On Electrons and Nuclei in a Magnetic Field

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0 Introduction

In this paper, we prove a lower bound for the energy of N electrons and M nuclei in a magnetic field. This bound, together with work of J. Fröhlich and G.-M. Graf, proves the H-stability of non-relativistic quantum electrodynamics (QED) with an ultraviolet cutoff. H-stability for a system with many particles says that the energy per (charged) particle remains bounded below, as the number of particles tends to infinity. This is a very natural requirement for physical systems. In this introduction, we begin by stating carefully the main inequality to be proven in this paper. We then give a quick sketch of the construction of non-relativistic QED with an ultraviolet cutoff. Next, we explain the relevance of our main estimate to QED, via the work of Fröhlich and Graf. The introduction concludes with a quick sketch of the main ideas in our proof. The results proven here are announced in [FFG2] and applied to QED in [FFG1]. See also Bugliaro-Fröhlich-Graf [BFG].

Our main result concerns the Pauli Hamiltonian for N quantized electrons and M fixed nuclei in a magnetic field. Suppose the nuclei are located at $y_1, y_2, \ldots, y_M \in \mathbb{R}^3$, and have atomic numbers $Z_1, Z_2, \ldots, Z_M$. Let Z be an upper bound for the Z_k. (In nature, we can take, say, $Z = 150$.) The magnetic field is given by a vector potential $A(x) = (A_\nu(x))_{\nu=1,2,3}$ on $\mathbb{R}^3$. To define the Pauli Hamiltonian, we use the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and form the Dirac operator

$$\sigma \cdot (i \bigtriangledown - A) = \sum_{\mu=1,2,3} \sigma_\mu \left(i \frac{\partial}{\partial x_\mu} - A_\mu(x) \right)$$

on $L^2(\mathbb{R}^3, \mathbb{C}^2)$.

On the N-fold tensor power $(L^2(\mathbb{R}^3, \mathbb{C}^2))^{\otimes N} = L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N})$, we define

$\sigma^{(k)} \cdot (i \bigtriangledown_{x_k} - A(x_k))$

(the Dirac operator for the $k^{\underline{\text{th}}}$ electron) as

$I \otimes \ldots \otimes I \otimes \{\sigma \cdot (i \bigtriangledown - A)\} \otimes I \otimes \ldots \otimes I,$

where $I =$ identity, and where $\{\sigma \cdot (i \bigtriangledown - A)\}$ occurs as the kth factor.

The Pauli Hamiltonian H_{Pauli} is defined as

$$H_{\text{Pauli}} = \sum_{k=1}^{N} [\sigma^{(k)} \cdot (i \nabla_{x_k} - A(x_k))]^2 + V_{\text{Coulomb}}, \tag{0.1}$$

with

$$V_{\text{Coulomb}} = \sum_{1 \le j < k \le N} |x_j - x_k|^{-1} + \sum_{1 \le j < k \le M} Z_j Z_k \, |y_j - y_k|^{-1} - \sum_{j=1}^{N} \sum_{k=1}^{M} Z_k |x_j - y_k|^{-1}. \tag{0.2}$$

This Hamiltonian acts on the Hillbert space

$$\mathcal{H}_{e\ell} = \bigwedge^N \left(L^2(\mathbb{R}^3, \mathbb{C}^2)\right) \subset L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N}),$$

where $\bigwedge^N$ denotes the N-fold antisymmetric tensor power. If the vector potential $A(x)$ is identically zero, then (0.1) reduces to the familiar Schrödinger operator $-\triangle + V_{\text{Coulomb}}$. An explanation of the Pauli Hamiltonian may be found in many textbooks on quantum mechanics.

Our main result concerns the energy $\langle H_{\text{Pauli}}\, \psi, \psi \rangle$ for a unit vector $\psi \in \mathcal{H}_{e\ell}$. It involves the magnetic field $B(x) = \text{curl } A$, and modifies previous estimates of the form

$$\langle H_{\text{Pauli}}\, \psi, \psi \rangle + \Gamma \int_U |B(x)|^2 dx \ge -C(N + M). \tag{0.3}$$

Here, U is the union of balls of radius 1 centered at the nuclei. Estimates (0.3) have been proven in [BFG] with constants Γ and C depending only on Z. (See also the closely related estimates in [LLS].)

One wants to modify (0.3) because it fails if Γ is taken too small. (Already, (0.3) may fail for $N = M = 1$; see [FFL, LY].) Consequently, (0.3) applies to QED only when the fine structure constant α is sufficiently small. (We will explain this later in the introduction.) To state our modification of (0.3), we introduce the function

$$D(x) = \text{distance to the nearest nucleus} \; = \min\{|x - y_k| \, : \, 1 \le k \le M\}.$$

In place of (0.3), we will prove the following estimate, valid for any $\Gamma > 0$ and for any positive $L < c\,(\Gamma, Z)$.

Theorem: $L < c\,(\Gamma, Z)$ *implies*

$$\text{(0.4)} \qquad \langle H_{\text{Pauli}}\,\psi, \psi\rangle \, + \, \Gamma \int\limits_{\mathbb{R}^3} |B(x)|^2 \, e^{-D(x)/L} \, dx \, + \, C(\Gamma, Z) \int\limits_{\mathbb{R}^3} L^2 \, |\nabla B(x)|^2 \, e^{-D(x)/L} \, dx$$

$$\ge \, - \, \tfrac{C'(\Gamma, Z)}{L} M.$$

Here, $c\,(\Gamma, Z)$, $C\,(\Gamma, Z)$, $C'\,(\Gamma, Z)$ are constants determined entirely by Γ and Z. (Actually, our result is sharper than (0.4), but we omit details from the introduction. See the next section for the full statement of our main result.) Estimate (0.4) has the same application to QED as (0.3), but without the restriction to small fine-structure constant.

