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Asymptotic Neutrality of Large Ions

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Abstract. It is proved that a nucleus of charge Z can bind at most $Z + O(Z^a)$ electrons, with $a = 47/56$.

Consider the Hamiltonian for a nucleus of charge Z and N quantized electrons,

$$H_{Z,N} = \sum_{i=1}^{N} \left[(-\Delta_{x_i}) - \frac{Z}{|x_i|} \right] + \frac{1}{2} \sum_{i \neq j} \frac{1}{|x_i - x_j|} = -\Delta + V_{\text{Coulomb}}.$$

The ground state energy is then

$$E(Z) = \inf_N E(Z, N) = \inf_N \inf_{\substack{\psi \in \mathscr{H} \\ \|\psi\|_2 = 1}} \langle H_{Z,N}\psi, \psi \rangle,$$

where $\mathscr{H} = \bigwedge_{i=1}^{N} (L^2(\mathbf{R}^3) \otimes \mathbf{C}^q)$ is the space of antisymmetric wave functions with q spins. Throughout this paper we will simply refer to them as "antisymmetric" wave functions.

For each Z, call $N(Z)$ the smallest number for which $E(Z) = E(Z, N)$. It is an interesting problem to obtain sharp estimates for $N(Z)$. The sharpest known result appears in [8], where the reader will find a discussion of the history of the problem. In particular, $N(Z)/Z \to 1$ as $Z \to \infty$, although there were no estimates for the rate of convergence. Our main result is the following:

Theorem.

$$N(Z) = Z + O(Z^\alpha) \quad \text{for} \quad \alpha = \frac{47}{56}.$$

We announced this result in [1]. We are grateful to V. Bach for pointing out a

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minor error in our announcement. The rest of the paper is devoted to the proof of this theorem.

For the proof we will be interested only in the case $Z \leqq N \leqq 2Z$. Lieb ([6] and [7]) has given a simple argument to handle the case $N > 2Z$. Thomas–Fermi theory will play a central role in the proof. We recall a few fundamental facts. For a nice detailed discussion see [5].

1. $E(Z) \sim C_{\mathrm{TF}} Z^{7/3}$ as $Z \to \infty$.
2. Let ρ_{TF} be Thomas–Fermi density. Then:

a. $\int_{\mathbf{R}^3} \rho_{\mathrm{TF}}(x)dx = Z$.
b. For $|x| > Z^{-1/3+\varepsilon}$, $\rho_{\mathrm{TF}}(x) \leqq C|x|^{-6}$.
c. $\int_{|x|>R} \rho_{\mathrm{TF}}(x)dx \leqq C_{\rho\mathrm{TF}} R^{-3}$ for $R > Z^{-1/3}$, for some constant $C_{\rho\mathrm{TF}}$.

1. Key Estimate

Fix N points in $\mathbf{R}^3$, $x_1, \ldots, x_N$. Take a radially symmetric function ϕ, supported in $B(0, \frac{1}{100} Z^{-2/3})$, $\int \phi = 1$, $\sup|\phi| \leqq CZ^2$, and set $\rho_{x_1,\ldots,x_N}(x) = \sum_i \phi(x - x_i)$. Observe that the subharmonicity and positive-definiteness of the Coulomb potential implies that

$$\begin{aligned}
\sum_{i<j} \frac{1}{|x_i - x_j|} &\geqq \tfrac{1}{2} \iint \frac{\rho_{x_1,\ldots,x_N}(x)\rho_{x_1,\ldots,x_N}(y)}{|x-y|} dx\,dy - CZ^{2/3} \cdot N \\
&= \tfrac{1}{2} \iint \frac{(\rho_{x_1,\ldots,x_N} - \rho_{\mathrm{TF}})(x)(\rho_{x_1,\ldots,x_N} - \rho_{\mathrm{TF}})(y)}{|x-y|} dx\,dy \\
&\quad + \iint \frac{\rho_{x_1,\ldots,x_N}(x)\rho_{\mathrm{TF}}(y)}{|x-y|} dx\,dy - \tfrac{1}{2} \iint \frac{\rho_{\mathrm{TF}}(x)\rho_{\mathrm{TF}}(y)}{|x-y|} dx\,dy - CZ^{2/3} \cdot N \\
&= c \int |\xi|^{-2} |\hat{\rho}_{x_1,\ldots,x_N}(\xi) - \hat{\rho}_{\mathrm{TF}}(\xi)|^2 d\xi \\
&\quad + \sum_j W(x_j) - \tfrac{1}{2} \iint \frac{\rho_{\mathrm{TF}}(x)\rho_{\mathrm{TF}}(y)}{|x-y|} dx\,dy - C/Z^{2/3} \cdot N
\end{aligned}$$

with

$$W(x) = \iint \frac{\phi(x-z)\rho_{\mathrm{TF}}(y)}{|z-y|} dz\,dy.$$

Let's set

$$K(x_1, \ldots, x_N) = \tfrac{1}{2} \iint \frac{(\rho_{x_1,\ldots,x_N} - \rho_{\mathrm{TF}})(x)(\rho_{x_1,\ldots,x_N} - \rho_{\mathrm{TF}})(y)}{|x-y|} dx\,dy$$

and note that $K \geqq 0$ pointwise. This provides the operator inequality

$$H_{Z,N} \geqq K + \sum_{i=1}^{N} \left[(-\Delta_{x_i}) - \frac{Z}{|x_i|} + W(x_i) \right] - \tfrac{1}{2} \iint \frac{\rho_{\mathrm{TF}}(x)\rho_{\mathrm{TF}}(y)}{|x-y|} dx\,dy - CZ^{5/3}$$

for $N \leqq 2Z$. We point out that similar inequalities were used in [2] and [4].

Let $\lambda_1, \lambda_2, \ldots$ be the negative eigenvalues of

$$(-\Delta_x) - \frac{Z}{|x|} + W(x),$$

and let

$$\tilde{E}(Z) = q \sum_{i=1}^{\infty} \lambda_i - \tfrac{1}{2} \iint \frac{\rho_{\mathrm{TF}}(x)\rho_{\mathrm{TF}}(y)}{|x-y|}\, dx\, dy.$$

It follows then that

$$H_{Z,N} \geqq \tilde{E}(Z) + O(Z^{5/3})$$

for all N between Z and $2Z$. From [3] we know that for some b between 1/3 and 2/3 we have

$$\tilde{E}(Z) \geqq C_{\mathrm{TF}} Z^{7/3} + \frac{q}{8} Z^2 + O(Z^{7/3-b}).$$

A careful exposition of Hughes' proof appears in [10]. Similarly, it follows from [7] that

$$E(Z,N) \leqq C_{\mathrm{TF}} Z^{7/3} + \frac{q}{8} Z^2 + O(Z^{7/3-b})$$

for all $N \geqq Z$.

Putting all this together we see that

$$\tilde{E}(Z) \geqq E(Z,N) + O(Z^{7/3-b})$$

for any N between Z and $2Z$. In particular, we have

$$H_{Z,N} \geqq E_0(Z) + K(x_1, \ldots, x_N) - C_{\mathrm{HSW}}(Z^{7/3-b}) \tag{1}$$

for

$$E_0(Z) = \inf_{N \leqq (1+\varepsilon^{\#})Z} E(Z,N),$$

where $\varepsilon^{\#}$ will be picked later, and some constant C_{HSW}. The constant b plays a crucial role in the analysis of the best possible power of Z for the excess charge. From [3] and [7] it follows that we can take $b = \frac{3}{8}$: this implies that we can take $\alpha = \frac{47}{56}$ in the statement of the theorem. Notice however that this value of b has been obtained using a much stronger result, namely the correct asymptotics for the energy. It is clear that one can do better and may be one can take $b = \frac{2}{3}$, which would allow us to take $\alpha = \frac{5}{7}$.

2. Estimates for a Ball

What we are planning to do now is conclude that if the number of electrons a particular state puts inside a ball is too different from what Thomas–Fermi theory predicts, then this state will have too much energy. This will be then generalized to random variables other than the number of electrons inside a ball. We need a few definitions.

Consider a ball $B(0, R)$. Define

$$N_R(x_1, \ldots, x_N) = \text{number of } x_i \in B(0, R).$$

Also, take a smooth function

$$\chi = \begin{cases} 1 & \text{for} \quad |x| < \frac{4}{3}R \\ 0 & \text{for} \quad |x| > \frac{5}{3}R \end{cases}$$

that we will call χ_R whenever we want to make it explicit which R is being used, and let

$$N_\chi(x_1, \ldots, x_N) = \sum_i \phi * \chi(x_i) = \int \rho_{x_1, \ldots, x_N}(x) \cdot \chi(x) dx.$$

Observe that $N_{R/2}(x_1, \ldots, x_N) \leqq N_\chi(x_1, \ldots, x_N) \leqq N_{2R}(x_1, \ldots, x_N)$, for all $x_1, \ldots, x_N$, provided $R > 2Z^{-2/3}$, which will certainly hold in our case, since we will be working with $R \geqq Z^{-1/3}$.

