Ground state energy of large atoms in a self-generated magnetic field

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Abstract
We consider a large atom with nuclear charge \(Z\) described by non-relativistic quantum mechanics with classical or quantized electromagnetic field. We prove that the absolute ground state energy, allowing for minimizing over all possible self-generated electromagnetic fields, is given by the non-magnetic Thomas-Fermi theory to leading order in the simultaneous \(Z \to \infty, \alpha \to 0\) limit if \(Z\alpha^2 \leq \kappa\) for some universal \(\kappa\), where \(\alpha\) is the fine structure constant.

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1 Introduction

The ground state energy of non-relativistic atoms and molecules with large nuclear charge $Z$ can be described by Thomas-Fermi theory to leading order in the $Z \to \infty$ limit \cite{LS}. Magnetic fields in this context were taken into account only as an external field, either a homogeneous one \cite{LSY1,LSY2} or an inhomogeneous one \cite{ES} but subject to certain regularity conditions. Self-generated magnetic fields, obtained from Maxwell’s equation are not known to satisfy these conditions. In this paper we extend the validity of Thomas-Fermi theory by allowing a self-generated magnetic field that interacts with the electrons. This means, we look for the absolute ground state of the system, after minimizing for both the electron wave function and for the magnetic field and we show that the additional magnetic field does not change the leading order Thomas-Fermi energy. Apart from finite energy, no other assumption is assumed on the magnetic field.

The nonrelativistic model of an atom in three spatial dimensions with nuclear charge $Z \geq 1$ and with $N$ electrons in a classical magnetic field is given by the Hamiltonian

$$H_{N,Z}^{cl}(A) = \sum_{j=1}^{N} \left[ T_j(A) - \frac{Z}{|x_j|} \right] + \sum_{i<j} \frac{1}{|x_i - x_j|} + \frac{1}{8\pi\alpha^2} \int_{\mathbb{R}^3} B^2$$

acting on the space of antisymmetric functions $\bigwedge^N \mathcal{H}$ with a single particle Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$. The coordinates of the $N$ electrons are denoted by $x = (x_1, x_2, \ldots, x_N)$. The vector potential $A : \mathbb{R}^3 \to \mathbb{R}^3$ generates the magnetic field $B = \nabla \times A$ and it can be chosen divergence-free, $\nabla \cdot A = 0$. The last term in (1.1) is the energy of the magnetic field. The kinetic energy of an electron is given by the Pauli operator

$$T(A) = [\sigma \cdot (p + A)]^2 = (p + A)^2 + \sigma \cdot B, \quad p = -i\nabla_x.$$ 

Here $\sigma$ is the vector of Pauli matrices. We use the convention that for any one-body operator $T$, the subscript in $T_j$ indicates that the operator acts on the $j$-th variable, i.e. $T_j(A) = [\sigma_j \cdot (-i\nabla_{x_j} + A(x_j))]^2$. The term $-Z|x_j|^{-1}$ describes the attraction of the $j$-th electron to the nucleus located at the origin and the term $|x_i - x_j|^{-1}$ is the electrostatic repulsion between the $i$-th and $j$-th electron.

Our units are $\hbar^2(2me^2)^{-1}$ for the length, $2me^4\hbar^{-2}$ for the energy and $2me^2c\hbar^{-1}$ for the magnetic vector potential, where $m$ is the electron mass, $e$ is the electron charge and $\hbar$ is the Planck constant. In these units, the only physical parameter that appears in (1.1) is the dimensionless fine structure constant $\alpha = e^2(\hbar c)^{-1}$. We will assume that $Z\alpha^2 \leq \kappa$ with some sufficiently small universal constant $\kappa \leq 1$ and we will investigate the simultaneous limit...
\[ Z \to \infty, \alpha \to 0. \] Note that the field energy is added to the total energy of the system and by the condition \( \nabla \cdot \mathbf{A} = 0 \) we have

\[
\int_{\mathbb{R}^3} \mathbf{B}^2 = \int_{\mathbb{R}^3} |\nabla \otimes \mathbf{A}|^2, \tag{1.2}
\]

where \( \nabla \otimes \mathbf{A} \) denotes the \( 3 \times 3 \) matrix of all derivatives \( \partial_i A_j \) and \( |\nabla \otimes \mathbf{A}|^2 = \sum_{i,j=1}^{3} |\partial_i A_j|^2 \). We will always assume that the vector potential belongs to the space of divergence free \( H^1 \)-vector fields

\[ \mathcal{A} := \{ \mathbf{A} \in H^1(\mathbb{R}^3, \mathbb{R}^3), \nabla \cdot \mathbf{A} = 0 \} \].

In the analogous nonrelativistic model of quantum electrodynamics, the electromagnetic vector potential is quantized. In the Coulomb gauge it is given by

\[ \mathbf{A}_\Lambda(x) = \mathbf{A}(x) = \mathbf{A}_-(x) + \mathbf{A}_-(x)^* \]

with

\[ \mathbf{A}_-(x) = \alpha^{1/2} \int_{\mathbb{R}^3} \frac{g(k)}{2\pi \sqrt{|k|}} \sum_{\lambda = \pm} a_\lambda(k) \mathbf{e}_\lambda(k) e^{ik \cdot x} dk. \]

Here \( g(k) \) is a cutoff function, satisfying \( |g(k)| \leq 1 \) and \( \text{supp} \ g \subset \{ k \in \mathbb{R}^3 : |k| \leq \Lambda \} \) with a constant \( \Lambda < \infty \) (ultraviolet cutoff). The field operators \( \mathbf{A}(x) \) depend on the cutoff function \( g(k) \) whose precise form is unimportant the only relevant parameter is \( \Lambda \). For each \( k \), the two polarization vectors \( \mathbf{e}_-(k), \mathbf{e}_+(k) \in \mathbb{R}^3 \) are chosen such that together with the direction of propagation \( k/|k| \) they are orthonormal. The operators \( a_\lambda(k), a_\lambda(k)^* \) are annihilation and creation operators acting on the bosonic Fock space \( \mathcal{F} \) over \( L^2(\mathbb{R}^3) \) and satisfying the canonical commutation relations

\[ [a_\lambda(k), a_{\lambda'}(k')] = [a_\lambda(k)^*, a_{\lambda'}(k')^*] = 0, \quad [a_\lambda(k), a_{\lambda'}(k')^*] = \delta_{\lambda\lambda'} \delta(k - k'). \]

The field energy is given by

\[ H_f = \alpha^{-1} \int_{\mathbb{R}^3} |k| \sum_{\lambda = \pm} a_\lambda(k)^* a_\lambda(k) dk. \]

The total Hamiltonian is

\[
H_{\text{N,Z}}^{\text{qed}} = \sum_{j=1}^{N} \left[ T_j(\mathbf{A}_\Lambda) - \frac{Z}{|x_j|} \right] + \sum_{i<j} \frac{1}{|x_i - x_j|} + H_f \tag{1.3}
\]

and it acts on \( (\wedge_1^{N} \mathcal{H}) \otimes \mathcal{F} \).
The stability of atoms in a classical magnetic field \([F, FLL, LL, LLS]\) implies that the operator \((1.1)\) is bounded from below uniformly in \(A\). If \(Z\alpha^2\) is small enough. It is known \([LY, ES2]\) that stability fails if \(Z\alpha^2\) is too large. The analogous stability result for quantized field \([BFG]\) states that \((1.3)\) is bounded from below if \(Z\alpha^2\) is small. In particular, we can for each fixed \(A\) define the operators in \((1.1)\) and \((1.3)\) as the Friedrichs extensions of these operators defined on smooth functions with compact support.

The ground state energy of the operator with a classical field is given by
\[
E_{N,Z}^{\text{cl}}(A) = \inf \left\{ \left\langle \Psi, H_{N,Z}^{\text{cl}}(A) \Psi \right\rangle : \Psi \in \bigwedge_1^N \left( C_0^\infty(\mathbb{R}^3) \otimes C^2 \right), \|\Psi\| = 1 \right\},
\]
and after minimizing in \(A\) we set
\[
E_{N,Z}^{\text{cl}} = \inf_{A \in A} E_{N,Z}^{\text{cl}}(A).
\]
We note that it is sufficient to minimize over all \(A \in A_0\) where \(A_0 = H^1_c(\mathbb{R}^3, \mathbb{R}^3)\) denotes the space of compactly supported \(H^1\) vector fields. It is easy to see that the Euler-Lagrange equations for the above minimizations in \(\Psi\) and \(A\) correspond to the stationary version of the coupled Maxwell-Pauli system, i.e., the eigenvalue problem \(H_{N,Z}^{\text{cl}}(A)\Psi = E_{N,Z}^{\text{cl}}\Psi\) together with the Maxwell equation \(\nabla \times B = 4\pi\alpha^2 J_{\Psi}\), where \(J_{\Psi}\) is the current of the wave function \(\Psi\). It is for this reason that it is natural to refer to \(B\) as a self-generated magnetic field in this context.

In the case of the quantized field, we define
\[
E_{N,Z}^{\text{qed}} = \inf \left\{ \left\langle \Psi, H_{N,Z}^{\text{qed}} \Psi \right\rangle : \Psi \in \bigwedge_1^N \left( C_0^\infty(\mathbb{R}^3) \otimes C^2 \right) \otimes F, \|\Psi\| = 1 \right\}.
\]
The stability results of \([F, FLL, LL, LLS, BFG]\) imply that \(E_{N,Z}^{\text{cl}} > -\infty\) and \(E_{N,Z}^{\text{qed}} > -\infty\) if \(Z\alpha^2\) is small enough.