We give a quick sketch of non-relativistic QED. This theory treats electrons, nuclei and photons. To begin with, suppose we have only photons. We will work in a Hilbert space $\mathcal{H}_{\text{photons}}$ with a distinguished unit vector Ω (the vacuum state). For each momentum vector $k \in \mathbb{R}^3 \backslash \{0\}$, we introduce two unit vectors $e_+(k)$, $e_-(k) \in \mathbb{R}^3$, orthogonal to each other and to k. We write $[e_\pm(k)]_\mu$ ($\mu = 1, 2, 3$) for the components of $e_\pm(k)$. Corresponding to $e_+(k), e_-(k)$, we introduce two operator-valued distributions $a_\pm(k)$. (For a particular k, $a_\pm(k)$ is not well-defined, but for suitable test functions $\theta(k)$, the smeared operator $\int\limits_{\mathbb{R}^3} \theta(k) a_\pm(k) dk$ is well-defined.)

Here, for $\lambda = \pm$, $a^*_\lambda(k)$ creates and $a_\lambda(k)$ annihilates a photon with momentum k and polarization $e_\lambda(k)$. The $a_\lambda(k)$ satisfy the commutation relations

$$[a_\lambda(k), \, a_{\lambda'}\,(k')] \, = \, [a^*_\lambda(k), \, a^*_{\lambda'}\,(k')] \, = \, 0,$$

$$[a_\lambda(k), \, a^*_{\lambda'}\,(k')] \, = \, \delta_{\lambda\lambda'}\, \delta(k - k'),$$

where $\delta_{\lambda\lambda'}$ is the Kronecker delta, and $\delta(k)$ is the Dirac delta on $\mathbb{R}^3$. Also, we have $a_\lambda(k)\Omega = 0$.

The Hilbert space $\mathcal{H}_{\text{photons}}$ is spanned by products of smeared creation operators, applied to the vacuum state Ω.

In terms of the basic operators $a_\lambda(k)$, the Hamiltonian for photons is

$$H_{ph} = \alpha^{-1} \sum_{\lambda=\pm} \int_{\mathbb{R}^3} a_\lambda^*(k)\, a_\lambda(k)\, |k|\, dk, \tag{0.5}$$

and the magnetic field is given in terms of the operator-valued vector potential

$$\begin{aligned} A_\mu(x) &= \frac{\alpha^{1/2}}{2\pi} \sum_{\lambda=\pm} \int_{\mathbb{R}^3} a_\lambda(k)\, [e_\lambda(k)]_\mu\, e^{ik\cdot x}\, \theta\left(\frac{k}{\wedge}\right) \frac{dk}{\sqrt{|k|}} \\ &+ \frac{\alpha^{1/2}}{2\pi} \sum_{\lambda=\pm} \int_{\mathbb{R}^3} a_\lambda^*(k)\, [e_\lambda(k)]_\mu\, e^{-ik\cdot x}\, \theta\left(\frac{-k}{\wedge}\right) \frac{dk}{\sqrt{|k|}}. \end{aligned} \tag{0.6}$$

Here, α is the fine-structure constant, $\wedge > 0$ is a cutoff parameter, and $\theta \in C_0^\infty(\mathbb{R}^3)$ with $\theta(0) = 1$. (The potential (0.6) is expressed in the Coulomb gauge.) The effect of the cutoff $\theta\left(\frac{k}{\wedge}\right)$ in (0.6) is that the integrals converge, so $A_\nu(x)$ makes sense, but the photons of momentum $|k| \gg \wedge$ do not contribute to the vector potential. It is physically reasonable to use (0.6) with $\wedge$ taken so large that a photon of momentum $\sim \wedge$ can create electron-positron pairs. This concludes our discussion of photons without electrons and nuclei.

We now explain the construction of QED when electrons and nuclei are present. Suppose there are N electrons and M nuclei. As before, we suppose that the nuclei are fixed at locations $y_1, \dots, y_M \in \mathbb{R}^3$ and have atomic numbers $Z_k \le Z$ $(1 \le k \le M)$. Our basic Hilbert space is

$\mathcal{H}_{QED} = \mathcal{H}_{\text{photons}} \otimes \mathcal{H}_{e\ell}$, and the Hamiltonian for QED is

$$H_{QED} = (H_{ph} \otimes I) + \sum_{k=1}^{N} \left[\sigma^{(k)} \cdot (i\nabla_{x_k} - A(x_k))\right]^2 + V_{\text{Coulomb}}, \tag{0.7}$$

with $A(x)$ given by (0.6).

Much of atomic, molecular, and condensed-matter physics amounts to the study of the Hamiltonian (0.7). This concludes our sketch of the construction of non-relativistic QED with ultraviolet cutoffs. See [BFS] for recent results on non-relativistic QED.

The purpose of this paper and of [FFG1] is to prove the H-stability of non-relativistic QED. More precisely, we have

$$H_{QED} \geq -CM, \tag{0.8}$$

with C depending only on $\alpha, Z, \wedge$. See [FFG1] for a more careful discussion of the physical meaning of (0.8), and of the dependence of C on $\wedge$ and α.