Define

$$N_\chi^{\mathrm{TF}} = \int \rho_{\mathrm{TF}}(x) \chi(x) dx.$$

Now, note that

$$N_\chi(x_1, \ldots, x_N) - N_\chi^{\mathrm{TF}} = \int (\rho_{x_1, \ldots, x_N} - \rho_{\mathrm{TF}})(x) \chi(x) dx = \int (\hat{\rho}_{x_1, \ldots, x_N} - \hat{\rho}_{\mathrm{TF}})(\xi) \hat{\chi}(\xi) d\xi.$$

Hence

$$|N_\chi - N_\chi^{\mathrm{TF}}|^2 \leqq \int |\hat{\chi}(\xi)|^2 \cdot |\xi|^2 d\xi \int |(\hat{\rho}_{x_1, \ldots, x_N} - \hat{\rho}_{\mathrm{TF}})|^2 \cdot |\xi|^{-2} d\xi \leqq CR \cdot K(x_1, \ldots, x_N).$$

Therefore, (1) implies

$$\langle H_{Z,N}\psi, \psi \rangle \geqq E_0(Z) + C_K \frac{\langle |N_\chi - N_\chi^{\mathrm{TF}}|^2 \psi, \psi \rangle}{R} - C_{\mathrm{HSW}}(Z^{7/3-b})$$

for some constant C_K. In particular, Cauchy–Schwarz implies

$$\langle H_{Z,N}\psi, \psi \rangle \geqq E_0(Z) + C_K \frac{|\langle N_\chi \psi, \psi \rangle - N_\chi^{\mathrm{TF}}|^2}{R} - C_{\mathrm{HSW}}(Z^{7/3-b}) \qquad \text{(A)}$$

for any antisymmetric ψ, $\|\psi\|_2 = 1$.

The previous argument can be generalized to yield the following result:

Lemma 2.1. *Given any function $\varphi(x) \in L^2(\mathbf{R}^3)$, we have*

$$\langle H_{Z,N}\psi, \psi \rangle \geqq E_0(Z) + C_K \frac{|\langle (\rho_\psi * \phi - \rho_{\mathrm{TF}}), \varphi \rangle|^2}{\|\nabla \varphi\|_2^2} - C_{\mathrm{HSW}}(Z^{7/3-b})$$

for $\psi \in \mathscr{H}$, $\|\psi\|_2 = 1$. Here,

$$\rho_\psi = N \int |\psi(x, x_2, \ldots, x_N)|^2 dx_2 \cdots dx_N$$

in the case of a fully antisymmetric ψ (i.e. $q = 1$) *and in general*

$$\rho_\psi(x) = \sum_{i=1}^{N} \int |\psi(x_1, \dots, x_{i-1}, x, x_{i+1}, \dots, x_N)|^2 \prod_{i \neq j} dx_j.$$

Now, we define a working variant of estimate (A).

Definition. *We say that* Estimate $(\bar{\varepsilon}, \varepsilon, R)$ *holds if for a nucleus of charge Z at the origin and N quantized electrons confirmed to the ball B* $(0, R)$ *we have*

$$\langle H_{Z,N}\psi, \psi\rangle \geqq E_0(Z) + \frac{\bar{\varepsilon}Z}{R}(N - (1 + \varepsilon)Z)$$

for normalized ψ, *where*

$$E_0(Z) = \inf_{0 \leqq N \leqq (1+\varepsilon^{\#})Z} E(Z, N)$$

for $\varepsilon^{\#}$ *to be picked later. By N quantized electrons confined to the ball* $B(0, R)$ *we mean that* $\psi = \psi(x_1, \dots, x_N)$ *is supported in the set* $x_i \in B(0, R)$ *for all* $i = 1, \dots, N$.

Now it will be necessary to introduce two parameters γ_1 and γ_2, in the proof. They are related to b by the relation

1. $\gamma_1 = \frac{3}{7}b$.
2. $\gamma_2 = b/7$.

The significance of γ_1 is that it represents the excess charge. Precisely

$$N(Z) = Z + O(Z^{1-\gamma_1}).$$

On the other hand, γ_2 is related to the radius of the largest ball for which we can obtain favourable estimates for its excess charge. This is clearly seen in the following lemma.

Lemma 2.2. *There exist constants* C_0 *and* c_0 *independent of Z, such that* Estimate $(\bar{\varepsilon}, \varepsilon, R)$ *holds for*

1. $\varepsilon^{\#} \geqq \varepsilon \geqq C_0 Z^{-\gamma_1}$,
2. $\bar{\varepsilon} \leqq c_0 Z^{-\gamma_1}$,
3. $R \leqq C_0 Z^{-1/3+\gamma_2}$.

Proof. Pick R, ε and $\bar{\varepsilon}$ within this range. Say ψ confines N electrons to $B(0, R)$. If $N \leqq (1 + \varepsilon)Z$, then

$$\begin{aligned}\langle H_{Z,N}\psi, \psi\rangle &\geqq E(Z, N) \geqq E_0(Z) \\ &\geqq E_0(Z) + \frac{\bar{\varepsilon}Z}{R}(N - (1 + \varepsilon)Z).\end{aligned}$$

If $N > (1 + \varepsilon)Z$, then

$$\langle N_\chi\psi, \psi\rangle > (1 + \varepsilon)Z$$

for $\chi = \chi_{2R}$. Since $N_\chi^{\mathrm{TF}} < Z$,

$$C_K \frac{|\langle N_\chi \psi, \psi\rangle - N_\chi^{\mathrm{TF}}|^2}{2R} > C_K \frac{|N-Z|^2}{2R} > C_K \frac{\varepsilon^2 Z^2}{2R}$$

$$> \frac{C_K C_0^2}{2C_0} Z^{7/3-(2\gamma_1+\gamma_2)} \geqq 2C_{\mathrm{HSW}} Z^{7/3-b}$$

for C_0 large enough; so,

$$\langle H_{Z,N}\psi, \psi\rangle \geqq E_0(Z) + C_K \frac{|N-Z|^2}{4R}.$$

On the other hand,

$$C_K \frac{|N-Z|^2}{4R} > \frac{\bar{\varepsilon} Z}{R}(N-(1-\varepsilon)Z) \quad \text{for} \quad N \geqq (1+\varepsilon)Z. \tag{2}$$

To see this, observe that it holds trivially at $N = (1+\varepsilon)Z$, because the right-hand side is zero; if now we differentiate both sides with respect to N, we obtain for the left-hand side

$$\frac{C_K(N-Z)}{2R} > \frac{C_K}{2} \cdot \frac{\varepsilon Z}{R}$$

and $\bar{\varepsilon} Z/R$ for the right-hand side. So Estimate $(\bar{\varepsilon}, \varepsilon, R)$ holds taking c_0 small enough.

Throughout the proof we will need a couple more conditions on C_0 and c_0 that will force us to take them to be larger and smaller respectively than what we needed for this lemma.

Lemma 2.3. *Let $R = Z^{-1/3+\gamma_2}$, and $\chi = \chi_R$. Say that for a number Y,*

$$\langle N_\chi \psi, \psi\rangle = Z + YZ^{1-\gamma_1}.$$

Then, for some universal constant c_1,

$$\langle H_{Z,N}\psi, \psi\rangle \geqq E_0(Z) + C_K \frac{(|Y|-c_1)_+^2 Z^{2-2\gamma_1}}{4R} - C_{\mathrm{HSW}} Z^{7/3-b}.$$

Proof. Observe that we have

$$N_\chi^{\mathrm{TF}} \geqq Z - \int_{|x| \geqq R/2} \rho_{\mathrm{TF}}(x)dx \geqq Z - 8C_{\rho\mathrm{TF}} Z^{1-3\gamma_2} = Z - 8C_{\rho\mathrm{TF}} Z^{1-\gamma_1}$$

and $N_\chi^{\mathrm{TF}} \leqq Z$. Thus,

$$\frac{|\langle N_\chi \psi, \psi\rangle - N_\chi^{\mathrm{TF}}|^2}{R} \geqq \frac{(\langle N_\chi \psi, \psi\rangle - N_\chi^{\mathrm{TF}})_+^2}{R} \geqq \frac{(Y)_+^2 Z^{2-2\gamma_1}}{R}$$

and

$$\frac{|\langle N_\chi \psi, \chi\rangle - N_\chi^{\mathrm{TF}}|^2}{R} \geqq \frac{(N_\chi^{\mathrm{TF}} - \langle N_\chi \psi, \psi\rangle)_+^2}{R} \geqq \frac{(-Y - 8C_{\rho\mathrm{TF}})_+^2 Z^{2-2\gamma_1}}{R}.$$

Applying (A) to both cases and averaging the resulting inequalities, we get

$$\langle H_{Z,N}\psi, \psi\rangle \geqq E_0(Z) + C_K Z^{2-2\gamma_1} \frac{(-Y - 8C_{\rho\mathrm{TF}})_+^2 + (Y)_+^2}{2R} - C_{\mathrm{HSW}} Z^{7/3-b}.$$

Elementary calculus says that

$$(-x-c)_+^2 + (x)_+^2 \geqq \frac{(|x|-c')_+^2}{2},$$

and this implies the conclusion of the lemma.

