline{\varphi_{\eta'}(x)} dx = (2D_\#)^{-3} \int\limits_{Q} \det \Phi'(x) \cdot \exp(i[\eta - \eta'] \cdot \Phi(x)) dx = (2D_\#)^{-3} \int\limits_{[-D_\#, +D_\#]^3} \exp(i[\eta - \eta'] \cdot y) dy = \{ ,,, 1 if \eta = \eta' 0 otherwise \}.$$

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

$$16\pi^2 \left[r_F \cdot \left(1 - (\rho|Q|)^{\varepsilon - 19}\right)\right]^3 \cdot (2D_\#)^3 + Error, 20$$

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

$$|D_\# - D| \leq C \left(\rho|Q|\right)^{\varepsilon - 19} D.$$

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

$$\underline{\mathrm{N}} = \rho|Q| + Error, with |Error| \leq C \left(\rho|Q|\right)^{\varepsilon + 89}.$$

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

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

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

$$\left|()ddt^m a\right| \le C_m(\tau B)^{-m} \left|()ddt^{m+1} g\right| \le C_m B^{-m,} \left|dgdt\right| \ge \tau, \quad with \quad 0 < \tau < 1.$$

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

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

Integration by parts gives

$$X = \pm i\lambda \int\limits_I \{ddt\,[a(t)g'(t)]\}\, e^{i\lambda g(t)} dt.20$$

bis

We estimate the derivatives of $ddt\,[a(t)g'(t)]$. The derivative $()ddt^m 1g'(t)$ is a sum of terms of the form

$$1[g'(t)]^{1+k} \prod_{\nu=1}^{k} ()ddt^{m_\nu} g'(t) \quad with$$

m$_\nu \ge 1$ and $m_1 + \cdots + m_k = m.21$

$$Inparticular,$$

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

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

Therefore,

$$|()ddt^m 1g'(t)| \le C_m \tau (\tau B)^{-m}.$$

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

$$|()ddt^m\,[a(t)g'(t)]| \le C'_m \tau \cdot (\tau B)^{-m}.$$

In particular,

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

Hence, equation (20 bis) gives

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

satisfying

$$|()ddt^m\tilde{a}(t)| \le C'_m\cdot(\tau B)^{-m},$$

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

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

with a_M supported on I, and

$$|()ddt^m a_M| \le C_{mM}(\tau B)^{-m}.$$

In particular,

$$|X| \le (\tau^2\lambda B)^{-M}\int\limits_I |a_M(t)|dt \le C_M|I|\cdot(\tau^2\lambda B)^{-M}, 22$$

with M as large as we please.

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

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

Suppose $|\xi| > r_F$ and $|\eta| \le r_F\cdot\left(1-(\rho|Q|)^{\varepsilon-19}\right)$. Set $\tau = (\rho|Q|)^{\varepsilon-19}$, $B = (\rho|Q|)^{\varepsilon-19}D$, $\lambda = |\xi|$,

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

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

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

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, $|\partial_x^\alpha(\nabla\Phi)| \le C_\alpha B^{-\alpha}$, again by the defining properties of θ. Since $|\eta| \le |\xi|$, equation (24) therefore implies

$$|\partial_x^\alpha\nabla g(x)| \le C_\alpha B^{-\alpha} \quad for$$

x$\in R^3$, α any multi-index. 26

$$Wepickanorthonormalbasis$$

e$_1$, e_2, e_3 of R^3 with $e_1 = \xi|\xi|$, 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,

$$\partial g \partial y_1 \geq 1 - |\eta||\xi|, \quad since$$

$|\nabla\Phi| \leq 127$

$$asoneseesatonceintheoriginalcoordinatesystem.Ourassumptionson$$

$|\xi|$ and $|\eta|$ yield $1 - |\eta||\xi| \geq \tau$, so (25), (26), (27) imply

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

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

$$\left| \int\limits_{-\infty}^{\infty} a(y_1, y_2, y_3) \exp(-i\lambda g(y_1, y_2, y_3)) dy_1 \right| \leq C_M D(\tau^2 \lambda B)^M,\ 4.5truecm$$

M$aslargeasweplease.29Theleft-handsidehereiszerofor|(y_2, y_3)| \geq CD$, in view of the fact that $a = (\det \Phi')^{1/2}$ is supported in Q.