The original strategy for proving (0.8) was to write

$$H_{QED} = \tilde{H}_{ph} \otimes I + \tilde{H}_{e\ell}, \ \text{ with} \tag{0.9}$$

$$\tilde{H}_{ph} = H_{ph} - \Gamma \int\limits_U |B(x)|^2 \, dx, \tag{0.10}$$

$$\tilde{H}_{e\ell} = \sum_{k=1}^N \left[\sigma^{(k)} \cdot (i\nabla_{x_k} - A(x_k))\right]^2 + V_{\text{Coulomb}} + \Gamma \int\limits_U |B(x)|^2 \, dx, \tag{0.11}$$

where $B(x) = \text{curl } A(x)$, $A(x)$ is given by (0.6), and Γ is a carefully picked constant. As before, $U = \cup_{1 \leq k \leq M} \{x \in \mathbb{R}^3 : |x - y_k| < 1\}$.

The point of this decomposition is that $\tilde{H}_{ph}$ involves only the photons, while $\tilde{H}_{e\ell}$ involves only the electrons and nuclei in an arbitrary classical vector potential $A_\mu(x)$. The idea of using (0.9), (0.10), (0.11) goes back to Fröhlich, who was led to conjecture (0.3) via the connection to QED. Fröhlich showed, using reflection positivity of the free photon theory, that

$\tilde{H}_{ph} \geq -C$ volume $(U) \geq -C'M$, provided one takes

$$\Gamma = \frac{\alpha^{-2}}{8\pi}. \text{ For larger } \Gamma,\ \tilde{H}_{ph} \text{ is unbounded below.} \tag{0.12}$$

Hence, if one can prove estimate (0.3) for the Pauli Hamiltonian, then (0.9), (0.10), (0.11) yield

$$H_{QED} \geq -C(N+M), \text{ provided } \alpha \text{ and } \Gamma \text{ are related by (0.12).} \tag{0.13}$$

The sharpest known result of the form (0.3) gives (0.13) for $\alpha \leq \frac{1}{132}, Z \leq 6$. (See Bugliaro-Fröhlich-Graf [BFG] , adapting the work of Lieb-Loss-Solovej [LLS] on a variant of (0.3) in which U is replaced by $\mathbb{R}^3$.) These results are of physical interest. However, one wants also to understand $\alpha \approx \frac{1}{137}$, $Z \leq 150$, as in nature. From a more fundamental viewpoint, one wants to know whether the truth of (0.13) really depends on the particular values of Z and α. This is the issue settled by this paper and [FFG1].

To get past the limitations of (0.9), (0.10), (0.11), Fröhlich and Graf proposed a different decomposition. A slight variant of their decomposition is as follows.

$$H_{QED} = H^{\#}_{ph} \otimes I + H^{\#}_{e\ell}, \text{ with} \tag{0.14}$$

$$H^{\#}_{ph} = H_{ph} - \Gamma \int_{\mathbb{R}^3} |B(x)|^2 e^{-D(x)}\, dx - \Gamma' \int_{\mathbb{R}^3} |\nabla B(x)|^2 e^{-D(x)} dx, \text{ and} \tag{0.15}$$

$$\begin{aligned} H^{\#}_{e\ell} &= \sum_{k=1}^{N} \left[\sigma^{(k)} \cdot (i\nabla_{x_k} - A(x_k))\right]^2 + V_{\text{Coulomb}} \\ &\quad + \Gamma \int_{\mathbb{R}^3} |B(x)|^2 e^{D(x)}\, dx + \Gamma' \int_{\mathbb{R}^3} |\nabla B(x)|^2 e^{-D(x)}\, dx. \end{aligned} \tag{0.16}$$

Here, $D(x)$ is the distance from x to the nearest nucleus, as in (0.4). In principle, one could try to bound the Hamiltonian (0.15) from below by again using reflection positivity. Instead, [FFG1] adapts an amazingly simple argument from Bugliaro-Fröhlich-Graf [BFG], to show that

(0.17) $$H^{\#}_{ph} \ge -C \int\limits_{\mathbb{R}^3} e^{-D(x)}\, dx \ge -C'M,$$

provided Γ, Γ' are chosen small enough. (Here, Γ depends only on α, while Γ' depends only on $\alpha, \wedge$.) This is analogous to the argument using (0.9), (0.10), (0.11). Now, however, one has

(0.18) $$H^{\#}_{e\ell} \ge -CM$$

for <u>any</u> constants $\Gamma, \Gamma' > 0$.

In fact, we simply pick $L < c\,(\Gamma, Z)$ as in our Theorem (0.4), making sure that L is so small that we have $C(\Gamma, Z)L^2 < \Gamma'$. The desired estimate (0.18) then follows at once from (0.4). Putting (0.17) and (0.18) into (0.14), we obtain (0.8), thus proving the H-stability of QED without restrictions on Z and α. So the H-stability of QED reduces to Theorem (0.4), and to the results in [FFG1].

Note that we have thrown away information in passing from (0.4) to (0.18), because the exponentials in (0.4) are $e^{-D(x)/L}$, while in (0.18) we have merely $e^{-D(x)}$. The actual argument in [FFG1] is careful to keep this extra information, to obtain good $\wedge$-dependence of the constant in (0.8). The exponential factors $e^{-D(x)/L}$ in (0.4) represent a significant idea. This concludes our discussion of the relevance of (0.4) to QED.