The previous estimates could have been done for R of the form $Z^{-1/3+\gamma}$ for $\gamma \leqq \gamma_2$, with the only effect of decreasing γ_1 and thus worsening a little the estimates for the excess charge. However, they cannot be carried out with these techniques for $\gamma > \gamma_2$, since whatever term we want to estimate will give a contribution so small to the energy that it will simply be lost in the $O(Z^{7/3-b})$. For radii this big we need a different approach in which we use in a more direct way the properties of the Coulomb potential. The goal of the next section is to analyze how estimates for a given ball imply corresponding estimates for its double.

3. Estimates for Spherical Shells

In this section we consider a system of N quantized electrons confined to $B(0,R)$, and N' electrons confined to $B(0,2R)-B(0,R/2)$. That is, we will be considering wave functions $\psi(x_1,\dots,x_N, x'_1,\dots,x'_{N'})$ supported on the set $x_1,\dots,x_N \in B(0,R)$, $x'_1,\dots,x'_{N'} \in B(0,2R)-B(0,R/2)$. We have to impose the extra condition that for fixed $x'_1,\dots,x'_{N'}$, ψ is antisymmetric in the $x_1,\dots,x_N$ and viceversa: that is, we will be considering vector-valued ψ, with domain $x'_1,\dots,x'_{N'} \in B(0,2R)-B(0,R/2)$, and values in $\mathscr{H}$ and vector-valued ψ, with domain $x_1,\dots,x_N \in B(0,R)$, and values in $\mathscr{H}$.

To stress the different role of the two sets of electrons, we rewrite the hamiltonian as

$$H_{Z,N+N'} = H_{Z,N} + H_{\text{extra}} = (-\Delta_{x_1,\dots,x_N} + V) + (-\Delta_{\text{extra}} + V_{\text{extra}})$$

with

$$\Delta_{\text{extra}} = \Delta_{x'_1,\dots,x'_{N'}},$$

$$V = -\sum_{i=1,\dots,N} \frac{Z}{|x_i|} + \frac{1}{2}\sum_{i\neq j} \frac{1}{|x_i - x_j|},$$

$$V_{\text{extra}} = -\sum_{i=1,\dots,N'} \frac{N}{|x'_i|} + \sum_{\substack{i=1,\dots,N'\\ j=1,\dots,N}} \frac{1}{|x'_i - x_j|} + \frac{1}{2}\sum_{\substack{i=1,\dots,N'\\ j=1,\dots,N'\\ i\neq j}} \frac{1}{|x'_i - x'_j|}.$$

Also, we restrict our attention to the case $R > C_0 R_* = C_0 Z^{-1/3+\gamma_2}$.

The content of the following lemma is as follows: We know from previous estimates that approximately Z of the electrons will organize themselves to be close to the nucleus; this will have the important effect of "screening" the nucleus. That is, all the other electrons will hardly feel any negative electrostatic potential; this has as a consequence that a lot more than Z electrons will only make the energy of the system grow above the ground state energy.

Lemma 3.1. *Assume that* $N + N' \geqq (1+\delta)Z$ *for*

$$C_0 Z^{-\gamma_1} \leqq \delta < (1+10^{-6}) C_0 Z^{-\gamma_1}.$$

Then, for some constant c,

$$\langle V_{\text{extra}}\psi,\psi\rangle \geqq \frac{c\delta Z}{R}N'$$

or else

$$\langle H_{Z,N+N'}\psi,\psi\rangle \geqq E_0(Z)+cZ^{7/3-7\gamma_2}.$$

Proof. We will assume that $N' \neq 0$ or else there is nothing to prove. Recall that $R_* = Z^{-1/3+\gamma_2}$. Let $\chi = \chi_{R_*}$. Note that

$$N_\chi = \sum_{i=1,\dots,N} \chi*\phi(\chi_i) + \sum_{j=1,\dots,N'} \chi*\phi(x_j') = \sum_{i=1,\dots,N} \chi*\phi(x_i)$$

as operators on our space of functions, since $\chi*\phi$ and ψ have disjoint support in the x_j' variables.

Let $V_{\text{extra}} = \sum_j V_j(x_1,\dots,x_N,x_1',\dots,x_{N'}')$ for

$$V_j = -\frac{Z}{|x_j'|} + \sum_{i=1,\dots,N}\frac{1}{|x_j'-x_i|} + \frac{1}{2}\sum_{\substack{i=1,\dots,N'\\ i\neq j}}\frac{1}{|x_i'-x_j'|}.$$

Note that

$$\sum_{i=1}^N \frac{1}{|x_j'-x_i|} = \sum_{i=1}^N \frac{\chi*\phi(x_i)}{|x_j'-x_i|} + \sum_{i=1}^N \frac{1-\chi*\phi(x_i)}{|x_j'-x_i|},$$

$$-\frac{Z}{|x_j'|} = -\frac{Z-N_\chi}{|x_j'|} - \sum_{i=1}^N \frac{\chi*\phi(x_i)}{|x_j'|},$$

and write

$$\begin{aligned} V_j(x_1,\dots,x_N,x_1',\dots,x_{N'}') &= -\frac{Z-N_\chi}{|x_j'|} + \sum_{i=1}^N \frac{1-\chi*\phi(x_i)}{|x_j'-x_i|} \\ &\quad + \frac{1}{2}\sum_{\substack{i=1,\dots,N'\\ i\neq j}}\frac{1}{|x_j'-x_i'|} + \sum_{i=1}^N\left(\frac{1}{|x_j'-x_i|}-\frac{1}{|x_j'|}\right)\cdot(\chi*\phi)(x_i) \\ &= T_1+T_2+T_3+T_4. \end{aligned}$$

Let's analyze this term by term:

·) $\langle T_1\psi,\psi\rangle \geqq -\dfrac{|Z-\langle N_\chi\psi,\psi\rangle|}{R/2}$.

·) $T_2 \geqq \dfrac{N-N_\chi}{8R}$ pointwise.

·) $\langle T_3\psi,\psi\rangle \geqq \dfrac{N'-1}{8R}$.

Therefore

$$\langle (T_1 + T_2 + T_3)\psi, \psi\rangle \geqq \frac{N + N' - \langle N_\chi \psi, \psi\rangle - 16|Z - \langle N_\chi \psi, \psi\rangle| - 1}{8R}$$

$$\geqq \frac{\delta Z - 20|Z - \langle N_\chi \psi, \psi\rangle| + \Omega}{9R}$$

for $\Omega = N + N' - \delta Z - Z$. Note that by hypothesis, $\Omega \geqq 0$. Summing over all j we obtain

$$\sum_{j=1}^{N'} \langle (T_1 + T_2 + T_3)\psi, \psi\rangle \geqq \frac{\delta Z - 20|Z - \langle N_\chi \chi, \psi\rangle| + \Omega}{9R} N'. \tag{3}$$

If we could prove that $|Z - \langle N_\chi \psi, \psi\rangle| < cZ^{1-\gamma_1}$ for some constant independent of C_0, then we would have

$$\langle (T_1 + T_2 + T_3)\psi, \psi\rangle \geqq \frac{\delta Z - 20|Z - \langle N_\chi \psi, \psi\rangle| + \Omega}{9R} \geqq \frac{\delta Z}{10R}$$

by simply taking C_0 large enough. So, the result will follow if we can prove that either

$$\langle H_{Z,N+N'}\psi, \psi\rangle \geqq E_0(Z) + cZ^{7/3 - 7\gamma_2}$$

or else:

$$\left|\sum_j \langle T_4 \cdot \psi, \psi\rangle\right| < \frac{\delta Z}{16R} N'$$

and

$$|Z - \langle N_\chi \psi, \psi\rangle| \leqq cZ^{1-\gamma_1}$$

with c independent of C_0.