Finally, we define the ground state energy with no magnetic field as
\[
E_{N,Z}^{\text{nf}} := E_{N,Z}^{\text{cl}}(A = 0).
\]
In all three cases we define
\[
E_Z^{\#} := \inf_{N \in \mathbb{N}} E_{N,Z}^{\#,}, \quad \# \in \{\text{cl, qed, nf}\},
\]
for the absolute (grand canonical) ground state energy. The main result of this paper states that the magnetic field does not change the leading term of the absolute ground state energy of a large atom in the \(Z \to \infty\) limit. In particular, Thomas-Fermi theory is correct to leading order even with including self-generated magnetic field.
Theorem 1.1. There exists a positive constant \( \kappa \) such that if \( Z^\alpha \leq \kappa \), then
\[
E_{\text{nf}}^Z \geq E_{\text{cl}}^Z \geq E_{\text{nf}}^Z - CZ^{\frac{5}{3}} - \frac{1}{63}.
\]
(1.4)

For the quantized case, if we additionally assume
\[
\Lambda \leq \kappa^{\frac{1}{4}} Z^{\frac{7}{12}} - \gamma \alpha^{-\frac{1}{4}}
\]
with some \( 0 \leq \gamma \leq \frac{1}{63} \), then
\[
E_{\text{nf}}^Z + CZ\alpha\Lambda^2 \geq E_{\text{nf}}^Z \geq E_{\text{nf}}^Z - CZ^{\frac{5}{3}} - \gamma.
\]
(1.6)

We note that \( Z\alpha\Lambda^2 \ll Z^{7/3} \) if \( \Lambda \ll \kappa^{-1/4} Z^{11/12} \) in the \( Z \to \infty \) limit.

Remark 1. The leading term asymptotics of the non-magnetic problem is given by the Thomas-Fermi theory and \( E_{\text{nf}}^Z = -c_{\text{TF}} Z^{\frac{7}{3}} + O(Z^2) \) as \( Z \to \infty \), where \( c_{\text{TF}} = 3.678 \cdot (3\pi^2)^{\frac{1}{2}} \) is the Thomas-Fermi constant. The leading order asymptotics was established in [LS] (see also [L]). The correction to order \( Z^2 \) is known as the Scott correction and was established in [H, SW1] and for molecules in [IS] (See also [SW2, SW3, SS]). The next term in the expansion of order \( Z^{5/3} \) was rigorously established for atoms in [FS].

Remark 2. The exponents in the error terms are far from being optimal. They can be improved by strengthening our general semiclassical result Lemma 1.3 for special Coulomb like potentials using multi-scale analysis.

Remark 3. For simplicity, we state and prove our results for atoms, but the same proofs work for molecules as well, if the number of nuclei \( K \) is fixed, each has a charge \( Z \), and assume that the nuclei centers \( \{ R_1, \ldots, R_K \} \) are at least at distance \( Z^{-1/3} \) away, i.e. \( |R_i - R_j| \geq cZ^{-1/3}, i \neq j \).

Remark 4. Theorem 1.1 holds for the magnetic Schrödinger operator as well, i.e. if we replace the Pauli operator \( T(A) = [\sigma \cdot (p + A)]^2 \) by \( T(A) = (p + A)^2 \) everywhere. The proof is a trivial modification of the Pauli case. The argument is in fact even easier; instead of the magnetic Lieb-Thirring inequality for the Pauli operator one uses the usual Lieb-Thirring inequality that holds for the magnetic Schrödinger operator uniformly in the magnetic field. We leave the details to the reader. Note that although the condition \( Z\alpha^2 \leq \kappa \) is not needed in order to ensure stability in the Schrödinger case, we still need it in the statement in Theorem 1.1. In the Schrödinger case this condition is not optimal.

The upper bound in (1.4) is trivial by using a non-magnetic trial state. The upper bound in (1.6) is obtained by a trial state that is the tensor product of a non-magnetic electronic trial function with the vacuum \( |\Omega\rangle \) of \( \mathcal{F} \). The field energy \( H_f \) and all terms that are linear in
A give zero expectation value in the vacuum. The only effect of the quantized field is in the nonlinear term $A^2$. A simple calculation shows that

$$
\langle \Omega | A^2 | \Omega \rangle \leq C \alpha^2.
$$

The main task is to prove the lower bounds. Using the results from [BFG], the result for the quantized field (1.6) will directly follow from an analogous result for a slightly modified Hamiltonian with a classical field. Let

$$
H_{N,Z}(A) = H_{N,Z,\alpha}(A) = \sum_{i=1}^{N} \left[ T_i(A) - \frac{Z}{|x_i|} \right] + \sum_{i<j} \frac{1}{|x_i - x_j|} + \frac{1}{8 \pi \alpha^2} \int_{|x| \leq 3r} |\nabla \otimes A|^2
$$

(1.7)

with some

$$
r = DZ^{-1/3} \text{ with } D \geq 1.
$$

(1.8)

Note that instead of the local field energy, the total local $H^1$-norm of $A$ is added in (1.7). By (1.2), we have

$$
H_{N,Z}^1(A) \geq H_{N,Z}(A)
$$

(1.9)

for any $A \in \mathcal{A}$. We define the ground state energy of the modified Hamiltonian (1.7)

$$
E_{N,Z}(A) := \inf \left\{ \langle \Psi, H_{N,Z}(A) \Psi \rangle : \Psi \in \bigotimes_{1}^{N} (C_0^\infty(\mathbb{R}^3) \otimes C^2), \| \Psi \| = 1 \right\},
$$

and set

$$
E_{N,Z} := \inf_{A \in \mathcal{A}} E_{N,Z}(A), \quad E_Z := \inf_{N} E_{N,Z},
$$

where the infimum for $A \in \mathcal{A}$ can again be restricted to compactly supported vector potentials $A \in \mathcal{A}_0$. For the modified classical Hamiltonian we have the following theorem:

**Theorem 1.2.** Let $Z \alpha^2 \leq \kappa$ and assume that $r = DZ^{-1/3}$ with $1 \leq D \leq Z^{1/63}$. Then

$$
E_{Z}^{\inf} \geq E_Z \geq E_{Z}^{\inf} - CZ^{7/3} D^{-1}.
$$

(1.10)

Taking into account (1.9), Theorem 1.2 immediately implies the lower bound in (1.4). The proof of the lower bound in (1.6) follows from Theorem 1.2 adapting an argument in [BFG] that we will review in Section 6 for completeness.

One of the key ingredients of the proof of Theorem 1.2 is the following semiclassical statement that is of interest in itself. The first version is formulated under general conditions but without an effective error term. In our proof we actually use the second version that has a quantitative error term.
Theorem 1.3. Let $T_h(A) = [\sigma \cdot (h\mathbf{p} + A)]^2$ or $T_h(A) = (h\mathbf{p} + A)^2$, $h \leq 1$, and $V \geq 0$.

1) If $V \in L^{5/2}(\mathbb{R}^3) \cap L^4(\mathbb{R}^3)$, then

$$
\text{Tr} [T_h(A) - V]_+ + h^{-2} \int_{\mathbb{R}^3} \mathbf{B}^2 \geq \text{Tr} [-h^2\Delta - V]_+ + o(h^{-3}) \quad \text{as } h \to 0.
$$

(1.11)

2) Assume that $\|V\|_{\infty} \leq K$ with some $1 \leq K \leq C h^{-2}$ and consider the operators with Dirichlet boundary condition on $\Omega \subset \mathbb{R}^3$. Let $B_R$ denote the ball of radius $R$ about the origin and let $\Omega_{\sqrt{h}} := \Omega + B_{\sqrt{h}}$ denote the $\sqrt{h}$-neighborhood of the set $\Omega$. We set $|\Omega_{\sqrt{h}}|$ for the Lebesgue measure of $\Omega_{\sqrt{h}}$. Then

$$
\text{Tr} [(T_h(A) - V)_{\Omega}]_+ + h^{-2} \int_{\mathbb{R}^3} \mathbf{B}^2 \\
\geq \text{Tr} [(-h^2\Delta - V)_{\Omega}]_+ - C h^{-3} K^{5/2} |\Omega_{\sqrt{h}}|(hK^{3/2})^{1/2} \left[1 + (hK^3/2)^{1/2}\right].
$$

(1.12)

Remark. Despite that the electrons are confined to $\Omega$, their motion generates a magnetic field in the whole $\mathbb{R}^3$, so the magnetic field energy in (1.12) is given by integration over $\mathbb{R}^3$.

We use the convention that letters $C, c$ denote positive universal constants whose values may change from line to line.

2 Reduction to the Main Lemmas

Proof of Theorem 1.2. We focus on the lower bound, the upper bound is trivial. We start with two localizations, one on scale $r \geq Z^{-1/3}$ and the other one on scale $d \leq Z^{-1/3}$. The first one is designed to address the difficulty that the $H^1$-norm of $A$ is available only locally around the nucleus. This step would not be needed for the direct proof of (1.4). The second localization removes the “Coulomb tooth”, i.e. the Coulomb singularity near the nucleus.

In this section we reduce the proof of the lower bound in Theorem 1.2 to two lemmas. Lemma 2.1 will show that the Coulomb tooth is indeed negligible. Lemma 2.2 shows that the magnetic field cannot substantially lower the energy for the problem without the Coulomb tooth. In the proof of Lemma 2.2 we will use Theorem 1.3.