We now sketch the ideas in the proof of Theorem (0.4). Our sketch will be correct in spirit, but oversimplified and inaccurate in detail. Without any real change in the ideas, we restrict attention to the case in which all the atomic numbers Z_k are equal to 1. We will combine known tricks from [FL] and [Min] with a new lower bound for the Pauli kinetic energy. (I would like to express my appreciation to W. Minicozzi for taking the excellent notes [Min] from lectures I gave at Stanford University. I am grateful also to the Stanford mathematics department for their hospitality.) Let me first explain the old tricks, then sketch the new kinetic energy inequality, and finally show how to mix the ingredients to prove Theorem (0.4).

To explain the old tricks, we first note that there are local potential and kinetic energies associated to a cube $Q \subset \mathbb{R}^3$. If A is a vector potential and $\psi \in L^2(\mathbb{R}^3, \mathbb{C}^2)$ is a one-electron wave function, then we write

$$T_{\text{Pauli}}(\psi, A, Q) = \int_Q |\sigma \cdot (i\nabla - A)\,\psi|^2\,dx \;\text{ and} \tag{0.19}$$

$$T(\psi, A, Q) = \int_Q |(i\nabla - A)\psi|^2\,dx. \tag{0.20}$$

These notions of local kinetic energy extend straightforwardly to N-electron wave functions. To localize the potential energy to a cube Q, let $x_1 \dots x_N \in \mathbb{R}^3$ and $y_1 \dots y_M \in \mathbb{R}^3$ be electrons and protons, respectively. Using an identity from [FL], we can define a localized Coulomb potential $V_Q\,(x_1 \dots x_N,\, y_1 \dots y_M)$. Roughly speaking (but not really), V_Q is the Coulomb energy arising from all the electrons and protons in Q. If $y_1 \dots y_M \in \mathbb{R}^3$ are fixed protons, and if $\psi \in L^2(\mathbb{R}^{3N},\, (\mathbb{C}^2)^{\otimes N})$ is an N-electron wave function, then the local potential energy is simply

$$PE(\psi, Q) = \langle V_Q\psi, \psi\rangle. \tag{0.21}$$

As Q expands to fill $\mathbb{R}^3$, one has

$$T_{\text{Pauli}}(\psi, A, Q) \to \left\langle \sum_{k=1}^N \left[\sigma^{(k)} \cdot (i\nabla_{x_k} - A(x_k))\right]^2 \psi, \psi \right\rangle \text{ and } PE(\psi, Q) \to \left\langle V_{\text{Coulomb}}\psi, \psi \right\rangle.$$

Moreover, if Q is decomposed into sub-cubes $\{Q_\nu\}$, then

$$T(\psi, A, Q) = \sum_\nu T(\psi, A, Q_\nu), \;\; T_{\text{Pauli}}(\psi, A, Q) = \sum_\nu T_{\text{Pauli}}\,(\psi, A, Q_\nu),$$

and also $PE(\psi, Q) \geq \sum_\nu PE(\psi, Q_\nu)$ modulo a controlled error. These remarks are immediate consequences of the definitions, provided one defines V_Q properly. See [Min].

One of the main technical results in [Min] is as follows.

<u>Local Stability of Matter:</u> If the vector potential A is <u>constant</u>, then

$$\begin{aligned}(0.22) \qquad & \delta \cdot T(\psi, A, Q) + PE(\psi, Q) \geq -\frac{C}{\delta}\langle \mathcal{N}_Q \psi, \psi \rangle, \text{ where} \\ & \delta = \text{side}(Q) \text{ and } \mathcal{N}_Q = (\text{number of electrons in } Q).\end{aligned}$$

Since [Min] is unpublished, we include a proof of (0.22) in this paper. ¿From now on (in the introduction), if Q is any cube in $\mathbb{R}^3$, then δ will denote side(Q), and $\mathcal{N}_Q$ will denote the number of electrons in Q.

The following estimate comes from a standard integration by parts.

<u>KE Comparison Lemma:</u> *Suppose the magnetic field $B = curl A$ is constant on Q. Then*

$$(0.23) \qquad T_{\text{Pauli}}(\psi, A, Q) \geq T(\psi, A, Q) - C(|B| + \delta^{-2})\langle \mathcal{N}_Q \psi, \psi \rangle.$$

This concludes our description of the old tricks.

The new kinetic energy inequality is as follows

<u>KE Lower Bound:</u> Let Q be the unit cube, and suppose the magnetic field $B = \text{curl } A$ is constant on Q. If $K > 1$, then

$$(0.24) \qquad T_{\text{Pauli}}(\psi, A, Q) \geq \left\langle \left(cK\mathcal{N}_Q - CK^{5/2}\{|B| + 1\}\right)\psi, \psi \right\rangle$$

We content ourselves here with a few remarks on the proof of (0.24). The KE Lower Bound is stated for N-electron wave functions, but it reduces to a one-electron estimate by separation of variables. To prove the one-electron estimate, we integrate by parts in (0.19) in two different ways, combine the results, and then break Q into thin rectangular tubes T_α parallel to the magnetic field. The tubes have dimension $\sim (|B| + 1)^{-1/2} \times (|B| + 1)^{-1/2} \times 1$. In effect, the restriction of ψ to a single T_α leads by a rescaling to a free electron in the unit cube. The proof of the KE Lower Bound is not hard. We warn the reader that the correct statement is not quite (0.24), and that this summary of our proof is correct only in spirit.