In order to analyze this, let's define

$$\psi_{x'_1,\ldots,x'_{N'}}(x_1, \ldots, x_N) = \psi(x_1, \ldots, x_N, x'_1, \ldots, x'_{N'})$$

together with its normalized version

$$\bar{\psi}_{x'_1,\ldots,x'_{N'}}(x_1, \ldots, x_N) = \|\psi_{x'_1,\ldots,x'_{N'}}\|^{-1}_{L^2(dx_1\cdots dx_N)} \psi_{x'_1,\ldots,x'_{N'}}(x_1, \ldots, x_N),$$

defined on the set

$$E = \{(x'_1, \ldots, x'_{N'}) \mid \|\psi_{x'_1,\ldots,x'_{N'}}\|_2 \neq 0\}.$$

Also, as in Lemma 2.1, define

$$\rho_{\psi_{x'_1,\ldots,x'_{N'}}}(y) = \sum_{i=1}^{N} \int |\psi(x_1, \ldots, x_{i-1}, y, x_{i+1}, \ldots, x_N, x'_1, \ldots, x'_{N'})|^2 \prod_{i \neq j} dx_j,$$

$$\rho_{\bar{\psi}_{x'_1,\ldots,x'_{N'}}}(y) = \sum_{i=1}^{N} \int |\bar{\psi}(x_1, \ldots, x_{i-1}, y, x_{i+1}, \ldots, x_N, x'_1, \ldots, x'_{N'})|^2 \prod_{i \neq j} dx_j.$$

Note also that since ρ_{TF} and χ are radially symmetric

$$\int\left(\frac{1}{|x_j'-y|}-\frac{1}{|x_j'|}\right)\rho_{\mathrm{TF}}(y)\chi(y)dy=0.$$

Then

$$\begin{aligned}
&\int T_4|\bar{\psi}(x_1,\ldots,x_N,x_1',\ldots,x_{N'}')|^2dx_1\cdots dx_N\\
&=\int\left(\frac{1}{|x_j'-y|}-\frac{1}{|x_j'|}\right)(\chi*\phi)(y)\rho_{\bar{\psi}_{x_1',\ldots,x_{N'}'}}(y)dy\\
&=\iint\left(\frac{1}{|x_j'-y|}-\frac{1}{|x_j'|}\right)\chi(z)\phi(y-z)\rho_{\bar{\psi}_{x_1',\ldots,x_{N'}'}}(y)dydz\\
&=\iint\left(\frac{1}{|x_j'-z|}-\frac{1}{|x_j'|}\right)\chi(z)\phi(y-z)\rho_{\bar{\psi}_{x_1',\ldots,x_{N'}'}}(y)dydz\\
&\quad-\iint\left(\frac{1}{|x_j'-z|}-\frac{1}{|x_j'-y|}\right)\chi(z)\phi(y-z)\rho_{\bar{\psi}_{x_1',\ldots,x_{N'}'}}(y)dydz\\
&=\int\left(\frac{1}{|x_j'-y|}-\frac{1}{|x_j'|}\right)\chi(y)(\phi*\rho_{\bar{\psi}_{x_1',\ldots,x_{N'}'}})(y)dy\\
&\quad-\iint\left(\frac{1}{|x_j'-z|}-\frac{1}{|x_j'-y|}\right)\chi(x)\phi(y-z)\rho_{\bar{\psi}_{x_1',\ldots,x_{N'}'}}(y)dydz.
\end{aligned}$$

Now observe that

$$\begin{aligned}
&\left|\iint\left(\frac{1}{|x_j'-z|}-\frac{1}{|x_j'-y|}\right)\chi(z)\phi(y-z)\rho_{\bar{\psi}_{x_1',\ldots,x_{N'}'}}(y)dydz\right|\\
&=\leqq 10\iint\frac{|z-y|}{R^2}\chi(z)\phi(y-z)\rho_{\bar{\psi}_{x_1',\ldots,x_{N'}'}}(y)dydz\\
&\leqq 10N\left\|\int\frac{|z-y|}{R^2}\chi(z)\phi(y-z)dz\right\|_{L^\infty(dy)}\\
&=N\frac{Z^{-2/3}}{R^2}\int\phi(z)dz\leqq 2\frac{Z^{1/3}}{R^2}.
\end{aligned}$$

Summing over all j we obtain that

$$\left|\sum_j\iint\left(\frac{1}{|x_j'-z|}-\frac{1}{|x_j'-y|}\right)\chi(z)\phi(y-z)\rho_{\bar{\psi}_{x_1',\ldots,x_{N'}'}}(y)dydz\right|\leqq 2\frac{Z^{1/3}}{R^2}N'.$$

Note that

$$\frac{Z^{1/3}}{R^2}N'\leqq\frac{Z^{2/3-\gamma_2}}{R}N'\ll\frac{\delta Z}{R}N' \tag{4}$$

as long as $\frac{2}{3}-\gamma_2<1-3\gamma_2$, that is, $\gamma_2<\frac{1}{6}$, or $b<\frac{7}{6}$, which certainly holds in this case. So

$$\begin{aligned}&\left|\sum_j \int T_4 |\bar{\psi}(x_1,\dots,x_N,x'_1,\dots,x'_{N'})|^2 dx_1\cdots dx_N\right|\\ &\leqq \left|\sum_j \int \left(\frac{1}{|x'_j-y|}-\frac{1}{|x'_j|}\right)\chi(y)(\rho_{\bar{\psi}_{x'_1,\dots,x'_{N'}}} * \phi)(y)dy\right| + 2\frac{Z^{1/3}}{R^2}N'\\ &= \left|\sum_j \int \left(\frac{1}{|x'_j-y|}-\frac{1}{|x'_j|}\right)\chi(y)(\rho_{\bar{\psi}_{x'_1,\dots,x'_{N'}}} * \phi(y)-\rho_{\mathrm{TF}}(y))dy\right| + 2\frac{Z^{1/3}}{R^2}N'\\ &= \left|\left\langle \sum_j \left(\frac{1}{|x'_j-y|}-\frac{1}{|x'_j|}\right)\cdot\chi, (\rho_{\bar{\psi}_{x'_1,\dots,x'_{N'}}} * \phi-\rho_{\mathrm{TF}}\right\rangle\right| + 2\frac{Z^{1/3}}{R^2}N'.\end{aligned}$$

So, if we define

$$\varphi(y)=\sum_j\left(\frac{1}{|x'_j-y|}-\frac{1}{|x'_j|}\right)\cdot\chi(y).$$

we have

$$\left|\sum_j \int T_4 |\bar{\psi}(x_1,\dots,x_N,x'_1,\dots,x'_{N'})|^2 dx_1\cdots dx_N\right| \leqq |\langle\varphi,(\rho_{\bar{\psi}_{x'_1,\dots,x'_{N'}}} * \phi-\rho_{\mathrm{TF}})\rangle| + 2\frac{Z^{1/3}}{R^2}N'.$$

In particular

$$\begin{aligned}&\left(\left|\sum_j \int T_4 |\bar{\psi}(x_1,\dots,x_N,x'_1,\dots,x'_{N'})|^2 dx_1\cdots dx_N\right| - 2\frac{Z^{1/3}}{R^2}N'\right)_+^2\\ &\leqq |\langle\varphi,(\rho_{\bar{\psi}_{x'_1,\dots,x'_{N'}}} * \phi-\rho_{\mathrm{TF}})\rangle|^2.\end{aligned}$$

Next, observe that

$$|\nabla_y\varphi| \leqq \begin{cases}\dfrac{CN'}{|x'_j-y|^2} & \text{for} \quad |y|\leqq R_* \\ \left(\dfrac{C}{|x'_j-y|^2}+\dfrac{C}{R_*R}\right)N' & \text{for} \quad R_*\leqq|y|\leqq 2\cdot R_* \\ 0 & \text{for} \quad |y|>2\cdot R_*\end{cases}.$$

In any case,

$$|\nabla_y\varphi| \leqq \frac{CN'}{RR_*},$$

therefore,

$$\|\nabla_y\varphi\|_2^2 \leqq CN'^2\frac{R_*}{R^2}.$$

By Lemma 2.1 applied to $\bar{\psi}$, we have for $(x'_1,\dots,x'_{N'})\in E$,

$$\langle H_{Z,N}\bar{\psi}_{x'_1,\ldots,x'_{N'}}, \bar{\psi}_{x'_1,\ldots,x'_{N'}}\rangle$$
$$\geqq E_0(Z) + C'\frac{R^2}{N'^2R_*}|\langle \rho_{\bar{\psi}_{x'_1,\ldots,x'_{N'}}} * \phi - \rho_{\mathrm{TF}}, \varphi\rangle|^2 - C_{\mathrm{HSW}}Z^{7/3-b}$$
$$\geqq E_0(Z) + C'\frac{R^2}{N'^2R_*}\left(\left|\left\langle \sum_j T_4\bar{\psi}_{x'_1,\ldots,x'_{N'}}, \bar{\psi}_{x'_1,\ldots,x'_{N'}}\right\rangle\right| - 2\frac{Z^{1/3}}{R^2}N'\right)_+^2 - C_{\mathrm{HSW}}Z^{7/3-b}.$$