Recall that $B_R$ denotes the ball of radius $R$ about the origin. We construct a pair of smooth cutoff functions satisfying the following conditions

$$
\theta_0^2 + \theta_1^2 \equiv 1, \quad \text{supp } \theta_1 \subset B_{2d}, \quad \theta_1 \equiv 1 \text{ on } B_d, \quad |\nabla \theta_0|, |\nabla \theta_1| \leq Cd^{-1}.
$$

We will choose

$$
d = \delta Z^{-1/3}
$$

(2.13)
with some \( \delta \leq 1 \), in particular \( d \leq r \).

We split the Hamiltonian as

\[
H_{N,Z}(A) = H^0_{N,Z}(A) + H^1_{N,Z}(A)
\]

with

\[
H^0_{N,Z}(A) = \sum_{i=1}^{N} \left[ \theta_0 \left( T(A) - \frac{Z}{|x_i|} - (|\nabla \theta_0|^2 + |\nabla \theta_1|^2) \right) \theta_0 \right]_i + \sum_{i<j} \frac{1}{|x_i - x_j|} + \frac{1}{16\pi\alpha^2} \int_{B_{3r}} |\nabla \otimes A|^2,
\]

\[
H^1_{N,Z}(A) = \sum_{i=1}^{N} \left[ \theta_1 \left( T(A) - \frac{Z}{|x_i|} - (|\nabla \theta_0|^2 + |\nabla \theta_1|^2) \right) \theta_1 \right] + \frac{1}{16\pi\alpha^2} \int_{B_{3r}} |\nabla \otimes A|^2,
\]

where we used the IMS localization formula that is valid for the Pauli operator as well as for the Schrödinger operator.

In Section 3 we deal with \( H^1_{N,Z} \), to prove that it is negligible:

**Lemma 2.1.** There is a positive universal constant \( \kappa \) such that for any \( Z, \alpha \) with \( Z\alpha^2 \leq \kappa \) we have

\[
\inf_N \inf_A H^1_{N,Z}(A) \geq -CZ^{7/3}\delta^{1/2} - Z^{2/3}\delta^{-2}
\]

if \( CZ^{-2/3} \leq \delta \leq D \) with a sufficiently large constant \( C \).

Starting Section 4 we will treat \( H^0_{N,Z}(A) \) and we prove the following

**Lemma 2.2.** There is a positive universal constant \( \kappa \) such that for any \( Z, \alpha \) with \( Z\alpha^2 \leq \kappa \) we have

\[
\inf_N \inf_A H^0_{N,Z}(A) \geq -c_{TF} Z^{7/3} - CZ^{7/3}[Z^{-1/30} + D^{-1}]
\]

with a sufficiently large constant \( C \) if \( Z^{-1/6} \leq \delta \leq 1 \) and \( D \leq Z^{1/24}\delta^{13/16} \).

The main ingredient in the proof is Theorem 1.3 that will be proven in Section 5. The proof of the lower bound in Theorem 1.2 then follows from Lemmas 2.1 and 2.2 after choosing \( \delta = Z^{-2/63} \). □
3 Estimating the Coulomb Tooth

Proof of the Lemma 2.1. Let \( \tilde{\chi}_0 \) be a smooth cutoff function supported on \( B_{3r} \) such that \( |\nabla \tilde{\chi}_0| \leq C r^{-1} \) and \( \tilde{\chi}_0 \equiv 1 \) on \( B_{2r} \). Let \( \langle A \rangle := |B_{3r}|^{-1} \int_{B_{3r}} A \). We define

\[
A_0 := (A - \langle A \rangle) \tilde{\chi}_0, \quad B_0 := \nabla \times A_0,
\]

then \( \nabla \otimes A_0 = \tilde{\chi}_0 \nabla \otimes A + (A - \langle A \rangle) \otimes \nabla \tilde{\chi}_0 \). Clearly

\[
\int_{\mathbb{R}^3} B_0^2 \leq \int_{\mathbb{R}^3} |\nabla \otimes A_0|^2 \leq 2 \int_{\mathbb{R}^3} \tilde{\chi}_0^2 |\nabla \otimes A|^2 + C r^{-2} \int_{B_{3r}} (A - \langle A \rangle)^2 \]

\[
\leq C_1 \int_{B_{3r}} |\nabla \otimes A|^2
\]

for some universal constant \( C_1 \), where in the last step we used the Poincaré inequality. Let \( \varphi \) be a real phase such that \( \nabla \varphi = \langle A \rangle \). Since \( \tilde{\chi}_0 \equiv 1 \) on the support of \( \theta_1 \) by \( D \geq \delta \), we have

\[
\theta_1 T(A) \theta_1 = \theta_1 e^{-i\varphi} T(A - \langle A \rangle) e^{i\varphi} \theta_1 = \theta_1 e^{-i\varphi} T(A_0) e^{i\varphi} \theta_1.
\]

After these localizations, we have

\[
H_{N,Z}^1(A) \geq \sum_{j=1}^N \left[ \theta_1 e^{-i\varphi} \left( T(A_0) - W(x) \right) e^{i\varphi} \theta_1 \right] + \frac{1}{2C_1 \alpha^2} \int B_0^2
\]

with

\[
W(x) = \left[ \frac{Z}{|x|} + C d^{-2} \right] 1(|x| \leq 2d).
\]

Now we use the “running energy scale” argument in [LLS].

\[
\sum_{j=1}^N \left[ \theta_1 e^{-i\varphi} \left[ T(A_0) - W \right] e^{i\varphi} \theta_1 \right] \geq - \int_0^\infty \mathcal{N}_e(T(A_0) - W) \, de
\]

\[
\geq - \int_0^\mu \mathcal{N}_e(T(A_0) - W) \, de - \int_\mu^\infty \mathcal{N}_0 \left( \frac{\mu}{e} T(A_0) - W + e \right) \, de
\]

\[
\geq - \int_0^\mu \mathcal{N}_e(T(A_0) - W) \, de - \int_\mu^\infty \mathcal{N}_0 \left( T(A_0) - \frac{e}{\mu} W + \frac{e^2}{\mu^2} \right) \, de,
\]

where \( \mathcal{N}_e(A) \) denotes the number of eigenvalues of a self-adjoint operator \( A \) below \( -e \).
In the first term we use the bound $T(A_0) \geq (p + A_0)^2 - |B_0|$ and the CLR bound:

$$\int_0^\mu \mathcal{N}_\epsilon(T(A_0) - W) \, d\epsilon \leq C \int_0^\mu \, d\epsilon \int_{\mathbb{R}^3} (W + |B_0| - \epsilon)^{3/2}$$

$$\leq C \int_0^\mu \, d\epsilon \int_{\mathbb{R}^3} (W - \epsilon/2)^{3/2} + C \int_0^\mu \, d\epsilon \int_{\mathbb{R}^3} (|B_0| - \epsilon^2/2\mu)^{3/2}$$

$$\leq C \int_{\mathbb{R}^3} W^{5/2} + C \mu^{1/2} \int_{\mathbb{R}^3} B_0^2$$

$$= CZ^{5/2}d^{1/2} + Cd^{-2} + C \mu^{1/2} \int_{\mathbb{R}^3} B_0^2.$$  \hfill (3.20)

In the second term of (3.19) we use

$$T(A_0) - \frac{e}{\mu} W \geq \frac{1}{2} \left[(p + A_0)^2 - \frac{2eZ}{\mu|x|}1(|x| \leq 2d)\right] + \frac{1}{2} (p + A_0)^2 - |B_0| - \frac{Ce}{\mu d^2}1(|x| \leq 2d),$$

and that

$$(p + A_0)^2 - \frac{2eZ}{\mu|x|}1(|x| \leq 2d) \geq (p + A_0)^2 - \frac{4eZ}{\mu|x|} = -\left(\frac{2eZ}{\mu}\right)^2$$  \hfill (3.21)

i.e.

$$T(A_0) - \frac{e}{\mu} W \geq \frac{1}{2} (p + A_0)^2 - 2\left(\frac{eZ}{\mu}\right)^2 - |B_0| - \frac{Ce}{\mu d^2}1(|x| \leq 2d).$$

We choose $\mu = 4Z^2$, then using $Ce/\mu d^2 \leq e^2/4\mu$ for $\mu \leq \epsilon$ (i.e. $C \leq (\delta Z^2/3)^2$), we get

$$\int_\mu^\infty \mathcal{N}_0 \left(T(A_0) - \frac{e}{\mu} W + \frac{e^2}{\mu}\right) \, d\epsilon \leq \int_\mu^\infty \mathcal{N}_0 \left(\frac{1}{2} (p + A_0)^2 - |B_0| + \frac{e^2}{4\mu}\right) \, d\epsilon$$

$$\leq C \int_0^\mu \, d\epsilon \int_{\mathbb{R}^3} (|B_0| - \epsilon^2/4\mu)^{3/2}$$

$$\leq C \mu^{1/2} \int_{\mathbb{R}^3} B_0^2.$$  \hfill (3.22)

Note that if $Z\alpha^2 \leq \kappa$ with some sufficiently small universal constant $\kappa$, then the magnetic energy terms in (3.20) and (3.22) can be controlled by the corresponding term in (3.18). Combining the estimates (3.18), (3.19), (3.20) and (3.22) we obtain

$$H_{N,Z}^1(A) \geq -CZ^{5/2}d^{1/2} - Cd^{-2}$$  \hfill (3.23)

and Lemma 2.1 follows. \hfill \Box
4 Removing the magnetic field

Proof of Lemma 2.2. We start with two preparations. In Section 4.1 we give an upper bound for the number of electrons $N$ in the truncated model described by $H_{N,Z}^{0}(A)$. In Section 4.2 we then reduce the problem to a one-body semiclassical statement on boxes. The semiclassical problem will be investigated in Section 5 and this will complete the proof of Lemma 2.2.