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

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

Putting this into (23) and recalling the definitions of τ, λ, B, we obtain for $|\xi| \geq r_F$, $|\eta| \leq r_F \cdot \left(1 - (\rho|Q|)^{\varepsilon - 19}\right)$ the estimate

$$|\widehat{\varphi}_\eta(\xi)| \leq C_M D^{3/2} \left\{(\rho|Q|)^{2\varepsilon - 29} |\xi| (\rho|Q|)^{\varepsilon - 19} D\right\}^{-M},$$

i.e.

$$|\widehat{\varphi}_\eta(\xi)| \leq C_M D^{32} \left\{(\rho|Q|)^{3\varepsilon - 13} |\xi| D\right\}^{-M} 30$$

Since $r_F \sim \rho^{1/3}$ and $D \sim |Q|^{13}$, $\rho|Q| \sim \underline{\mathrm{N}}$, we have

$$(\rho|Q|)^{3\varepsilon-13}|\xi|D = r_F^{-1}|\xi| \cdot (r_F D)(\rho|Q|)^{3\varepsilon-13} \qquad \sim r_F^{-1}|\xi|(\rho|Q|)^{1/3} \cdot (\rho|Q|)^{3\varepsilon-13} \sim \underline{\mathrm{N}}^{3\varepsilon}|\xi|r_F^{-1},$$

so that (30) may be rewritten as

$$|\widehat{\varphi}_\eta(\xi)| \leq C_M |Q|^{1/2} (\underline{\mathrm{N}}^{3\varepsilon} |\xi| r_F^{-1})^{-M},\ 4.5truecmwith$$

M$aslargeasweplease.31 Estimate (31) holds for |\xi| \geq r_F,\ |\eta| \leq r_F \cdot \left(1-(\rho|Q|)^{\varepsilon-19}\right)$.

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

$$\int\limits_{Q_\xi} (r_F|\zeta|)^M \, d\zeta \geq c_M \, (r_F|\xi|)^M \, L^{-3} \quad for \quad |\xi| \geq r_F.$$

Therefore, (31) implies

$$\sum_{\xi \in \Lambda B(0,r_F)} L^{-3}|\widehat{\varphi}_\eta(\xi)|^2 \leq C_M|Q|\underline{\mathrm{N}}^{-3\varepsilon M} \sum_{\xi \in \Lambda B(0,r_F)} (r_F|\xi|)^M \, L^{-3} 32 \leq C'_M|Q|\underline{\mathrm{N}}^{-3\varepsilon M} \sum_{\xi \in \Lambda B(0,r_F)} \int\limits_{Q_\xi} (r_F|\zeta|)^M \, d\zeta \leq C''_M|Q|\underline{\mathrm{N}}^{-3\varepsilon M} \int\limits_{R^3 B(0,cr_F)} (r_F|\zeta|)^M \, d\zeta \leq C'''_M|Q|\underline{\mathrm{N}}^{-3\varepsilon M} r_F^3 \quad for \quad M > 3.$$

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

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

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

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

completing the proof of conclusion (B).

Turning to conclusion (C), we take $x, y \in 34Q$. Then Φ is the identity map near x and near y, so that

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

Hence

$$\sum_\eta \varphi_\eta(x)\overline{\varphi_\eta(y)} = (2D_\#)^{-3} \sum_{\eta \in 2\pi(2D_\#)Z^3} \exp(i\eta\cdot[x-y]) 33 |\eta| < r_F \cdot \left(1-(\rho|Q|)^{\varepsilon-19}\right)$$

Set $\tilde{r}_F = r_F \cdot \left(1-(\rho|Q|)^{\varepsilon-19}\right)$, and introduce a cube Q_η centered at $\eta \in 2\pi(2D_\#)Z^3$, with side$2\pi(2D_\#)$. We have

$$|\exp(i\eta\cdot[x-y]) - (2D_\#)^3(2\pi)^3 \int\limits_{Q_\eta} \exp(i\zeta\cdot[x-y])d\zeta| \leq C|x-y|diam\, Q_\eta \sim C|x-y|diam\, Q,$$

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

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

$$|(2D_{\#})^{-3}\sum \eta \in 2\pi 2D_{\#}Z^3|\eta| < \tilde{r}_F \exp(i\eta\cdot[x-y]) - \int\limits_E \exp(i\zeta\cdot[x-y])d\zeta(2\pi)^3| \leq 34C|x-y| diam\, QD_{\#}^{-3}\cdot[Number of$$

$\eta \in 2\pi 2D_{\#}Z^3$ with $|\eta| < \tilde{r}_F]$.