In other words,

$$\langle H_{Z,N}\psi_{x'_1,\ldots,x'_{N'}}, \psi_{x'_1,\ldots,x'_{N'}}\rangle$$
$$\geqq \|\psi_{x'_1,\ldots,x'_{N'}}\|_2^2 \cdot \left(E_0(Z) - C_{\mathrm{HSW}}Z^{7/3-b} + C'\frac{R^2}{N'^2R_*} \cdot\frac{\left(\left|\left\langle \sum_j T_4\psi_{x'_1,\ldots,x'_{N'}}, \psi_{x'_1,\ldots,x'_{N'}}\right\rangle\right| - 2\frac{Z^{1/3}}{R^2}N'\cdot\|\psi_{x'_1,\ldots,x'_{N'}}\|_2^2\right)_+^2}{\|\psi_{x'_1,\ldots,x'_{N'}}\|_2^4}\right)$$
$$= (E_0(Z) - C_{\mathrm{HSW}}Z^{7/3-b})\|\psi_{x'_1,\ldots,x'_{N'}}\|_2^2$$
$$+ C'\frac{R^2}{N'^2R_*}\frac{\left(\left|\left\langle \sum_j T_4\psi_{x'_1,\ldots,x'_{N'}}, \psi_{x'_1,\ldots,x'_{N'}}\right\rangle\right| - 2\frac{Z^{1/3}}{R^2}N'\cdot\|\psi_{x'_1,\ldots,x'_{N'}}\|_2^2\right)_+^2}{\|\psi_{x'_1,\ldots,x'_{N'}}\|_2^2}.$$

Now, integrate with respect to $(x'_1,\ldots,x'_{N'})\in E$ to obtain

$$\langle H_{Z,N}\psi,\psi\rangle \geqq E_0(Z) - C_{\mathrm{HSW}}Z^{7/3-b} + C'\frac{R^2}{N'^2R_*}$$
$$\cdot\int_E \frac{\left(\left|\left\langle \sum_j T_4\psi_{x'_1,\ldots,x'_{N'}}, \psi_{x'_1,\ldots,x'_{N'}}\right\rangle\right| - 2\frac{Z^{1/3}}{R^2}N'\cdot\|\psi_{x'_1,\ldots,x'_{N'}}\|_2^2\right)_+^2}{\|\psi_{x'_1,\ldots,x'_{N'}}\|_2^2}dx'_1\cdots dx'_{N'}.$$

Now use Cauchy–Schwarz and the fact that

$$\int (f(x))_+\,dx \geqq \left(\int f(x)dx\right)_+ \geqq 0$$

to realize that

$$\left(\left|\left\langle \sum_j T_4\psi,\psi\right\rangle\right| - 2\frac{Z^{1/3}}{R^2}N'\right)_+^2$$
$$\leqq \left(\int_E\left(\left|\left\langle \sum_j T_4\psi_{x'_1,\ldots,x'_{N'}}, \psi_{x'_1,\ldots,x'_{N'}}\right\rangle\right| - 2\frac{Z^{1/3}}{R^2}N'\cdot\|\psi_{x'_1,\ldots,x'_{N'}}\|_2^2\right)dx'_1\cdots dx'_{N'}\right)_+^2$$
$$\leqq \left(\int_E\left(\left|\left\langle \sum_j T_4\psi_{x'_1,\ldots,x'_{N'}}, \psi_{x'_1,\ldots,x'_{N'}}\right\rangle\right| - 2\frac{Z^{1/3}}{R^2}N'\cdot\|\psi_{x'_1,\ldots,x'_{N'}}\|_2^2\right)_+dx'_1\cdots dx'_{N'}\right)^2$$
$$\leqq \left(\int \|\psi_{x'_1,\ldots,x'_{N'}}\|_2^2 dx'_1\cdots dx'_{N'}\right)$$

$$\cdot \int_E \frac{\left(\left| \left\langle \sum_j T_4 \psi_{x'_1,\ldots,x'_{N'}}, \psi_{x'_1,\ldots,x'_{N'}} \right\rangle \right| - 2\frac{Z^{1/3}}{R^2} N' \cdot \| \psi_{x'_1,\ldots,x'_{N'}} \|_2^2 \right)_+^2}{\| \psi_{x'_1,\ldots,x'_{N'}} \|_2^2} dx'_1 \cdots dx'_{N'}$$

$$= \int_E \frac{\left(\left| \left\langle \sum_j T_4 \psi_{x'_1,\ldots,x'_{N'}}, \psi_{x'_1,\ldots,x'_{N'}} \right\rangle \right| - 2\frac{Z^{1/3}}{R^2} N' \cdot \| \psi_{x'_1,\ldots,x'_{N'}} \|_2^2 \right)_+^2}{\| \psi_{x'_1,\ldots,x'_{N'}} \|_2^2} dx'_1 \cdots dx'_{N'}.$$

Therefore

$$\langle H_{Z,N} \psi, \psi \rangle \geqq E_0(Z) + C' \frac{R^2}{N'^2 R_*} \left(\left| \left\langle \sum_j T_4 \psi, \psi \right\rangle \right| - 2\frac{Z^{1/3}}{R^2} N' \right)_+^2 - C_{\mathrm{HSW}} Z^{7/3-b}.$$

Recall that

$$H_{Z,N} + H_{\mathrm{extra}} = H_{Z,N+N'}$$

to obtain

$$\begin{aligned} \langle H_{Z,N+N'} \psi, \psi \rangle &\geqq E_0(Z) + \langle H_{\mathrm{extra}} \psi, \psi \rangle \\ &\quad + C' \frac{R^2}{N'^2 R_*} \left(\left| \left\langle \sum_j T_4 \psi, \psi \right\rangle \right| - 2\frac{Z^{1/3}}{R^2} N' \right)_+^2 - C_{\mathrm{HSW}} Z^{7/3-b}. \end{aligned}$$

Using (3) we get

$$\begin{aligned} \langle H_{Z,N+N'} \psi, \psi \rangle &\geqq E_0(Z) + \frac{\delta Z - 20|Z - \langle N_\chi \psi, \psi \rangle| + \Omega}{9R} N' + \left\langle \sum_j T_4 \psi, \psi \right\rangle \\ &\quad + C' \frac{R^2}{N'^2 R_*} \left(\left| \left\langle \sum_j T_4 \psi, \psi \right\rangle \right| - 2\frac{Z^{1/3}}{R^2} N' \right)_+^2 - C_{\mathrm{HSW}} Z^{7/3-b}. \qquad (5) \end{aligned}$$

Similarly, since

$$\langle \mathrm{N}_\chi \psi, \psi \rangle = \int \langle N_\chi \psi_{x'_1,\ldots,x'_{N'}}, \psi_{x'_1,\ldots,x'_{N'}} \rangle dx'_1 \cdots dx'_{N'},$$

if we let, for $(x'_1, \ldots, x'_{N'}) \in E$,

$$\langle N_\chi \bar{\psi}_{x'_1,\ldots,x'_{N'}}, \bar{\psi}_{x'_1,\ldots,x'_{N'}} \rangle = Z + Z^{1-\gamma_1} Y(x'_1, \ldots, x'_{N'})$$

and

$$\langle N_\chi \psi, \psi \rangle = Z + Y Z^{1-\gamma_1},$$

then

$$Y = \int_E Y(x'_1, \ldots, x'_{N'}) \| \psi_{x'_1,\ldots,x'_{N'}} \|_2^2 dx'_1 \cdots dx'_{N'}.$$

Now, Lemma 2.3 implies that

$$\langle H_{Z,N} \bar{\psi}_{x'_1,\ldots,x'_{N'}}, \bar{\psi}_{x'_1,\ldots,x'_{N'}} \rangle \geqq E_0(Z) + \frac{C_K}{4} Z^{7/3-b} (|Y(x'_1, \ldots, x'_{N'})| - c_1)_+^2 - C_{\mathrm{HSW}} Z^{7/3-b}$$

for $(x'_1, \ldots, x'_{N'}) \in E$.

Arguing just as before we see that

$$(|Y|-c_1)_+^2 \leqq \left(\int_E (|Y(x'_1,\dots,x'_{N'})|-c_1)\|\psi_{x'_1,\dots,x'_{N'}}\|_2^2 dx'_1\cdots dx'_{N'}\right)_+^2$$
$$\leqq \left(\int_E (|Y(x'_1,\dots,x'_{N'})|-c_1)_+\|\psi_{x'_1,\dots,x'_{N'}}\|_2^2 dx'_1\cdots dx'_{N'}\right)^2$$
$$\leqq \int_E (|Y(x'_1,\dots,x'_{N'})|-c_1)_+^2\|\psi_{x'_1,\dots,x'_{N'}}\|_2^2 dx'_1\cdots dx'_{N'}.$$

Therefore,

$$\langle H_{Z,N}\psi,\psi\rangle \geqq E_0(Z)+\left(\frac{C_K}{4}(|Y|-c_1)_+^2 - C_{\mathrm{HSW}}\right)Z^{7/3-b},$$

and using (3) we see that

$$\langle H_{Z,N+N'}\psi,\psi\rangle \geqq E_0(Z)+\frac{\delta Z-20|Z-\langle N_\chi\psi,\psi\rangle|+\Omega}{9R}N'+\left\langle \sum_j T_4\psi,\psi\right\rangle$$
$$+\left(\frac{C_K}{4}(|Y|-c_1)_+^2 - C_{\mathrm{HSW}}\right)Z^{7/3-b}.$$

Therefore, averaging this expression with (5), we get that

$$\langle H_{Z,N+N'}\psi,\psi\rangle \geqq E_0(Z)+\frac{\delta Z-20|Z-\langle N_\chi\psi,\psi\rangle|+\Omega}{9R}N'+\left\langle \sum_j T_4\psi,\psi\right\rangle$$
$$+(C'(|Y|-c_1)_+^2 - C_{\mathrm{HSW}})Z^{7/3-b}$$
$$+C'\frac{R^2}{R_*}\left(\left|\frac{1}{N'}\left\langle \sum_j T_4\psi,\psi\right\rangle\right|-2\frac{Z^{1/3}}{R^2}\right)_+^2, \tag{6}$$

possibly with a different constant C'.