4.1 Upper bound on the number of electrons $N$

Let

$$E_{N,Z}^{0}(A) := \inf \left\{ \langle \Psi, H_{N,Z}^{0}(A) \Psi \rangle : \Psi \in \bigwedge_{1}^{N} \left( C_{0}^{\infty}(\mathbb{R}^{3}) \otimes \mathbb{C}^{2} \right), \| \Psi \| = 1 \right\}$$

be the ground state energy of the truncated Hamiltonian $H_{N,Z}^{0}(A)$ defined in (2.14). The following lemma shows that we can assume $N \leq CZ$ when taking the infimum over $N$ in (2.15). The proof is a slight modification of the proof of the Ruskai-Sigal theorem as presented in [CFKS]. We note that the original proof was given for the non-magnetic case and it can be trivially extended to the Schrödinger operator with a magnetic field but not to the Pauli operator. This is because a key element of the proof, the standard lower bound on the hydrogen atom, $-\Delta - Z/|x| \geq -Z^{2}/4$, is valid if $-\Delta = p^{2}$ replaced by $(p + A)^{2}$ but there is no lower bound for the ground state energy of the hydrogen atom with the Pauli kinetic energy that is independent of the magnetic field. However, for the truncated Coulomb potential the trivial lower bound can be used.

Lemma 4.1. There exist universal constants $c$ and $C$ such that for any fixed $A \in A_{0}$ and $Z$ we have

$$E_{N,Z}^{0}(A) = E_{N-1,Z}^{0}(A)$$

whenever $N \geq CZ$ and $Z^{-1/6} \leq \delta \leq c$. In particular

$$\inf_{N} \inf_{A \in A_{0}} E_{N,Z}^{0}(A) = \inf_{N \leq CZ} \inf_{A \in A_{0}} E_{N,Z}^{0}(A) \quad (4.24)$$

if $Z^{-1/6} \leq \delta \leq c$.

Proof. We mostly follow the proof of Theorem 3.15 in [CFKS] and we will indicate only the necessary changes. For any $x = (x_{1}, x_{2}, \ldots, x_{N}) \in \mathbb{R}^{3N}$ we define

$$x_{\infty}(x) := \max \{|x_{i}| : i = 1, 2, \ldots, N\}$$

$$A_{0} := \{ x : |x_{j}| < \varrho \ \forall \ j = 1, 2, \ldots, N \}$$

$$A_{i} := \{ x : |x_{i}| \geq (1 - \zeta) x_{\infty}(x), \ x_{\infty}(x) > \frac{\varrho}{2} \}$$
for some fixed positive $\rho$ and $\zeta < 1/2$ to be chosen later. According to Lemma 3.16 in [CFKS], there is partition of unity $\{J_i\}_{i=0,1,...,N}$, with $\sum_i J_i^2 \equiv 1$, supp $J_i \subset A_i$ such that the gradient estimates

$$L(x) = \sum_{i=0}^{N} |\nabla J_i(x)|^2 \leq \frac{CN^{1/2}}{\rho^2}$$ if $x \in A_0$$

$$L(x) = \sum_{i=0}^{N} |\nabla J_i(x)|^2 \leq \frac{CN^{1/2}}{\rho x_{\infty}(x)}$$ if $x \in A_j, j \geq 1$$

hold with a suitable universal constant $C$. Moreover, $J_0$ is symmetric in all variables, while $J_i, i \geq 1$, is symmetric in all variables except $x_i$.

We subtract the local field energy that is an irrelevant constant, i.e. define

$$H_N := H_{N,Z}^0 - \frac{1}{16\pi\alpha^2} \int_{B_3} |\nabla \otimes A|^2$$

and $E_N = \inf \text{Spec } H_N$. We will show that $E_N = E_{N-1}$ for $N \geq CZ$. By removing one electron to infinity, clearly $E_N \leq E_{N-1} \leq 0$; here we used the fact that $A$ is compactly supported.

By the IMS localization

$$H_N = J_0(H_N - L)J_0 + \sum_{i=1}^{N} J_i(H_N - L)J_i.$$  \hfill (4.25)

In the first term we use that on the support of $\theta_0$ we have $-Z|x|^{-1} \geq -Zd^{-1}$. Hence

$$J_0(H_N - L)J_0 \geq J_0 \left(-CZN d^{-1} - CN d^{-2} + \frac{N(N - 1)}{4\rho} - \frac{CN^{1/2}}{\rho^2} \right) J_0.$$  \hfill (4.26)

Choosing $\rho = 8d$ we see that $J_0(H_N - L)J_0 \geq 0$ if $N \geq CZ$ with a constant $C$ if $\delta \geq CZ^{-2/3}$.

To estimate the terms $J_i(H_N - L)J_i$ for $i \neq 0$, we define

$$H_{N-1}^{(i)} := \sum_{j=1}^{N} \left[ \theta_0 \left(T(A) - \frac{Z}{|x|} \right) - (|\nabla\theta_0|^2 + |\nabla\theta_i|^2) \right] \theta_0_j + \sum_{k<j, k,j \neq i} \frac{1}{|x_k - x_j|}.$$
On the support of $J_i$ we have $|x_i| \geq \varrho/4 = 2d$, so $\nabla \theta_0$ and $\nabla \theta_1$ vanish. Then we can estimate
\[
J_i (H_N - L) J_i \geq J_i \left( H_{N-1}^{(i)} - \frac{Z}{|x_i|} + \frac{N - 1}{2x_1(x)} - \frac{CN^{1/2}}{x_{\infty}(x)\varrho} \right) J_i \\
\geq J_i \left( E_{N-1} + \frac{1}{|x_i|} \left[ \frac{N - 1}{2} (1 - \zeta) - Z - \frac{CN^{1/2}Z^{1/3}}{\delta} \right] \right) J_i \\
\geq J_i E_{N-1} J_i
\]
(4.27)
if $N \geq CZ$ and $N$ is large. Thus we conclude from (4.25), (4.26) and (4.27) that $E_N \geq E_{N-1}$ if $N \geq CZ$. □

4.2 Reduction to a one-body problem

We start by presenting an abstract lemma whose proof is given in Appendix A.

Lemma 4.2. Let $\mathfrak{h}$ be a one-particle operator on $\mathcal{H} = L^2(\mathbb{R}^3)$ and let $W$ be a two-particle operator defined on $\mathcal{H} \wedge \mathcal{H}$. We assume that the domains of $\mathfrak{h}$ and $W$ include the $C_0^\infty$ functions. Let $\theta \in C^\infty(\mathbb{R}^3)$ with compact support $\Omega := \text{supp} \theta$. Then
\[
\inf \left\{ \left\langle \Psi, \sum_{i=1}^N \theta_i \mathfrak{h}_i \theta_i + \sum_{1 \leq i < j \leq N} \theta_i \theta_j W_{ij} \theta_j \theta_i \right\rangle \Psi : \Psi \in \bigwedge_{1}^N C_0^\infty(\mathbb{R}^N), \| \Psi \| = 1 \right\} \\
\geq \inf_{n \leq N} \inf \left\{ \left\langle \Phi, \left( \sum_{i=1}^n \mathfrak{h}_i + \sum_{1 \leq i < j \leq n} W_{ij} \right) \Phi \right\rangle : \Phi \in \bigwedge_{1}^n C_0^\infty(\Omega), \| \Phi \| = 1 \right\},
\]
(4.28)
where $\mathfrak{h}_i$ denotes the operator $\mathfrak{h}$ acting on the $i$-th component of the tensor product, and similar convention is used for the two-particle operators. The same result holds with obvious changes if $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$.

To continue the proof of Lemma 2.2 we first localize $H_{N,Z}^0(\Lambda)$ onto a ball $B_r$ of radius $r = DZ^{-1/3}$ (see (1.8)) and we also localize the magnetic field as in Section 3. We introduce smooth cutoff functions $\chi_0$ and $\chi_1$ with
\[
\chi_0^2 + \chi_1^2 \equiv 1, \quad \text{supp} \chi_0 \subset B_{2r}, \quad \chi_0 \equiv 1 \quad \text{on} \ B_r, \quad |\nabla \chi_0|, |\nabla \chi_1| \leq Cr^{-1}.
\]

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We get

\[
H_{0,N,Z}^0(A) \geq \sum_{i=1}^{N} \theta_0 \chi_0 e^{-i\varphi_0} \left[ T_i(A_0) - \frac{Z}{|x_i|} \right] e^{i\varphi_0} \chi_0 \theta_0 + \sum_{i<j} \frac{1}{|x_i - x_j|} + \frac{1}{C\alpha^2} \int_{\mathbb{R}^3} B_0^2 - CNd^{-2} - CNZr^{-1}
\]  

(4.29)

using that the new localization error \(|\nabla \chi_1|^2 + |\nabla \chi_0|^2 \leq Cr^{-2} \leq Cd^{-2}\) and that \(-Z/|x| \geq -Zr^{-1}\) on the support of \(\chi_1\). We also used (3.17).