We are ready to mix the above ingredients to prove (0.4). The first main idea is to establish the following

LOCAL PAULI STABILITY (Constant Magnetic Fields): Let B_0 be a large constant, to be picked later. Suppose the magnetic field $B = \operatorname{curl} A$ is constant on Q, and satisfies $|B| \leq CB_0\delta^{-2}$ on Q. Then

$$CB_0^{1/2}\delta \cdot T_{\text{Pauli}}(\psi, A, Q) + PE(\psi, Q) \geq -CB_0^{3/2}\delta^{-1}. \tag{0.25}$$

A crucial point here is that B_0 appears on the right-hand side, raised to a power less than 2. To prove (0.25), we subdivide Q into sub-cubes $\{Q_\alpha\}$ of side $\sim B_0^{-1/2}\delta$. After a suitable gauge transformation, one can show that the vector potential is approximately constant on each Q_α. Hence, we may apply Local Stability of Matter to each Q_α, which shows that

$$B^{-1/2}\delta \cdot T(\psi, A, Q_\alpha) + PE(\psi, Q_\alpha) \geq -CB_0^{1/2}\,\delta^{-1}\,\langle \mathcal{N}_{Q_\alpha}\psi, \psi\rangle.$$

Summing over α, we obtain

$$B_0^{-1/2}\,\delta \cdot T(\psi, A, Q) + PE(\psi, Q) \geq -CB_0^{1/2}\,\delta^{-1}\langle \mathcal{N}_Q\psi, \psi\rangle. \tag{0.26}$$

Also, the KE Comparison Lemma gives

$$B_0^{-1/2}\,\delta \cdot T_{\text{Pauli}}(\psi, A, Q) \geq B_0^{-1/2}\,\delta \cdot T(\psi, A, Q) - CB_0^{1/2}\,\delta^{-1}\langle \mathcal{N}_Q\psi, \psi\rangle. \tag{0.27}$$

Putting (0.27) into (0.26), we find that

$$B_0^{-1/2}\,\delta \cdot T_{\text{Pauli}}(\psi, A, Q) + PE(\psi, Q) \geq -CB_0^{1/2}\,\delta^{-1}\langle \mathcal{N}_Q\psi, \psi\rangle. \tag{0.28}$$

On the other hand, the KE Lower Bound (0.24) gives

$$B_0^{1/2}\,\delta \cdot T_{\text{Pauli}}(\psi, A, Q) \geq cKB_0^{1/2}\,\delta^{-1}\langle \mathcal{N}_Q\psi, \psi\rangle - CK^{5/2}B_0^{3/2}\,\delta^{-1}, \tag{0.29}$$

by a simple rescaling from the unit cube to Q. Adding (0.28) and (0.29), we obtain

$$CB_0^{1/2}\,\delta\cdot T_{\text{Pauli}}(\psi,A,Q)\;+\;PE(\psi,Q)\;\geq \\ [cK\;-C']\,B_0^{1/2}\delta^{-1}\,\langle\mathcal{N}_Q\psi,\psi\rangle-CK^{5/2}B_0^{3/2}\,\delta^{-1}. \tag{0.30}$$

If we take K to be a large enough universal constant, then the first term on the right side of (0.30) will be non-negative, since $[cK\;-C']>0$. Hence, (0.30) implies (0.25), completing the proof of Local Pauli Stability for constant fields.

Next, we pass from constant magnetic fields to fields that vary slightly on Q. By elementary potential theory, one can write the vector potential A in the form $A=A_c+A^{\#}$ on Q, where A_c has a constant magnetic field, and $A^{\#}$ is small. We may then apply Local Pauli Stability (0.25) to the vector potential A_c, and regard $A^{\#}$ as a small perturbation. In this spirit, we can extend (0.25) as follows

<u>Local Pauli Stability</u> (Slightly Varying Magnetic Fields): Let B_0 be a large constant, to be picked later. Suppose the magnetic field $B\;=\;\operatorname{curl}A$ satisfies

$$\int_Q |B(x)|^2\,dx\;\leq\;B_0^2\,\delta^{-1}\quad\text{and} \tag{0.31}$$

$$\int_Q |B(x)\;-\operatorname{mean}_Q B|^2\,dx\;<\;cB_0^{-1/3}\,\delta^{-1}. \tag{0.32}$$

Then we have

$$CB_0^{1/2}\,\delta\cdot T_{\text{Pauli}}(\psi,A,Q)\;+\;PE(\psi,Q)\;\geq\;-C'B_0^{3/2}\,\delta^{-1}. \tag{0.33}$$

We omit all discussion of the proof, but just point out that (0.31), (0.32) suggest that

$$\int_Q |B(x)\;-\operatorname{mean}_Q B|^2\,dx \ll \int_Q |B(x)|^2 dx, \text{ so that } B \text{ varies only slightly on } Q.$$