Let's say now that, for some numbers S and V,

$$\left\langle \sum_j T_4\cdot\psi,\psi\right\rangle = -S\frac{\delta Z N'}{R},$$
$$N' = V\delta Z\frac{R}{R_*} > C_0 V\delta Z.$$

Thus $V\geqq 0$. Note that if $|S|<\frac{1}{16}$ and $|Y|$ is bounded above independently of C_0 we are done. This follows from the remarks following (3).

Observe that

$$\Omega = N'+N-Z-\delta Z \geqq (N'+\langle N_\chi\psi,\psi\rangle - Z-\delta Z)_+$$
$$\geqq \left(C_0 V - \frac{2|Y|}{C_0}-1\right)_+\delta Z.$$

Using (4) we can rewrite (6) to obtain

$$\langle H_{Z,N+N'}\psi,\psi\rangle \geqq E_0(Z)+F(S,Y,V)\cdot Z^{7/3-b}$$

for

$$F(S,Y,V)=\frac{C_0^2V}{9}-\frac{20}{9}(1+10^{-6})C_0V|Y|+\left(\frac{C_0^3V^2-2C_0V|Y|-C_0^2V}{9}\right)_+$$
$$-(1+10^{-6})^2C_0^2|S|V+C'((|Y|-c_1)_+^2+(C_0|S|-10^{-6})_+^2)-C_{\mathrm{HSW}}$$
$$\geqq \tfrac{1}{9}(C_0^2V-30C_0V|Y|+(C_0^3V^2-2C_0V|Y|-C_0^2V)_+-10C_0^2|S|V$$
$$+C''((|Y|-c_1)_+^2+(C_0|S|-10^{-6})_+^2)-9C_{\mathrm{HSW}}).$$

Observe that we can assume that $C''<1$ and c_1 is so big that

$$c_1^2C''-18C_{\mathrm{HSW}}>2. \tag{7}$$

The rest of the lemma is devoted to proving that either $|S|<\frac{1}{16}$ and $|Y|<$ some constant or else $F>$ some other constant. In order to understand why this is so, we deal with different cases:

Case 1. $|S|>\frac{1}{16}$ $|Y|<2c_1$ $V<\frac{C''}{24}|S|$.

Since $|S|>\frac{1}{16}$, for $C_0>64$ we have $(C_0|S|-10^{-6})_+^2>\frac{1}{2}C_0^2S^2$. Thus,

$$9F\geqq -\tfrac{5}{2}C''c_1C_0|S|-\tfrac{5}{12}C''C_0^2S^2+\tfrac{1}{2}C''C_0^2S^2-9C_{\mathrm{HSW}}$$
$$\geqq -40C''c_1C_0S^2+\tfrac{1}{12}C''C_0^2S^2-9C_{\mathrm{HSW}}$$
$$\geqq C''C_0S^2(-40c_1+\tfrac{1}{12}C_0)-9C_{\mathrm{HSW}}$$
$$\geqq \frac{C''}{16^2}C_0(-40c_1+\tfrac{1}{12}C_0)-9C_{\mathrm{HSW}},$$

and pick C_0 large enough so that this is at least 1.

Case 2. $|S|>\frac{1}{16}$ $|Y|<2c_1$ $V\geqq\frac{C''}{24}|S|$.

$$9F\geqq -60c_1VC_0+(C_0^3V^2-4c_1C_0V-C_0^2V)_+-10VC_0^2|S|-9C_{\mathrm{HSW}}.$$

Pick now C_0 large enough so that

$$(C_0^3V^2-4c_1C_0V-C_0^2V)_+>\tfrac{1}{2}C_0^3V^2 \quad \text{for} \quad V>\frac{C''}{24\cdot 16},$$

then

$$9F\geqq -60c_1VC_0+\tfrac{1}{2}C_0^3V^2-\frac{240}{C''}V^2C_0^2-9C_{\mathrm{HSW}}$$
$$\geqq V^2\left(\frac{-60\cdot 24\cdot 16c_1}{C''}C_0+\tfrac{1}{2}C_0^3-\frac{240}{C''}C_0^2\right)-9C_{\mathrm{HSW}},$$

and again pick C_0 large enough so that this is at least 1 for $V>C''/24\cdot 16$.

Case 3. All $|S|$ $|Y|>2c_1$ $V<10^{-6}C''$.

If $|S|\geqq\frac{1}{16}$, observe that $-10C_0^2V|S|+C''/2C_0^2|S|^2$ is increasing in $|S|$ as long as

$V < C''/160$, which is true in our case. So it is enough to consider the case $|S| < \frac{1}{16}$. Observe that

$$C_0^2 V - 10C_0^2 V|S| \geqq \tfrac{3}{8}C_0^2 V \quad \text{if} \quad |S| < \tfrac{1}{16}$$

$$(|Y| - c_1)_+^2 \geqq \frac{Y^2}{4} \qquad \text{if} \quad |Y| \geqq 2c_1. \tag{8}$$

Therefore

$$\begin{aligned}
9F &\geqq \tfrac{3}{8}C_0^2 V - 30C_0 V|Y| + \frac{C''}{4}Y^2 - 9C_{\mathrm{HSW}} \\
&= \tfrac{3}{8}C_0^2 V + \left(\sqrt{\frac{C''}{4}}\,Y - \frac{15C_0}{\sqrt{C''/4}}\,V\right)^2 - \frac{900}{C''}C_0^2 V^2 - 9C_{\mathrm{HSW}} \\
&\geqq C_0^2\left(\tfrac{3}{8}V - \frac{900}{C''}V^2\right) - 9C_{\mathrm{HSW}} \\
&\geqq C_0^2\left(\tfrac{3}{8}V - \frac{900}{C''}10^{-6}C''V\right) - 9C_{\mathrm{HSW}} \\
&\geqq C_0^2 V(\tfrac{3}{8} - 900\cdot 10^{-6}) - 9C_{\mathrm{HSW}}.
\end{aligned}$$

Now, if $V > 100C_{\mathrm{HSW}}C_0^{-2}$ we are done. Otherwise,

$$\begin{aligned}
9F &\geqq -3000C_{\mathrm{HSW}}C_0^{-1}|Y| + \frac{C''}{4}Y^2 - 9C_{\mathrm{HSW}} \\
&\geqq Y^2\left(-\frac{3000C_{\mathrm{HSW}}}{2c_1 C_0} + \frac{C''}{4}\right) - 9C_{\mathrm{HSW}} \\
&\geqq \frac{C''}{8}Y^2 - 9C_{\mathrm{HSW}} \geqq \frac{c_1^2 C''}{2} - 9C_{\mathrm{HSW}} \geqq 1
\end{aligned}$$

by (7) and for C_0 large enough.

Case 4. $|S| < \frac{1}{16}$ $|Y| > 2c_1$ $10^{-13}C''^2 C_0^{1/3} \geqq V \geqq 10^{-6}C''$.

If $|Y| > C_0^{5/3}$, by (8)

$$\begin{aligned}
9F &\geqq -30C_0 V|Y| + \frac{C''}{4}Y^2 - 9C_{\mathrm{HSW}} \\
&\geqq -3\cdot 10^{-12}C''^2 C_0^{4/3}|Y| + \frac{C''}{4}Y^2 - 9C_{\mathrm{HSW}}.
\end{aligned}$$

Differentiate with respect to $|Y|$ to realize that for $C_0 > 216\cdot 10^{-36}C''^3$ the right-hand side is increasing for $|Y| \geqq C_0^{5/3}$. So,

$$9F \geqq -3\cdot 10^{-12}C''^2 C_0^{9/3} + \frac{C''}{4}C_0^{10/3} - 9C_{\mathrm{HSW}}, \tag{9}$$

and pick C_0 big enough so that this is at least 1. If, on the contrary, $|Y| \leqq C_0^{5/3}$, we have

$$2C_0V|Y|+C_0^2V\leqq 10^{-13}C''^2(2C_0^3+C_0^{7/3})\leqq 3\cdot 10^{-13}C''^2C_0^3\leqq \tfrac{3}{10}C_0^3V^2.$$

So, using (8) again

$$9F\geqq -30C_0V|Y|+\tfrac{1}{2}C_0^3V^2-9C_{\mathrm{HSW}}\geqq -30C_0^{8/3}V+\tfrac{1}{2}C_0^3V^2-9C_{\mathrm{HSW}}, \tag{10}$$

and pick C_0 so that this is bigger than 1 for $V\geqq 10^{-6}C''$.