Let \(A_{d,r} = \{ x : d \leq |x| \leq r \} \subset \mathbb{R}^3\). Using (4.24), the positivity of the Coulomb repulsion \(|x_i - x_j|^{-1} > 0\) and Lemma 4.2 with \(\theta := \theta_0 \chi_0\) we obtain

\[
\inf_N \inf_{A \in A_0} H_{0,N,Z}^0(A) \geq \inf_{N \leq CZ} \inf_{A_0 \in A_0} \left\{ \inf_{\Psi} \left\langle \Psi, \left[ \sum_{i=1}^{N} \left[ T_i(A_0) - \frac{Z}{|x|} \right] + \sum_{i<j} \frac{1}{|x_i - x_j|} \right] \right\rangle_{A_{d,r}} \Psi \right\} + \frac{1}{C\alpha^2} \int_{\mathbb{R}^3} B_0^2 - C \frac{5}{3} \delta^{-2} - C \frac{7}{3} D^{-1},
\]

(4.30)

where the infimum is over all antisymmetric wave functions \(\Psi \in \bigwedge_1^N C_0^\infty(A_{d,r}) \otimes \mathbb{C}^2\) with \(\|\Psi\|_2 = 1\). The notation \([H]_Q\) indicates the \(N\)-particle operator \(H\) with Dirichlet boundary condition on the domain \(Q^N \subset \mathbb{R}^{3N}\).

We define

\[
D(f,g) := \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(x)g(y)}{|x-y|} \, dx \, dy.
\]

**Lemma 4.3.** There is a universal constant \(C_0 > 0\) such that for any \(\Psi \in \bigwedge_1^N C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^2\) with \(\|\Psi\|_2 = 1\), for any nonnegative function \(\varrho : \mathbb{R}^3 \rightarrow \mathbb{R}\) with \(D(\varrho, \varrho) < \infty\), for any \(A \in A_0\) and for any \(\varepsilon > 0\) we have

\[
\left\langle \Psi, \left[ \sum_{i=1}^{N} T_i(A) + \sum_{i<j} \frac{1}{|x_i - x_j|} \right] \Psi \right\rangle + C_0 \int_{\mathbb{R}^3} B^2 \geq -D(\varrho, \varrho) + \left\langle \Psi, \sum_{i=1}^{N} \left( \varrho * |x_i|^{-1} \right) \Psi \right\rangle - C\varepsilon^{-1} N.
\]

(4.31)
Proof. By the Lieb-Oxford inequality \[\text{LO}\] and by the positivity of the quadratic form \(D(\cdot, \cdot)\)

\[
\left\langle \Psi, \sum_{i<j} \frac{1}{|x_i - x_j|} \Psi \right\rangle \geq D(\varrho, \varrho) - C \int_{\mathbb{R}^3} \frac{\varrho^{4/3}}{\Psi} \\
\geq -D(\varrho, \varrho) + \left\langle \Psi, \sum_{i=1}^{N} (\varrho * |x_i|^{-1}) \Psi \right\rangle - C \int_{\mathbb{R}^3} \frac{\varrho^{4/3}}{\Psi}
\]

where \(\varrho(x)\) is the one-particle density of \(\Psi\).

The error term is controlled by the following kinetic energy inequality for the Pauli operator

\[
\left\langle \Psi, \left[ \sum_{i=1}^{N} [T(A) - U] \right] \Psi \right\rangle \geq c \int_{\mathbb{R}^3} \min\{\varrho^{5/3} + \gamma \varrho^{4/3}, \gamma \varrho^{4/3}\} - \gamma \int_{\mathbb{R}^3} B^2
\]

with some positive universal constant \(c\) and for any \(\gamma > 0\). For the proof of (4.33) use the magnetic Lieb-Thirring inequality

\[
\left\langle \Psi, \left[ \sum_{i=1}^{N} [T(A) - U] \right] \Psi \right\rangle \geq -C \int_{\mathbb{R}^3} U^{5/2} - C \gamma^{-3} \int_{\mathbb{R}^3} U^4 - \gamma \int_{\mathbb{R}^3} B^2.
\]

With the choice \(U = \beta \min\{\varrho^{2/3} + \gamma \varrho^{1/3}\}\) we can ensure that \(\frac{1}{2} \beta \varrho \geq C U^{5/2} + C \gamma^{-3} U^4\) if \(\beta\) is sufficiently small (independent of \(\gamma\)) and this proves (4.33).

Thus

\[
\int_{\mathbb{R}^3} \varrho^{4/3} \leq \gamma^{-1} \int_{\mathbb{R}^3} \min\{\varrho^{5/3} + \gamma \varrho^{4/3}, \gamma \varrho^{4/3}\} + \gamma \int_{\mathbb{R}^3} \varrho
\]

\[
\leq (c\gamma)^{-1} \left\langle \Psi, \left[ \sum_{i=1}^{N} [T(A) - U] \right] \Psi \right\rangle + c^{-1} \int_{\mathbb{R}^3} B^2 + \gamma N
\]

so choosing \(\gamma = C \varepsilon^{-1}\) with a sufficiently large constant \(C\), we obtain (4.31). \(\square\)

Using Lemma 4.3 we can continue the estimate (4.30) (with writing \(A\) instead of \(A_0\) in the infimum) as

\[
\inf \inf_{N} H_{N,Z}^{0}(A) \geq (1 - \varepsilon) \inf_{N \leq C \varepsilon} \inf_{A \in A_0} \left\{ \inf_{\Psi} \left\langle \Psi, \left[ \sum_{i=1}^{N} [T(A) + W] \right]_{A_{d,r}} \Psi \right\rangle + \frac{1}{C \alpha^2} \int_{\mathbb{R}^3} B^2 \right\}
\]

\[
- D(\varrho, \varrho) - C \varepsilon^{-1} Z - C Z^{5/3} \delta^{-2} - C Z^{7/3} D^{-1}
\]

(4.35)
with
\[ W(x) := \frac{1}{1 - \varepsilon} \left[ -\frac{Z}{|x|} + \varrho * |x|^{-1} \right] \]
and assuming that \( \alpha \leq \alpha_0 \) with some small universal \( \alpha_0 \).

We now perform a rescaling: \( x = Z^{-1/3} X, \ p = Z^{1/3} P \) and
\[
\tilde{A}(X) = Z^{-2/3} A(Z^{-1/3} X), \quad \tilde{B}(X) = \nabla \times \tilde{A}(X) = Z^{-1} B(Z^{-1/3} X)
\]
Introducing \( h = Z^{-1/3} \) and \( T_h(\tilde{A}) := [(hP + \tilde{A}) \cdot \sigma]^2 \), we obtain that the kinetic energy changes as
\[
[(\mathbf{p} + A) \cdot \sigma]^2 = Z^{1/3} [(Z^{-1/3} \mathbf{P} + \tilde{A}) \cdot \sigma]^2 = Z^{4/3} T_h(\tilde{A})
\]
and the field energy changes as
\[
\int_{\mathbb{R}^3} B^2(x) dx = Z \int_{\mathbb{R}^3} \tilde{B}^2(X) dX.
\]
The new potential energy is
\[
\tilde{W}(X) = Z^{-4/3} W(Z^{-1/3} X) = \frac{1}{1 - \varepsilon} \left[ -\frac{1}{|X|} + \tilde{\varrho} * |X|^{-1} \right],
\]
where \( \tilde{\varrho}(X) = Z^{-2} \varrho(Z^{-1/3} X) \) and \( D(\tilde{\varrho}, \tilde{\varrho}) = Z^{-7/3} D(\varrho, \varrho) \). After rescaling, we get from (4.35)
\[
\inf_N \inf_{A \in A_0} \frac{1}{N} H^0_{N,Z}(A) \geq (1 - \varepsilon) Z^{4/3} \inf_{N \leq CZ} \inf_{A \in A_0} \left\{ \inf_{\Psi} \left[ \Psi, \sum_{i=1}^N \left[ T_h(\tilde{A}) + \tilde{W} \right]_{A_{\delta,D}} \Psi \right] + \frac{h^2}{CZ\alpha^2} \int_{\mathbb{R}^3} \tilde{B}^2 \right\} \quad (4.36)
\]
\[
- Z^{7/3} D(\tilde{\varrho}, \tilde{\varrho}) - C \varepsilon^{-1} Z - CZ^{5/3} \delta^{-2} - CZ^{7/3} D^{-1},
\]
where \( A_{\delta,D} = \{ X : \delta \leq |X| \leq D \} \) and \( \inf_{\Psi} \) denotes infimum over all normalized antisymmetric functions. Using (1.12) from Theorem (1.3) and the fact that \( Z\alpha^2 \leq \kappa \), we get
\[
\inf_N \inf_A H^0_{N,Z}(A) \geq (1 - \varepsilon) Z^{4/3} \text{Tr} \left[ (-h^2 \Delta + \tilde{W})_{A_{\delta,D}} \right] - CZ^{13/6} D^3 \delta^{-13/4}
\]
\[
- Z^{7/3} D(\tilde{\varrho}, \tilde{\varrho}) - C \varepsilon^{-1} Z - CZ^{5/3} \delta^{-2} - CZ^{7/3} D^{-1} \quad (4.37)
\]
assuming \( \delta \geq Z^{-2/9} \). By standard semiclassical result for Coulomb-like potentials (see e.g. the result in Section V.2 of [L]):
\[
\text{Tr} \left[ (-h^2 \Delta + \tilde{W})_{A_{\delta,D}} \right] \geq \text{Tr} \left[ -h^2 \Delta + \tilde{W} \right] \geq -C_{sc} h^{-3} \int_{\mathbb{R}^3} \tilde{W}_{-5/2}^2 - Ch^{-3+1/10}. \quad (4.38)
\]
where \( C_{sc} = 2/(15\pi^2) \) is the Weyl constant in semiclassics. The \( \frac{1}{10} \) exponent in the error term is far from being optimal; the methods developed to prove the Scott correction can yield an exponent up to one (see Remark 1 after Theorem 1.1).