$$The right-hand side of (34) has the order of magnitude$$

C$|x-y| diam\, QD_{\#}^{-3}\cdot[D_{\#}^3 r_F^3]$, 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

$$\left|\sum_\eta \varphi_\eta(x)\overline{\varphi_\eta(y)} - \int\limits_E \exp(i\eta\cdot[x-y])d\zeta(2\pi)^3\right| \leq C|x-y| diam\, Q r_F^3 35 \leq C'\rho|x-y| diam\, Q$$

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

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

Consequently,

$$\left|\int\limits_E \exp(i\zeta\cdot[x-y])d\zeta(2\pi)^3 - \int\limits_{B(0,\tilde{r}_F)} \exp(i\zeta\cdot[x-y])d\zeta(2\pi)^3\right| 36 \leq \int\limits_{B(0,\tilde{r}_F+100D^{-1})B(0,\tilde{r}_F-100D^{-1})} |\exp(i\zeta\cdot[x-y])| d\zeta(2\pi)^3 \leq C r_F^2 D^{-1}.$$

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

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

Hence, (35) and (36) yield

$$\left|\sum_\eta \varphi_\eta(x)\overline{\varphi_\eta(y)} - \int\limits_{B(0,\tilde{r}_F)} \exp(i\zeta\cdot[x-y])d\zeta(2\pi)^3\right| \leq C\rho\left(|x-y| diam\, Q + \underline{\mathrm{N}}^{-13}\right).37$$

Also,

$$\left|\int\limits_{B(0,\tilde{r}_F)} \exp(i\zeta\cdot[x-y])d\zeta(2\pi)^3 - \int\limits_{B(0,r_F)} \exp(i\zeta\cdot[x-y])d\zeta(2\pi)^3\right| \leq vol\{B(0,r_F)B(0,\tilde{r}_F)\} \leq C r_F^2\cdot(r_F - \tilde{r}_F) \sim C\rho\cdot(\rho|Q|)^{\varepsilon-19} \sim C\rho\underline{\mathrm{N}}^{\varepsilon-19}.$$

Combining this with (37), we obtain

$$\left|\sum_{\eta}\varphi_{\eta}(x)\overline{\varphi_{\eta}(y)} - \int\limits_{B(0,r_F)} \exp(i\zeta\cdot[x-y])d\zeta(2\pi)^3\right| \leq C\rho\left(|x-y|diam\, Q + \underline{N}^{\varepsilon-19}\right).$$

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

For each spin s $(1 \leq s \leq q)$, define the density $\rho_s = N_s L^3$ of particles with spin s, and define the Fermi radius r_F^s by $\rho_s = 16\pi^2(r_F^s)^3$ as in (18). Let Q be a cube in R^3, centered at 0, with $diam\, Q < 110L$ but $\rho_s|Q| > C_\varepsilon$ (as in Lemma 4) for each s. Lemma 4 constructs a finite orthonormal family $\varphi_{1,s}(x)$, $\varphi_{2,s}(x)$, , $\varphi_{\underline{N}_s,s}(x)$ of smooth functions supported in Q. According to Lemma 4, we have

$1\; |\underline{N}_s - \rho_s|Q|\,| \leq C_\varepsilon(\rho_s|Q|)^{89+3\varepsilon} 38 |\widehat{\varphi}_{\alpha,s}(\xi)| \leq C|Q|^{1/2} \quad forall \quad \xi,\ 1 \leq \alpha \leq \underline{N}_s 39 \sum\limits_{\xi\in\Lambda B(0,r_F^s)} |\widehat{\varphi}_{\alpha,s}(\xi)|^2 L^3 \leq C_{m\varepsilon}\underline{N}_s{}^{-m} \quad (any$

m¿0)$for \quad 1 \leq \alpha \leq \underline{N}_s.40 \left|\sum\limits_{1\leq\alpha\leq\underline{N}_s} \varphi_{\alpha,s}\overline{\varphi_{\alpha,s}(y)} - \mathrm{S}_{\rho_s}(x-y)\right| \leq C_\varepsilon\rho_s\cdot\left(\underline{N}_s^{-19+3\varepsilon} + |x-y|diam\, Q\right) 41 \qquad forx,y\in$

$34Q$, with S_ρ(z) defined by (19).