Case 5. $|S|\geqq\frac{1}{16}$ $|Y|>2c_1\ 10^{-13}C''^2C_0^{1/3}\geqq V\geqq 10^{-6}C''$.

In this case, argue as in Case 4, with the only difference that $C_0^2(V-10|S|V+\frac{1}{2}C''S^2)$ need no longer be positive, and we have to include it in (9) and (10), which will be replaced respectively by

$$9F\geqq -3\cdot 10^{-12}C''^2C_0^{9/3}+\frac{C''}{4}C_0^{10/3}+C_0^2(V-10|S|V+\tfrac{1}{2}C''S^2)-9C_{\mathrm{HSW}}$$

and

$$9F\geqq -30C_0^{8/3}V+\tfrac{1}{2}C_0^3V^2+C_0^2(V-10|S|V+\tfrac{1}{2}C''S^2)-9C_{\mathrm{HSW}}.$$

Note that

$$C_0^2(V-10|S|V+\tfrac{1}{2}C''S^2)\geqq -\frac{100}{C''}C_0^2V^2, \tag{11}$$

since, for given V,

$$\min_{|S|}(V-10|S|V+\tfrac{1}{2}C''|S|^2)$$

is attained when $10V=C''|S|$: so,

$$\min_{|S|}(V-10|S|V+\tfrac{1}{2}C''|S|^2)\geqq -\frac{100}{C''}V^2.$$

Therefore, in our range of V, (11) is at least $-10^{-24}C''^3C_0^{8/3}$, so, for C_0 big enough it doesn't affect the result since V is bounded below by a constant independent of C_0.

Case 6. All $|S|$ $|Y|>2c_1\ 10^{-13}C''^2C_0^{1/3}\leqq V$.

If $|Y|>(200/C'')C_0V$, and $|S|<\frac{1}{16}$, by (8),

$$9F\geqq -30C_0V|Y|+\frac{C''}{4}Y^2-9C_{\mathrm{HSW}}.$$

Again the derivative of this with respect to $|Y|$ is positive for $|Y|>(200/C'')C_0V$. So, plugging in for $|Y|$ the value $|Y|=(200/C'')C_0, V$, we obtain

$$9F\geqq C_0^2V^2\left(-\frac{6000}{C''}+\frac{10{,}000}{C''}\right)-9C_{\mathrm{HSW}}\geqq\frac{4000}{C''}C_0^2V^2-9C_{\mathrm{HSW}}.$$

If $|S|\geqq\frac{1}{16}$, by (11) we have to subtract $(100/C'')C_0^2V^2$, that does not alter the result. Now, if $|Y|\leqq(200/C'')C_0V$, observe that

$$C_0^3V^2-2C_0V|Y|-C_0^2V\geqq C_0^3V^2-\frac{400}{C''}C_0^2V^2-C_0^2V\geqq\tfrac{1}{2}C_0^3V^2$$

for C_0 big enough, since $V \geqq 1$. So, for $|S| < \frac{1}{16}$ we have

$$\begin{aligned} 9F &\geqq -30C_0 V|Y| + \tfrac{1}{2}C_0^3 V^2 - 9C_{\mathrm{HSW}} \\ &\geqq -\frac{6000}{C''} C_0^2 V^2 + \tfrac{1}{2}C_0^3 V^2 - 9C_{\mathrm{HSW}}, \end{aligned}$$

and as usual we pick C_0 so that this is at least 1. If $|S| \geqq \frac{1}{16}$, we have to subtract $(100/C'')C_0^2 V^2$, which again is harmless for C_0 big enough. This proves that either both $|S| \leqq \frac{1}{16}$ and $|Y| \leqq 2c_1$ or

$$\langle H_{Z,N+N'}\psi, \psi \rangle \geqq E_0(Z) + cZ^{7/3-b},$$

which concludes the lemma.

4. The Bootstrap

In Sect. two we obtained estimates for wave functions supported on balls, where the ball was to be of a certain size. The estimates from the previous section will help us obtain essentially the same kind of estimates for a ball of twice their size, and by induction, to all balls in $\mathbf{R}^3$.

Lemma 4.1. *Let* $R \geqq C_0 Z^{-1/3+\gamma_2}$, $\bar{\varepsilon} = c_0 Z^{-\gamma_1}$ *and*

$$C_0 Z^{-\gamma_1} \leqq \varepsilon \leqq (1 + 10^{-12}) C_0 Z^{-\gamma_1}.$$

If Estimate$(\bar{\varepsilon}, \varepsilon, R)$ *holds, then* Estimate$(\bar{\varepsilon}, \varepsilon', 2R)$ *also holds, with*

$$\varepsilon' = \varepsilon + \frac{2C}{\bar{\varepsilon} R Z},$$

provided that $\varepsilon' \leqq \varepsilon^{\#} < 1$.

Proof. We consider a partition of unity given by two smooth functions, θ_0 and θ_1, satisfying

$$\theta_0(x) = \begin{cases} 1 & \text{if } |x| < R/2 \\ 0 & \text{if } |x| > R \end{cases},$$

$$\theta_0^2(x) + \theta_1^2(x) = 1.$$

Given a wave function $\psi(x_1, \ldots, x_N)$ supported on $B(0, 2R)$, and given any sequence $i_1, \ldots, i_N$ of 0's and 1's, we define

$$\psi_{i_1,\ldots,i_N} = \theta_{i_1}(x_1) \cdots \theta_{i_N}(x_N) \psi(x_1, \ldots, x_N).$$

Assume for simplicity that $i_j = 0$ for $j = 1, \ldots, N_1$ and $i_j = 1$ for $j = N_1 + 1, \ldots, N$; let $N_2 = N - N_1$. We define $\psi_{x_{N_1+1},\ldots,x_N}$ to be ψ, where the variables $x_{N_1+1}, \ldots, x_N$ are fixed. It is thus an antisymmetic wave function supported on $(B(0,R))^{N_1}$. Since Estimate$(\bar{\varepsilon}, \varepsilon, R)$ holds, we have

$$\langle H_{Z,N_1} \psi_{x_{N_1+1},\ldots,x_N}, \psi_{x_{N_1+1},\ldots,x_N} \rangle \geqq \left(E_0(Z) + \frac{\bar{\varepsilon} Z}{R}(N_1 - (1+\varepsilon)Z) \right) \| \psi_{x_{N_1+1},\ldots,x_N} \|_2^2.$$

Integrate this against $dx_{N_1+1}, \ldots, dx_N$ to obtain

$$\langle H_{Z,N_1}\psi_{i_1,\ldots,i_N}, \psi_{i_1,\ldots,i_N}\rangle \geqq \left(E_0(Z) + \frac{\bar{\varepsilon}Z}{R}(N_1 - (1+\varepsilon)Z)\right)\|\psi_{i_1,\ldots,i_N}\|_2^2. \tag{12}$$

Our goal now is to prove that

$$\begin{aligned}&\langle H_{Z,N_1+N_2}\psi_{i_1,\ldots,i_N}, \psi_{i_1,\ldots,i_N}\rangle \\ &\geqq \left(E_0(Z) + \frac{\bar{\varepsilon}Z}{R}(N_1 + N_2 - (1+\varepsilon)Z)\right)\|\psi_{i_1,\ldots,i_N}\|_2^2.\end{aligned} \tag{13}$$

This is trivial if $N = N_1 + N_2 \leqq (1+\varepsilon)Z$, since $\varepsilon \leqq \varepsilon^{\#}$. If $N \geqq (1+\varepsilon)Z$, we can apply Lemma 3.1, with $\delta = \varepsilon$. If

$$\langle H_{Z,N_1+N_2}\psi_{i_1,\ldots,i_N}, \psi_{i_1,\ldots,i_N}\rangle \geqq (E_0(Z) + cZ^{7/3-b})\|\psi_{i_1,\ldots,i_N}\|_2^2,$$

then, either

$$cZ^{7/3-b} > \frac{\bar{\varepsilon}Z}{R}(N - (1+\varepsilon)Z)$$

in which case (13) is proved, or

$$cZ^{7/3-b} \leqq \frac{\bar{\varepsilon}Z}{R}(N - (1+\varepsilon)Z). \tag{14}$$

If this is the case, just like in (2), note that provided $c_0 < cC_{\mathrm{K}}/(8C_{\mathrm{HSW}})$, where c is the constant in Lemma 3.1 (we can assume $c < 1$ and $C_{\mathrm{HSW}} > 1$),

$$cC_{\mathrm{K}}\frac{|N-Z|^2}{8C_{\mathrm{HSW}}R} > \frac{\bar{\varepsilon}Z}{R}(N - (1+\varepsilon)Z). \tag{15}$$

Equation (14) then implies that

$$C_{\mathrm{K}}\frac{|N-Z|^2}{4R} > 2C_{\mathrm{HSW}}Z^{7/3-b}.$$

Estimate (A) then with $\chi = \chi_{2R}$ implies that

$$\begin{aligned}\langle H_{Z,N_1+N_2}\psi_{i_1,\ldots,i_N}, \psi_{i_1,\ldots,i_N}\rangle &\geqq \left(E_0(Z) + C_{\mathrm{K}}\frac{|N-Z|^2}{8R}\right)\|\psi_{i_1,\ldots,i_N}\|_2^2 \\ &\geqq \left(E_0(Z) + cC_{\mathrm{K}}\frac{|N-Z|^2}{8C_{\mathrm{HSW}}R}\right)\|\psi_{i_1,\ldots,i_N}\|_2^2,\end{aligned}$$

and (15) again implies (13).