Taking the optimal \( \tilde{\rho} \) to be the Thomas-Fermi density for \( Z = 1 \) \( \tilde{\rho} = \rho_{\text{TF}} \) (see, e.g. Section II of [L]) and defining the Thomas-Fermi constant as

\[
c_{\text{TF}} := D(\tilde{\rho}, \tilde{\rho}) + C_{sc} \int_{\mathbb{R}^3} \left( -\frac{1}{|X|} + \tilde{\rho} * |X|^{-1} \right)^{5/2}
\]

we get

\[
\inf_{N} \inf_{A} H_{N,Z}^{0}(A) \geq (1 - \varepsilon)^{-3/2} Z^{7/3} \left( - D(\tilde{\rho}, \tilde{\rho}) - C_{sc} \int_{\mathbb{R}^3} \left( -\frac{1}{|X|} + \tilde{\rho} * |X|^{-1} \right)^{5/2} \right)
\]

\[
- C Z^{7/3 - 1/30} - C Z^{13/6} D^{3} \delta^{-13/4} - C \varepsilon^{-1} Z - C Z^{5/3} \delta^{-2} - C Z^{7/3} D^{-1}
\]

\[
\geq -(1 - \varepsilon)^{-3/2} c_{\text{TF}} Z^{7/3} - C Z^{7/3 - 1/30} - C \varepsilon^{-1} Z - C Z^{5/3} \delta^{-2} - C Z^{7/3} D^{-1}
\]

\[
\geq -c_{\text{TF}} Z^{7/3} - C Z^{7/3} \left[ Z^{-1/30} + D^{-1} \right]
\]

where we optimized for \( \varepsilon \) and we used that \( D \leq 1/24 \delta^{13/16} \) and \( Z^{-1/6} \leq \delta \leq 1 \). This completes the proof of Lemma 2.2. \( \square \)

5 Semiclassics: proof of Theorem 1.3

We present the Schrödinger and Pauli cases in parallel. We prove the statement with Dirichlet boundary conditions (1.12) in details and in Section 5.4 we comment on the necessary changes for the proof of the (1.11). The potential \( V \) is defined only on \( \Omega \), but we extend it to be zero on \( \mathbb{R}^3 \setminus \Omega \) we continue to denote by \( V \) its extension.

5.1 Localization onto boxes

We choose a length \( L \) with \( h \leq L \leq \frac{1}{3} h^{1/2} \). Let \( \Omega_L = \Omega + B_L \) be the \( L \)-neighborhood of \( \Omega \). Let \( Q_k = \{ y \in \mathbb{R}^3 : \|y - k\|_{\infty} < L/2 \} \) with \( k \in (L\mathbb{Z})^3 \cap \Omega_L \) denote a non-overlapping covering of \( \Omega \) with boxes of size \( L \). In this section the index \( k \) will always run over the set \( (L\mathbb{Z})^3 \cap \Omega_L \).

Let \( \xi_k \) be a partition of unity, \( \sum_k \xi_k^2 \equiv 1 \), subordinated to the collection of boxes \( Q_k \), such that

\[
\text{supp} \xi_k \subset (2Q)_k, \quad |\nabla \xi_k| \leq CL^{-1}
\]
where \((2Q)_k\) denotes the cube of side-length \(2L\) with center \(k\). Let \(\bar{\xi}_k\) be a cutoff function such that \(\bar{\xi}_k \equiv 1\) on \((2Q)_k\) (i.e. on the support of \(\xi_k\)), \(\text{supp} \bar{\xi}_k \subset \bar{Q}_k := (3Q)_k\) and \(|\nabla \bar{\xi}_k| \leq CL^{-1}\).

Let \(\langle A \rangle_k = |\bar{Q}_k|^{-1} \int_{\bar{Q}_k} A\). Similarly to (3.16), we define \(A_k := (A - \langle A \rangle_k)\bar{\xi}_k\) and \(B_k := \nabla \times A_k\), then

\[
\int_{\mathbb{R}^3} B_k^2 \leq C \int_{\bar{Q}_k} |\nabla \otimes A|^2
\]

as in (3.17). From the IMS localization with \(\psi_k\) satisfying \(h \nabla \psi_k = \langle A \rangle_k\) we have

\[
\text{Tr} \left[ [T_h(A) - V]_{\Omega} \right] + h^{-2} \int_{\mathbb{R}^3} B^2 = \inf_{\gamma} \text{Tr} \left( \gamma [T_h(A) - V] \right) + h^{-2} \int_{\mathbb{R}^3} |\nabla \otimes A|^2 \\
\geq \inf_{\gamma} \sum_{k \in (LZ)^3 \cap \Omega} \mathcal{E}_k(\gamma)
\]

with

\[
\mathcal{E}_k(\gamma) := \text{Tr} \left[ \gamma \xi_k e^{-i\psi_k} [T_h(A - \langle A \rangle_k) - V] e^{i\psi_k} \xi_k - \gamma |h \nabla \xi_k|^2 \right] + c_0 h^{-2} \int_{\bar{Q}_k} |\nabla \otimes A|^2
\]

with some universal constant \(c_0\). Here \(\inf_{\gamma}^*\) denotes infimum over all density matrices \(0 \leq \gamma \leq 1\) that are supported on \(\Omega\), i.e. they are operators on \(L^2(\Omega) \otimes \mathbb{C}^2\). We also used \(\int_{\mathbb{R}^3} B^2 = \int_{\mathbb{R}^3} |\nabla \otimes A|^2\) and we reallocated the second integral. We introduce the notation

\[
\mathcal{F}_k := c_0 h^{-2} \int_{\bar{Q}_k} |\nabla \otimes A|^2.
\]

### 5.2 Apriori bound on the local field energy

In case of the Pauli operator, for each fixed box \(\bar{Q}_k\) we apply the magnetic Lieb-Thirring inequality [LLS] together with (5.40) and with the bound \(||V||_\infty \leq K\) to obtain that for any density matrix \(\gamma\)

\[
\mathcal{E}_k(\gamma) \geq \text{Tr} \left[ [T_h(A_k) - V - Ch^2 L^{-2}]_{\bar{Q}_k} \right] + \mathcal{F}_k \\
\geq -Ch^{-3} \int_{\bar{Q}_k} [V + Ch^2 L^{-2}]^{5/2} - C \left( \int_{\bar{Q}_k} [V + Ch^2 L^{-2}]^4 \right)^{1/4} \left( h^{-2} \int_{\bar{Q}_k} B_k^2 \right)^{3/4} + \mathcal{F}_k \\
\geq -C [h^{-3} K^{5/2} L^3 + h^3 L^2 + K^4 L^3 + h^8 L^{-5}] - \frac{c_0}{2} h^{-2} \int_{\bar{Q}_k} |\nabla \otimes A|^2 + \mathcal{F}_k \\
\geq -Ch^{-3} K^{5/2} L^3 + \frac{1}{2} \mathcal{F}_k
\]

(5.42)
using $h \leq L$ and $1 \leq K \leq Ch^{-2}$. In the Schrödinger case we use the usual Lieb-Thirring inequality \cite{LT} that holds with a magnetic field as well. The estimate \eqref{5.42} is then valid even without the third term in the second line.

Let $S \subset (LZ)^3 \cap \Omega_L$ denote the set of those $k$ indices such that

$$
F_k \leq Ch^{-3}K^{5/2}L^3. \tag{5.43}
$$

holds with some large constant $C$. In particular

$$
\mathcal{E}_k(\gamma) \geq 0, \quad \text{for all } k \not\in S \text{ and for any } \gamma. \tag{5.44}
$$

\section{Improved bound}

We use the Schwarz inequality in the form

$$
T_h(A - \langle A \rangle_k) \geq -(1 - \varepsilon_k)h^2 \Delta - C\varepsilon_k^{-1}(A - \langle A \rangle_k)^2,
$$

with some $0 < \varepsilon_k < \frac{1}{3}$. We have for any $\gamma$ supported on $\Omega$ that

$$
\mathcal{E}_k(\gamma) \geq \text{Tr} \left[ 1_\Omega \xi_k [- (1 - 2\varepsilon_k)h^2 \Delta - V - Ch^2L^{-2}]\xi_k 1_\Omega \right] - \text{Tr} \left[ 1_{\tilde{Q}_k} [- \varepsilon_k h^2 \Delta - C\varepsilon_k^{-1}(A - \langle A \rangle_k)^2] 1_{\tilde{Q}_k} \right] + \mathcal{F}_k \tag{5.45}
$$