Our plan in proving Theorem (0.4) is to make a Calderón-Zygmund decomposition of $\mathbb{R}^3$ into cubes $\{Q_\nu\}$ that satisfy (0.31) and (0.32). We then apply local Pauli stability (0.33) to each Q_ν, and sum the result over ν. To construct the $\{Q_\nu\}$, we proceed as follows. Partition $\mathbb{R}^3$ into a grid of cubes $\{Q^0_\alpha\}$ of side L, with L as in (0.4). We retain all the Q_α that satisfy (0.31), (0.32), and cut all the other Q^0_α into sub-cubes of side $\frac{L}{2}$. Thus, we obtain a collection $\{Q^1_\alpha\}$ of cubes of side $L/2$. We retain all the Q^1_α that satisfy (0.31), (0.32), and cut all the other Q^1_α into sub-cubes of side $L/4$. Thus, we obtain a collection $\{Q^2_\alpha\}$ of cubes of side $L/4$. We retain all the Q^2_α that satisfy (0.31), (0.32), and we cut all the other Q^2_α into cubes of side $L/8$. Thus, we obtain a collection $\{Q^3_\alpha\}$ of cubes of side $L/8$. We continue in this way, and let $\{Q_\nu\}$ denote the collection of all the Q^j_α (j, α arbitrary) retained during the above construction. Thus, $\mathbb{R}^3$ is partitioned into cubes $\{Q_\nu\}$ that satisfy (0.31), (0.32). Let $\delta_\nu =$ side (Q_ν); note that $\delta_\nu \le L$.

Next, we bring in the function $D(x) = \min\{|x - y_k| : 1 \le k \le M\}$ from (0.4). We set

$$\theta_\nu \; = \; \max_{x\in Q_\nu} \exp(-D(x)/L). \tag{0.34}$$

The basic estimates for our Calderón-Zygmund cubes are (0.31), (0.32) and the following

$$\sum_\nu \theta_\nu \delta_\nu^{-1} \le C B_0^{-2} \int\limits_{\mathbb{R}^3} |B(x)|^2\, e^{-D(x)/L}\, dx + C B_0^{1/3} \int\limits_{\mathbb{R}^3} L^2 |\nabla B(x)|^2\, e^{-D(x)/L}\, dx \; + \; \frac{C}{L} M. \tag{0.35}$$

The proof of (0.35) is based on the following idea. If $\delta_\nu < L$, then Q_ν arose by cutting a cube Q^+_ν of side $2\delta_\nu$, for which at least one of (0.31), (0.32) must fail (or else we would not have cut Q^+_ν). If (0.31) fails for Q^+_ν, then, roughly speaking, we have

$$\int\limits_{Q_\nu} |B(x)|^2\, dx \; \ge \; c B_0^2\, \delta_\nu^{-1}. \tag{0.36}$$

Since side $(Q_\nu) = \delta_\nu \le L$, (0.34) gives $c\theta_\nu \le \exp(-D(x)/L) \le \theta_\nu$ on Q_ν, so (0.36) implies

$$B_0^{-2} \int\limits_{Q_\nu} |B(x)|^2 \, e^{-D(x)/L} \, dx \;\geq\; c\theta_\nu \delta_\nu^{-1}. \tag{0.37}$$

Summing (0.37) over all the ν to which it applies, we see that

$$\sum_{\nu \in \mathcal{A}} \theta_\nu \delta_\nu^{-1} \leq C B_0^{-2} \int\limits_{\mathbb{R}^3} |B(x)|^2 \, e^{-D(x)/L} \, dx,$$

where $\mathcal{A}$ denotes the set of ν for which (0.31) fails for Q_ν^+. Similarly, the $|\nabla B(x)|^2$ term in (0.35) arises from the cubes Q_ν for which (0.32) fails for Q_ν^+. The last term on the right in (0.35) arises from the Q_ν with $\delta_\nu = L$. We dispense with further details, and accept (0.35).

At last we are ready to prove Theorem (0.4). For each ν, we have

$$C B_0^{1/2} \, \delta_\nu \cdot T_{\text{Pauli}} \, (\psi, A, Q_\nu) \;+\; PE(\psi, Q_\nu) \;\geq\; -C B_0^{3/2} \, \theta_\nu \, \delta_\nu^{-1}. \tag{0.38}$$

In fact, (0.38) reduces to Local Pauli Stability (0.33) if Q_ν contains at least one nucleus, since then $\theta_\nu = 1$ by (0.34). On the other hand, if Q_ν contains no nuclei, then the Coulomb energy arising from particles in Q_ν consists purely of repulsion of electrons, so it is plausible that $PE(\psi, Q_\nu) \geq 0$. Actually, the correct definition of V_Q in (0.21) immediately gives $PE(\psi, Q_\nu) = 0$ when Q_ν contains no nuclei. Hence, in that case, the left side of (0.38) is positive, while the right side is negative. So (0.38) holds, whether Q_ν contains nuclei or not. Summing (0.38) over all ν, and applying (0.35), we find that

$$\begin{aligned} C B_0^{1/2} \cdot \sum_\nu \delta_\nu \cdot T_{\text{Pauli}} \, (\psi, A, Q_\nu) \;+\; \Big\langle V_{\text{Coulomb}} \, \psi, \psi \Big\rangle \;\geq \\ - C B_0^{-1/2} \int\limits_{\mathbb{R}^3} |B(x)|^2 \, e^{-D(x)/L} \, dx \;-\; C B_0^{11/6} \int\limits_{\mathbb{R}^3} L^2 |\nabla B(x)|^2 \, e^{-D(x)/L} \, dx \\ - \frac{C}{L} \, B_0^{3/2} \, M. \end{aligned} \tag{0.39}$$