The alternative left from Lemma 3.1 is that

$$\langle H_{\mathrm{extra}}\psi_{i_1,\ldots,i_N}, \psi_{i_1,\ldots,i_N}\rangle \geqq \frac{c\varepsilon Z}{R}N_2\|\psi_{i_1,\ldots,i_N}\|_2^2. \tag{16}$$

Since

$$H_{Z,N_1+N_2} = H_{Z,N_1} + H_{\mathrm{extra}}$$

and $c\varepsilon > \bar{\varepsilon}$ (for $c_0 < c \cdot C_0$), (12) and (16) imply

$$\langle H_{Z,N_1+N_2}\psi_{i_1,\ldots,i_N}, \psi_{i_1,\ldots,i_N}\rangle \geqq \left(E_0(Z) + \frac{\bar{\varepsilon}Z}{R}(N_1 + N_2 - (1+\varepsilon)Z)\right) \cdot \|\psi_{i_1,\ldots,i_N}\|_2^2,$$

and (13) is proved.

Putting all these estimates together, we see that

$$\sum_{i_1,\ldots,i_N} \langle H_{Z,N_1+N_2}\psi_{i_1,\ldots,i_N}, \psi_{i_1,\ldots,i_N}\rangle \geqq E_0(Z) + \frac{\bar{\varepsilon}Z}{R}(N_1 + N_2 - (1+\varepsilon)Z).$$

Now,

$$\sum_{i_1,\ldots,i_N} \langle V_{\text{Coulomb}}\psi_{i_1,\ldots,i_N}, \psi_{i_1,\ldots,i_N}\rangle = \langle V_{\text{Coulomb}}\psi, \psi\rangle.$$

For $-\Delta$, we have

$$\begin{aligned}
&\sum_{i_1,\ldots,i_N} \langle -\Delta_{x_1,\ldots,x_N}\psi_{i_1,\ldots,i_N}, \psi_{i_1,\ldots,i_N}\rangle \\
&= \sum_{i_1,\ldots,i_N} \sum_k \langle -\Delta_{x_k}\psi_{i_1,\ldots,i_N}, \psi_{i_1,\ldots,i_N}\rangle \\
&= \sum_{i_1,\ldots,i_N} \sum_k \left\langle \prod_{j\neq k} \theta_{ij}^2(x_j)\cdot(-\Delta_{x_k}\theta_{i_k}(x_k)\psi), (\theta_{x_k}(x_k)\psi)\right\rangle \\
&= \sum_k \sum_{i_k} \langle -\Delta_{x_k}(\theta_{i_k}(x_k)\psi), (\theta_{i_k}(x_k)\psi)\rangle \\
&= \sum_{i,k} \langle \theta_i^2(x_k)(-\Delta_{x_k}\psi), \psi\rangle + \sum_{i,k} \langle \psi(-\Delta_{x_k}\theta_i(x_k)), \theta_i(x_k)\psi\rangle \\
&\quad - 2\sum_{i,k} \langle \nabla_{x_k}\psi \cdot \nabla_{x_k}\theta_i(x_k), \psi\theta_i(x_k)\rangle \\
&= \langle -\Delta\psi, \psi\rangle + \left\langle \sum_{i,k} \theta_i(x_k)(-\Delta_{x_k}\theta_i(x_k))\psi, \psi\right\rangle - \sum_{i,k} \langle \nabla_{x_k}\theta_i^2(x_k)\cdot\nabla_{x_k}\psi, \psi\rangle.
\end{aligned}$$

The last term on the right is zero, since

$$\sum_i \nabla_{x_k}\theta_i^2(x_k) = \nabla_{x_k}\sum_i \theta_i^2(x_k) = \nabla 1 = 0.$$

Hence, if we define

$$W(x) = \sum_i \theta_i(x)\Delta\theta_i(x),$$

we get

$$\sum_{i_1,\ldots,i_N} \langle -\Delta_{x_1,\ldots,x_N}\psi_{i_1,\ldots,i_N}, \psi_{i_1,\ldots,i_N}\rangle = \langle -\Delta\psi, \psi\rangle - \left\langle \sum_k W(x_k)\psi, \psi\right\rangle.$$

As result, we get

$$\langle H_{Z,N}\psi, \psi\rangle - \left\langle \sum_k W(x_k)\psi, \psi\right\rangle \geqq E_0(Z) + \frac{\bar{\varepsilon}Z}{R}(N - (1+\varepsilon)Z).$$

Observe now that

$$|W(x)| \leqq \frac{C}{R^2}.$$

Thus it follows that

$$\left|\left\langle \sum_k W(x_k)\psi, \psi \right\rangle\right| \leqq \frac{CN}{R^2}.$$

Thus we have

$$\langle H_{Z,N}\psi, \psi \rangle \geqq E_0(Z) + \frac{\bar{\varepsilon}Z}{R}(N - (1+\varepsilon)Z) - \frac{CN}{R^2}.$$

So we have only left to investigate when

$$\frac{\bar{\varepsilon}Z}{R}(N - (1+\varepsilon)Z) - \frac{CN}{R^2} \geqq \frac{\bar{\varepsilon}Z}{2R}(N - (1+\varepsilon')Z). \tag{17}$$

Observe that the derivative with respect to N of the left-hand side is bigger than the derivative of the right-hand side. This amounts to checking that

$$\frac{\bar{\varepsilon}Z}{R} - \frac{C}{R^2} \geqq \frac{\bar{\varepsilon}Z}{2R},$$

which is equivalent to

$$\frac{C}{R} \leqq \frac{\bar{\varepsilon}Z}{2},$$

which will hold as long as $R \geqq 2C/\bar{\varepsilon}Z$. This certainly holds in our case, since

$$R > Z^{-1/3+\gamma_2} \gg Z^{-1+\gamma_1}.$$

So it is enough to prove that (17) holds for the smallest value of N in which we are interested. For $N = (1+\varepsilon')Z$, (17) is equivalent to

$$C\frac{1+\varepsilon'}{R} \leqq \bar{\varepsilon}Z(\varepsilon' - \varepsilon),$$

i.e.

$$\varepsilon' \geqq \varepsilon + \frac{C(1+\varepsilon')}{\bar{\varepsilon}ZR}.$$

So, Estimate$(\bar{\varepsilon}, \varepsilon', 2R)$ holds with

$$\varepsilon' = \varepsilon + \frac{2C}{\bar{\varepsilon}ZR}.$$

Corollary. *There exist* $\bar{\varepsilon}^{\#}, \varepsilon^{\#}$ *such that* Estimate$(\bar{\varepsilon}^{\#}, \varepsilon^{\#}, R)$ *holds for all* $R \geqq C_0 Z^{-1/3+\gamma_2}$.

Proof. Define

$$\varepsilon_0 = C_0 Z^{-\gamma_1}, \quad \bar{\varepsilon}_0 = c_0 Z^{-\gamma_1},$$

$$R_0 = C_0 Z^{-1/3+\gamma_2}, \quad \varepsilon_n = \varepsilon_{n-1} + \frac{2C}{\bar{\varepsilon}_0 Z R_n}, \quad R_n = 2^n R_0.$$

Note that

$$\varepsilon_n \leqq \varepsilon_0 + \sum_{k=0}^{\infty} \frac{4C}{\bar{\varepsilon}_0 Z 2^k R_0} < C^{\#} \varepsilon_0 \stackrel{\text{def}}{=} \varepsilon^{\#}$$

for Z large enough, provided $b < \frac{14}{15}$ (which is true in our discussion), with $C^{\#} \leqq (1 + 10^{-12})$.

By Lemma 2.2 we see that Estimate $(\bar{\varepsilon}_0, \varepsilon_0, R_0)$ holds. Therefore, by the previous lemma, if we make $\bar{\varepsilon}^{\#} = \bar{\varepsilon}_0$, Estimate $(\bar{\varepsilon}_0, \varepsilon_n, R_n)$ holds for all n, and the corollary follows. This implies that

$$\langle H_{Z,N}\psi, \psi \rangle \geqq E_0(Z),$$

and therefore

$$N(Z) \leqq Z + \varepsilon^{\#} Z = Z + O(Z^{1-\gamma_1}).$$

From [11] it follows that

$$N(Z) \geqq Z,$$

and therefore,

$$N(Z) = Z + O(Z^{1-\gamma_1})$$

which proves the theorem.

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