We will show at the end of the section that

$$
\text{Tr} \left[ 1_\Omega \xi_k [- (1 - 2\varepsilon_k)h^2 \Delta - V - Ch^2L^{-2}]\xi_k 1_\Omega \right] - \text{Tr} \left[ 1_{\tilde{Q}_k} [- \varepsilon_k h^2 \Delta - C\varepsilon_k^{-1}(A - \langle A \rangle_k)^2] 1_{\tilde{Q}_k} \right] \geq Ch^{-3}K^{5/2}(\varepsilon_k + h^2L^{-2})|\tilde{Q}_k|. \tag{5.46}
$$

Using \eqref{5.44} and \eqref{5.46},

$$
\inf_{\gamma}^* \sum_k \mathcal{E}_k(\gamma) \geq \inf_{\gamma}^* \sum_{k \in S} \mathcal{E}_k(\gamma) \geq \sum_k \text{Tr} \left[ 1_\Omega \xi_k [- h^2 \Delta - V] \xi_k 1_\Omega \right] - \sum_{k \in S} \mathcal{D}_k \tag{5.47}
$$
with

\[ D_k := \text{Tr} \left[ [ -\varepsilon_k h^2 \Delta - C \varepsilon_k^{-1} (A - \langle A \rangle_k)^2 ] \tilde{Q}_k \right] - Ch^{-3} K^{5/2} |\tilde{Q}_k| (\varepsilon_k + h^2 L^{-2}) + F_k. \] (5.48)

In the last step in (5.47) we used that for any collection of density matrices \(\gamma_k\), the density matrix \(\sum_k \Omega \xi_k \gamma_k \xi_k^\dagger \Omega\) is admissible in the variational principle

\[ \text{Tr} \left[ ( -h^2 \Delta - V ) \right] = \inf \left\{ \text{Tr} \gamma [ -h^2 \Delta - V ] : 0 \leq \gamma \leq 1, \text{supp} \gamma \subset \Omega \right\}. \] (5.49)

We estimate \(D_k\) for \(k \in S\) as follows

\[ D_k \geq -C \varepsilon_k^{-4} h^{-3} \int \tilde{Q}_k (A - \langle A \rangle_k)^5 - Ch^{-3} K^{5/2} |\tilde{Q}_k| (\varepsilon_k + h^2 L^{-2}) + F_k \] (5.50)

\[ \geq F_k - C \varepsilon_k^{-4} h^2 L^{1/2} F_k^{5/2} - Ch^{-3} K^{5/2} |\tilde{Q}_k| (\varepsilon_k + h^2 L^{-2}). \]

In the first step we used Lieb-Thirring inequality, in the second step Hölder and Sobolev inequalities in the form

\[ \int \tilde{Q}_k (A - \langle A \rangle_k)^5 \leq CL^{1/2} \left( \int \tilde{Q}_k |\nabla \otimes A|^2 \right)^{5/2}. \]

We choose

\[ \varepsilon_k = hL^{-1/2} K^{-1/2} F_k^{1/2} \]

and using the apriori bound (5.43), we see that

\[ \varepsilon_k \leq Ch^{-1/2} L K^{3/4}. \]

Thus, assuming

\[ L \leq ch^{1/2} K^{-3/4} \] (5.51)

with a sufficiently small constant \(c\), we get \(\varepsilon_k \leq 1/3\). With this choice of \(\varepsilon_k\), and recalling \(|\tilde{Q}_k| = 9|Q_k| = 9L^3\), we have

\[ D_k \geq F_k - Ch^{-2} L^{5/2} K^2 F_k^{1/2} - Ch^{-3} K^{5/2} L^3 h^2 L^{-2} \]

\[ \geq -Ch^{-3} L^3 K^{5/2} \left( h^{-1} L^2 K^{3/2} + h^2 L^{-2} \right). \] (5.52)

If we choose \(L = h^{3/4} K^{-3/8}\), then

\[ D_k \geq -Ch^{-3} L^3 K^{5/2} \left( h^{3/2} K^{3/2} \right)^{1/2}. \]
This choice is allowed by (5.51) if $K \leq ch^{-2/3}$. If $ch^{-2/3} \leq K \leq h^{-2}$, then we choose $L = ch^{1/2}K^{-3/4}$ and we get from (5.52)

$$D_k \geq -Ch^{-3}L^3K^{5/2}(1 + hK^{3/2}).$$

Combining these two inequalities, we get that

$$D_k \geq -Ch^{-3}L^3K^{5/2}(1 + hK^{3/2})$$

always holds. Summing up (5.53) for all $k$ and using that

$$\sum_{k \in (LZ)^3 \cap \Omega_L} L^3 \leq C|\Omega_{3L}| \leq C|\Omega_{\sqrt{h}}|$$

(recall that $\Omega_{\sqrt{h}}$ is a $\sqrt{h}$-neighborhood of $\Omega$ and $3L \leq h^{1/2}$), we obtain from (5.47) and (5.53)

$$\inf_{\gamma} \sum_{k} \mathcal{E}_k(\gamma) \geq \text{Tr} \left[ (-h^2\Delta - V)\Omega \right] - Ch^{-3}K^{5/2} |\Omega_{\sqrt{h}}|(hK^{3/2})^{1/2}[1 + (hK^{3/2})^{1/2}]$$

(5.54)

and this proves (1.12).

Finally, we prove (5.46). Let $\gamma$ be a trial density matrix for the left hand side of (5.46). We can assume that

$$0 \geq \text{Tr} \left[ \gamma \Omega \xi_k[-(1 - 2\varepsilon_k)h^2\Delta - V - Ch^2L^{-2}]\xi_k \Omega \right]$$

Then

$$0 \geq \text{Tr} \left[ \gamma \Omega \xi_k[-\frac{1}{6}h^2\Delta + K]\xi_k \Omega \right] + \text{Tr} \left[ \gamma \Omega \xi_k[-\frac{1}{6}h^2\Delta - V - Ch^2L^{-2} - K]\xi_k \Omega \right]$

$$\geq \text{Tr} \left[ \gamma \Omega \xi_k[-\frac{1}{6}h^2\Delta + K]\xi_k \Omega \right] - Ch^{-3} \int_{\tilde{Q}_k} [V + K + Ch^2L^{-2}] \frac{5}{2},$$

(5.55)

where we used Lieb-Thirring inequality. Thus, using $|V| \leq K$, $h \leq L$ and $K \geq 1$, we have

$$\text{Tr} \left[ \gamma \Omega \xi_k[-\frac{1}{6}h^2\Delta + K]\xi_k \Omega \right] \leq Ch^{-3}K^{5/2}|\tilde{Q}_k|.$$

Therefore

$$\text{Tr} \left[ \gamma \Omega \xi_k[-(1 - 2\varepsilon_k)h^2\Delta - V - Ch^2L^{-2}]\xi_k \Omega \right]$$

$$\geq \text{Tr} \left[ \gamma \Omega \xi_k[-h^2\Delta - V]\xi_k \Omega \right] - Ch^{-3}K^{5/2}(|\varepsilon_k + h^2L^{-2})|\tilde{Q}_k|.$$

(5.56)

Now (5.46) follows by variational principle. □
5.4 Reduction of (1.11) to (1.12)

We approximate \( V \in L^{5/2} \cap L^4 \) by a bounded potential \( \widetilde{V} \), \( \| \widetilde{V} \|_\infty \leq K \), that is supported on a ball \( B_{R/2} \) and \( \widetilde{V} \leq V \). By choosing \( K \) and \( R \) sufficiently large, we can make \( \| V - \widetilde{V} \|_{5/2} + \| V - \widetilde{V} \|_4 \) arbitrarily small. We choose a cutoff function \( \chi_R \) that is supported on \( B_R \) and \( \chi_R \equiv 1 \).

Borrowing a small part of the kinetic energy, by IMS localization we have

\[
T_h(A) - V \geq (1 - \varepsilon) \chi_R [T_h(A) - \widetilde{V}] \chi_R
+ \varepsilon T_h(A) - (V - (1 - \varepsilon) \widetilde{V}) - |\nabla \chi_R|^2 - |\nabla \widetilde{\chi}_R|^2
\]

Using the magnetic Lieb-Thirring inequality \([LLS]\) to estimate the second term, we get

\[
\text{Tr} [T_h(A) - V] - (1 - \varepsilon) \text{Tr} [T_h(A) - \widetilde{V}]_{BR} - C \varepsilon^{-3/2} h^{-3} \int_{\mathbb{R}^3} |U|^{5/2} - C \int_{\mathbb{R}^3} |U|^4 - \frac{1}{2} h^{-2} \int_{\mathbb{R}^3} B^2
\]

with

\[
U := (V - (1 - \varepsilon) \widetilde{V}) + |\nabla \chi_R|^2 + |\nabla \widetilde{\chi}_R|^2.
\]

For the first term in (5.58) we use (1.12) (and that it holds even with a 1/2 in front of \( \int B^2 \)) and the fact that

\[
\text{Tr} [(-h^2 \Delta - \widetilde{V})_{BR}] \geq \text{Tr} [-h^2 \Delta - V]
\]

by monotonicity, \( \widetilde{V} \leq V \). The second and the third terms in (5.58) can be made arbitrarily small compared with \( h^{-3} \) for any fixed \( \varepsilon \) if \( R \) and \( K \) are sufficiently large and \( h \) is small. Finally, choosing \( \varepsilon \) sufficiently small, we proved (1.11).