If we restrict L by requiring

$$\left(CB_0^{1/2}\right) L \le 1 \text{ with } C \text{ as in (0.39), then } CB_0^{1/2}\,\delta_\nu \le 1 \text{ for all } \nu, \tag{0.40}$$

so we have trivially

$$\left\langle \sum_{k=1}^{N} \left[\sigma^{(k)} \cdot (i\,\nabla_{x_k} - A(x_k))\right]^2 \psi, \psi \right\rangle = \sum_\nu T_{\text{Pauli}}\,(\psi, A, Q_\nu) \ge$$

$$CB_0^{1/2} \sum_\nu \delta_\nu \cdot T_{\text{Pauli}}\,(\psi, A, Q_\nu),$$

and consequently (0.39) implies

$$\left\langle H_{\text{Pauli}}\psi, \psi \right\rangle + CB_0^{-1/2} \int_{\mathbb{R}^3} |B(x)|^2\, e^{-D(x)/L} dx + CB_0^{11/6} \int_{\mathbb{R}^3} L^2 |\nabla B(x)|^2\, e^{-D(x)/L}\, dx \ge -\frac{C}{L}\, B_0^{3/2}\, M. \tag{0.41}$$

Thus, (0.40) implies (0.41). To finish the proof of (0.4), we simply take B_0 large enough that $CB_0^{-1/2} \le \Gamma$, with C as in (0.41) and Γ as in (0.4). This step works, thanks to the negative power of B_0 in (0.41), which in turn arises because B_0 appears on the right of (0.25) with an exponent less than 2.

The proof of (0.4) is complete. Again, we warn the reader not to take at face value anything we say in the introduction about the proof of (0.4).

For correct statements and complete proofs, the reader may consult sections 1 through 9 below, and reference [FFG1].

It would be interesting to simplify our proof of (0.4). In particular, it is natural to suppose that one can prove it in the spirit of the Lieb-Thirring inequality.

I am grateful to Gerree Pecht for expertly TeXing this paper.

1 Statement of the Main Result

In this section, we state our main estimate for the Pauli kinetic energy, which is sharper than the Theorem (0.4) given in the introduction. We show how the theorem stated here easily implies (0.4), and then give an elementary (and standard) reduction of our main result to the case in which all the nuclei have the same atomic number Z. The rest of the paper is devoted to the proof of our main theorem.

Our basic result is as follows.

Main Theorem: *Let $\Gamma, Z > 0$ be given. For constants $c(\Gamma, Z)$, $C_1(\Gamma, Z)$, $C_2(\Gamma, Z)$ depending only on Γ and Z, the following holds.*

Let $A(x)$ be a vector potential, and let $L > 0$ be a length. Assume $L < c(\Gamma, Z)$. Define

$B(x) = \operatorname{curl} A(x)$ *(the magnetic field),*

$\bar{B}_L(x) = \left(\frac{4\pi}{3} L^3\right)^{-1} \int\limits_{|y-x|<L} B(y)dy$ *(the mean of B over a ball about x),*

$S_L(x) = \left\{ \left(\frac{4\pi}{3} L^3\right)^{-1} \int\limits_{|y-x|<L} |B(y) - \bar{B}_L(x)|^2 \, dy \right\}^{1/2}$ *(the standard deviation of B on a ball about x).*

Let $y_1, \ldots, y_M \in \mathbb{R}^3$ and $Z_1, \ldots, Z_M \geq 0$ be given.

Assume $Z_k \leq Z$ for all $k = 1, 2, \ldots, M$. Define

$D(x) = \min\{|x - y_k| : 1 \leq k \leq M\}$ *for $x \in \mathbb{R}^3$, and*

$V_{\text{Coulomb}}(x_1 \ldots x_N) = \sum\limits_{1\leq j<k\leq N} |x_j - x_k|^{-1} + \sum\limits_{1\leq j<k\leq M} Z_j Z_k |y_j - y_k|^{-1} - \sum\limits_{j=1}^{N} \sum\limits_{k=1}^{M} Z_k |x_j - y_k|^{-1}.$

Finally, let $\psi \in L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N})$ be antisymmetric with norm 1, and let

$$H_{\text{Pauli}} = \sum_{k=1}^{N} \left[\sigma^{(k)} \cdot (i\nabla_{x_k} - A(x_k))\right]^2 + V_{\text{Coulomb}} \qquad \text{(Pauli Hamiltonian)}.$$

Then

$$\left\langle H_{\mathrm{Pauli}}\psi, \psi \right\rangle + \Gamma \int_{\mathbb{R}^3} |B(x)|^2 \, e^{-D(x)/L} \, dx + C_1(\Gamma, Z) \int_{\mathbb{R}^3} (S_L(x))^2 \, e^{-D(x)/L} \, dx \tag{1.1}$$

$$\geq -C_2(\Gamma, Z) \, \tfrac{M}{L}.$$

This sharpens (0.4), because we use $S_L(x)$ in place of $L^2|\nabla B(x)|^2$ in (1.1). It is easy to deduce (0.4) from (1.1). In fact, we have

$|D(x) - D(y)| \leq |x - y|$ by definition, and

$(S_L(x))^2 \leq CL^{-1} \int_{|y-x|<L} |\nabla B(y)|^2 \, dy$ by the Poincaré inequality.