Here

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

For each s, we complete $\varphi_{1,s}\ldots\varphi_{\underline{N}_s,s}$ to an orthonormal basis $(\varphi_{\alpha,s})_{1\leq\alpha<\infty}$ 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 $(\varphi_{\alpha,s})_{-\infty<\alpha\leq 0}$ be an orthonormal basis for the L^2 functions supported in TQ, for each fixed s. Thus, for each s, $(\varphi_{\alpha,s})_{-\infty<\alpha<\infty}$ is an orthonormal basis for $L^2(T)$. For each z $\in T$ we form the translates $\varphi^{\mathrm{z}}_{\alpha,s}(x) = \varphi_{\alpha,s}(x-\mathrm{z})$. Thus for fixed z and s, the $(\varphi^{\mathrm{z}}_{\alpha,s})_{-\infty<\alpha<\infty}$ form an orthonormal basis of $L^2(T)$, with $\varphi^{\mathrm{z}}_{\alpha,s}$ supported in $Q+\mathrm{z}$ when $\alpha \geq 1$, and supported in $T(Q+\mathrm{z})$ when $\alpha \leq 0$.

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

$$\Psi(x_1\ldots x_N) = \sum_{\alpha_1\ldots\alpha_N} C^{\mathrm{z}}_{\alpha_1\ldots\alpha_N}\prod_{s=1}^{q}\Bigg(\prod_{spin(j)=s}\varphi^{\mathrm{z}}_{\alpha_j,s}(x_j)\Bigg).42$$

Note that

$$\sum_{\alpha_1\ldots\alpha_N}|C^{\mathrm{z}}_{\alpha_1\ldots\alpha_N}|^2 = 1, 43$$

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

We also make a standard Fourier expansion of Ψ:

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

We have

$$\sum_{\xi_1\ldots\xi_N\in\Lambda}|A_{\xi_1\ldots\xi_N}|^2=1,45$$

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 $spin(j)=s$ are all distinct.

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

$$\sum_{(\alpha_1\ldots\alpha_N)\notin \mathrm{B}}|C^{\mathrm{z}}_{\alpha_1\ldots\alpha_N}|^2\quad issmallcomparedto$$

$1.Toprovethis, weintroducethenumbers\mu_s(\mathrm{z},\alpha)$, defined by setting

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

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

$$\int\limits_T\overline{\varphi^{\mathrm{z}}_{\alpha,s_0}(x_j)}\Psi(x_1\ldots x_N)dx_j=\sum_{\alpha_1\ldots\alpha_N}\chi_{\alpha_j=\alpha}C^{\mathrm{z}}_{\alpha_1\ldots\alpha_N}\prod_{s=1}^{q}\left(\prod spin(i)=si\neq j\varphi^{\mathrm{z}}_{\alpha_i,s}(x_i)\right)$$

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

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

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

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

This and (43) yield

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

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

$$\mathrm{B}_{\alpha,s}=\{(\alpha_1\ldots\alpha_N)|\alpha_j=\alpha forsome$$

$j with \mathrm{spin}\, s\ \}, 48 equation (47) becomes \mu_s(\mathrm{z},\alpha) = \sum_{(\alpha_1\ldots\alpha_N)\notin \mathrm{B}_{\alpha,s}} |C^{\mathrm{z}}_{\alpha_1\ldots\alpha_N}|^2 .49$

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

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

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

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

so (44) implies

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

which in turn gives

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

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

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

In view of (45), this is equivalent to

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

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

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

with

$$\mathrm{A}_s(\xi_1 \ldots \xi_N) = \{\xi_j \ \big|\ spin(j) = s\} .53$$

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

$$\left(1 - \sum_{spin(j)=s} |\widehat{\varphi}_{\alpha,s}(\xi_j)|^2 L^3\right) = \sum_{\xi\in\Lambda\mathrm{A}_s(\xi_1\ldots\xi_N)} |\widehat{\varphi}_{\alpha,s}(\xi)|^2 L^3 54 \leq \left[\sum_{\xi\in\Lambda B(0,r_F^s)} |\widehat{\varphi}_{\alpha,s}(\xi)|^2 L^3\right] + \sum_{\xi\in\Lambda\cap B(0,r_F^s)\mathrm{A}_s(\xi_1\ldots\xi_N)} |\widehat{\varphi}_{\alpha,s}(\xi)|^2 L^3 \leq \left[\sum_{\xi\in\Lambda B(0,r_F^s)} |\widehat{\varphi}_{\alpha,s}(\xi)|^2 L^3\right] + \|\widehat{\varphi}_{\alpha,s}\|^2_{L^\infty} L^3 H_s(\xi_1\ldots\xi_N),$$

with $H_s(\xi_1\ldots\xi_N)$ equal to the number of points of $\Lambda\cap B(0,r_F^s)$ not belonging to $\mathrm{A}_s(\xi_1\ldots\xi_N)$. That is, $H_s(\xi_1\ldots\xi_N)$ 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

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

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

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

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

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

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

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

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

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

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

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