6 Proof of the quantized field case

For the proof of the lower bound in (1.16), we follow the argument of \([BFC]\) to reduce the problem to the classical bound (1.10). We set

\[
H_g = \alpha^{-1} \int_{\mathbb{R}^3} |g(k)|^2 |k| \sum_{\lambda = \pm} a_\lambda(k)^* a_\lambda(k) dk.
\]

to be the cutoff field energy, then \( H_f \geq H_g \) and only the modes appearing in \( H_g \) interact with the electron. By Lemma 3 of \([BFC]\), for any real function \( f \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3) \) we have

\[
\frac{1}{8\pi} \int_{\mathbb{R}^3} f(x) |\nabla \otimes A(x)|^2 dx \leq \alpha^2 \| f \|_{\infty} H_g + C \alpha A^4 \| f \|_1.
\]

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Applying it with \( f \) being the characteristic function of the ball \( B_3r \) with \( r = DZ^{-1/3} \) (the radius of the ball is here chosen differently from \([BFG]\)) and using \( Z\alpha^2 \leq \kappa \) we get

\[
H_f \geq H_g \geq \left( \frac{Z\alpha^2}{\kappa} \right) H_g \geq \frac{Z}{8\pi \kappa} \int_{B_3r} |\nabla \otimes A(x)|^2 \, dx - C\kappa^{-1} \alpha \Lambda^4 D^3.
\]

Setting \( \tilde{\alpha} = (\kappa/Z)^{1/2} \), i.e. \( Z\tilde{\alpha}^2 = \kappa \), we have for \( \kappa \) sufficiently small

\[
E_{\text{ed}}^{\text{N,Z}} \geq E_{\text{N,Z,}\tilde{\alpha}} - C\kappa^{-1} \alpha \Lambda^4 D^3,
\]

where \( E_{\text{N,Z,}\tilde{\alpha}} \) is the ground state energy of the Hamiltonian \((1.7)\) with fine structure constant \( \tilde{\alpha} \). Applying \((1.10)\) to this Hamiltonian, we get

\[
E_{\text{ed}}^{\text{N,Z}} \geq E_{\text{N}}^{\text{nf}} \geq C\kappa^{-1} \alpha \Lambda^4 D^3
\]

whenever \( 1 \leq D \leq Z^{1/3} \). Writing \( D = Z^{\gamma} \) and applying the upper bound \((1.5)\) on \( \Lambda \), we obtain the lower bound in \((1.6)\). \( \square \)

### A Proof of Lemma 4.2

Let the function \( \chi(x) \in C^\infty(\mathbb{R}^3) \) be defined such that \( \theta^2(x) + \chi^2(x) \equiv 1 \). For any subset \( \alpha \subset \{1, 2, \ldots, N\} \) we denote by \( x_\alpha \) the collection of variables \( \{x_i : i \in \alpha\} \) and define

\[
\Theta_\alpha = \Theta_\alpha(x_\alpha) := \prod_{i \in \alpha} \theta(x_i), \quad \Xi_\alpha = \Xi_\alpha(x_\alpha) := \prod_{i \in \alpha} \chi(x_i).
\]

We set the notation \( \alpha^c = \{1, 2, \ldots, N\} \setminus \alpha \) for the complement of the set \( \alpha \) and set \( \underline{n} := \{1, 2, \ldots, n\} \). Let \( |\alpha| \) denote the cardinality of the set \( \alpha \).

For an arbitrary function \( \Psi \in \bigwedge_1^N C_0^\infty(\mathbb{R}^3) \), \( \|\Psi\| = 1 \), and for \( 0 \leq n \leq N \) we define

\[
\Gamma^n := \Theta_{\underline{n}} \left( \text{Tr}_{\underline{n}^c} \left[ \Xi_{\underline{n}^c} |\Psi\rangle \langle \Psi| \Xi_{\underline{n}^c} \right] \right) \Theta_{\underline{n}},
\]

where \( \text{Tr}_{\underline{n}^c} \) denotes taking partial trace for the \( x_{n+1}, x_{n+2}, \ldots, x_N \) variables. Define the fermionic Fock space as \( \mathcal{F} = \bigoplus_{n=0}^N \mathcal{H}_n \) with \( \mathcal{H}_n := \bigwedge^n \mathcal{H} \) and we define a density matrix

\[
\Gamma := \sum_{\alpha \subset \{1, 2, \ldots, N\}} \Gamma^{[\alpha]} = \sum_{n=0}^N \binom{N}{n} \Gamma^n \quad \text{on} \quad \mathcal{F}.
\]
We first prove that $\Gamma \leq I$ on $\mathcal{F}$. It is sufficient to show that $\Gamma \leq I$ on the $n$-particle sectors for each $n$. Let $n \leq N$, choose $\Phi \in \mathcal{H}_n$, and compute

$$
\sum_{\alpha \subset \{1,2,\ldots,N\} \atop |\alpha|=n} \langle \Phi, \Gamma^{\alpha}|\Phi \rangle = \sum_{\alpha \subset \{1,2,\ldots,N\}} \int dx_\alpha dx'_\alpha \overline{\Phi}(x_\alpha)\Gamma^n(x_\alpha, x'_\alpha)\Phi(x'_\alpha)
$$

$$
= \sum_{\alpha} \int dx_\alpha dx'_\alpha dy_{a\epsilon} \overline{\Phi}(x_\alpha)\Theta_\alpha(x_\alpha)\Xi_{a\epsilon}(y_{a\epsilon})\Psi(x_\alpha, y_{a\epsilon})\overline{\Psi}(x'_\alpha, y_{a\epsilon})\Xi_{a\epsilon}(y_{a\epsilon})\Theta_\alpha(x'_\alpha)\Phi(x'_\alpha)
$$

$$
\leq \sum_{\alpha} \int dx_\alpha dx'_\alpha dy_{a\epsilon} \Theta_\alpha^2(x_\alpha)\Xi_{a\epsilon}^2(y_{a\epsilon})|\Psi(x_\alpha, y_{a\epsilon})|^2|\Phi(x'_\alpha)|^2
$$

$$
= \|\Phi\|_2^2 \int dx|\Psi(x)|^2 \sum_{\alpha} \Theta_\alpha^2(x_\alpha)\Xi_{a\epsilon}^2(x_{a\epsilon})
$$

$$
= \|\Phi\|_2^2
$$

(A.59)

using Schwarz inequality and that $1 \equiv \prod_{j=1}^N[\theta^2(x_j) + \chi^2(x_j)] = \sum_{\alpha} \Theta_\alpha^2(x_\alpha)\Xi_{a\epsilon}^2(x_{a\epsilon})$.

Second, for a fixed $n \leq N$, we compute

$$
\text{Tr}_\mathcal{F}\left[ \Gamma \bigoplus_{n=0}^N \sum_{i=1}^n \mathfrak{h}_i \right] = \sum_{n=0}^N \binom{N}{n} \text{Tr}_\mathcal{F}\left[ \Gamma^n \sum_{i=1}^n \mathfrak{h}_i \right]
$$

$$
= \sum_{\alpha} \sum_{i \in \alpha} \int dx_\alpha dx_{a\epsilon} \overline{\Psi}(x_\alpha, x_{a\epsilon})\Theta_{\alpha}(x_\alpha)\Xi_{a\epsilon}(x_{a\epsilon})\mathfrak{h}_i \left( \Theta_\alpha(x_\alpha)\Xi_{a\epsilon}(x_{a\epsilon})\Psi(x_\alpha, x_{a\epsilon}) \right)
$$

$$
= \sum_{i=1}^N \sum_{\alpha : i \in \alpha} \int dx \overline{\Psi}(x_\alpha, x_{a\epsilon})\Theta_{\alpha\setminus\{i\}}^2(x_{\alpha\setminus\{i\}})\Xi_{a\epsilon}^2(x_{a\epsilon})\theta(x_i)\mathfrak{h}_i \left( \theta(x_i)\Psi(x_\alpha, x_{a\epsilon}) \right)
$$

$$
= \sum_{i=1}^N \langle \Psi, \theta_i \mathfrak{h}_i \theta_i \Psi \rangle
$$

(A.60)

where the trace on the left hand side is computed on $\mathcal{F}$. In the last step we used that for any fixed $i$, we have $1 \equiv \prod_{j\neq i}[\theta^2(x_j) + \chi^2(x_j)] = \sum_{\hat{\alpha}} \Theta_{\hat{\alpha}}^2\Xi_{\hat{\alpha}\epsilon}^2$ where the summation is over all $\hat{\alpha} \subset \{1,2,\ldots,N\} \setminus \{i\}$ and $\hat{\alpha}\epsilon = \{1,2,\ldots,N\} \setminus \{i\} \setminus \alpha$.

A similar calculation for the two-body potential shows that

$$
\text{Tr}_\mathcal{F}\left[ \Gamma \bigoplus_{n=0}^N \sum_{1 \leq i < j \leq n} W_{ij} \right] = \sum_{1 \leq i < j \leq N} \langle \Psi, \theta_i \theta_j W_{ij} \theta_j \theta_i \Psi \rangle.
$$

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Thus, by the variational principle,

\[
\langle \Psi, \left( \sum_{i=1}^{N} \theta_i \theta_i + \sum_{1 \leq i < j \leq N} \theta_i \theta_j W_{ij} \theta_j \theta_i \right) \Psi \rangle \geq \inf_{\Gamma} \text{Tr} \left[ \Gamma \bigoplus_{n=0}^{N} \left( \sum_{i=1}^{n} \theta_i + \sum_{1 \leq i < j \leq n} W_{ij} \right) \right].
\]

Since \( \Gamma \) is a density matrix supported on \( \Omega \), we obtain (4.28). \( \square \)

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