Hence,

$$\int_{\mathbb{R}^3} (S_L(x))^2 \, e^{-D(x)/L} \, dx \leq CL^{-1} \iint_{|x-y|<L} |\nabla B(y)|^2 \, e^{-D(x)/L} \, dy \, dx$$

$$\leq C' L^{-1} \iint_{|x-y|<L} |\nabla B(y)|^2 \, e^{-D(y)/L} \, dy \, dx$$

$$= C'' \int_{\mathbb{R}^3} L^2 |\nabla B(y)|^2 \, e^{-D(y)/L} \, dy.$$

Therefore, (1.1) implies

$$\left\langle H_{\mathrm{Pauli}}\psi, \psi \right\rangle + \Gamma \int_{\mathbb{R}^3} |B(x)|^2 \, e^{-D(x)/L} dx + C_1'(\Gamma, Z) \int_{\mathbb{R}^3} L^2 |\nabla B(x)|^2 \, e^{-D(x)/L} \, dx \tag{1.2}$$

$$\geq -C_2(\Gamma, Z) \, \tfrac{M}{L}.$$

Thus, we obtain (0.4). This easy argument reduces (0.4) to (1.1).

In proving our main theorem, we may assume without loss of generality that Z exceeds a large, universal constant. We may also assume without loss of generality that all the $Z_k(1 \le k \le M)$ are equal to Z. To see this, fix $L, \Gamma, Z, y_1, \dots, y_M, A(x), \psi$, and regard the left-hand side of (1.1) as a function of $Z_1, \dots, Z_M$; let us call it $F(Z_1, \dots, Z_M)$. Thus, F is defined on the cube $([0, Z])^M$. We want to prove estimate (1.1), i.e.,

$$F(Z_1, \dots, Z_M) \ge -C_2(\Gamma, Z)\,\frac{M}{L} \text{ for } (Z_1, \dots, Z_M) \in ([0, Z])^M. \tag{1.3}$$

One checks that F is linear in each Z_k when all the other Z_j are held fixed.

It follows by induction on J that (1.3) may be reduced to the special case in which each $Z_j(1 \le j \le J)$ is either 0 or Z. The constant $C_2(\Gamma, Z)$ in (1.3) does not change in the induction step. Taking $J = M$, we have reduced (1.3) to the special case in which each Z_k is either zero or Z. Thus, (1.1) is reduced to this same special case. Moreover, any nuclei with atomic number $Z_k = 0$ may be simply deleted without affecting the left-hand side of (1.1). This completes the reduction of our Main Theorem (1.1) to the special case in which all the Z_k are equal to Z. The rest of this paper is dedicated to the proof of (1.1) in that special case.

2 Notation and Preliminary Remarks

Let Z be an integer, bounded below by a large enough absolute constant. Our Coulomb system consists of electrons and nuclei of charge $+Z$. Throughout our proof, we will carry along two large, positive constants, K and B_0. We write c, C, C', etc., for constants independent of Z, K, B_0. At the very end of our proof, we will take K to be a large enough universal constant, and then pick B_0 depending on Z, Γ in the statement of our main result. Note that we are justified, say, in asserting that $c - \frac{C}{B_0} > \frac{1}{2}c$, since c and C are constants independent of B_0, and B_0 is taken large enough. We will repeatedly use this reasoning without necessarily explaining it further.

We use the following notation. If $Q \subset \mathbb{R}^3$ is a cube of side δ, then for $(x_1, \dots, x_N) \in \mathbb{R}^{3N}$, we set

$$\mathcal{N}_Q = \mathcal{N}_Q(x_1 \ldots x_N) = \sum_{k=1}^N \chi_Q(x_k) \quad \text{where } \chi_Q \text{ denotes the characteristic function.}$$

Similarly, if $y_1 \ldots y_M \in \mathbb{R}^3$ are given (we think of the y_k as the positions of nuclei), then we set

$$\mathcal{M}_Q = \sum_{k=1}^M \chi_Q(y_k) = (\text{number of } y_k \text{ in } Q).$$

If $z \in \mathbb{R}^3$ and $R > 0$, then $B(z,R)$ denotes the ball in $\mathbb{R}^3$ with center z and radius R. We set

$$N_{zR} = N_{zR}(x_1 \ldots x_N) = \sum_{k=1}^N \chi_{B(z,R)}(x_k) \quad \text{and}$$

$$M_{zR} = \sum_{k=1}^M \chi_{B(z,R)}(y_k) = (\text{number of } y_k \text{ in } B(z,R)).$$

Also, we define

$$\Omega_{zR} = N_{zR}(N_{zR}-1) + Z^2 M_{zR}(M_{zR}-1) - 2ZN_{zR}M_{zR}.$$

Since $\Omega_{zR} = \left[\left(N_{zR} - ZM_{zR} - \frac{1}{2}\right)^2 - \frac{1}{4}\right] - (Z^2+Z)M_{zR}$, we have trivially

$$\Omega_{zR} \geq -2Z^2 M_{zR}. \tag{2.1}$$

The quantity Ω_{zR} enters by virtue of the following identity (see [FL]). Set

$$V_{\text{Coulomb}} = \sum_{1\leq j<k\leq N} |x_j - x_k|^{-1} + Z^2 \sum_{1\leq j<k\leq M} |y_j - y_k|^{-1} - Z\sum_{j=1}^N \sum_{k=1}^M |x_j - y_k|^{-1}.$$

Then we have

$$V_{\text{Coulomb}} = \frac{1}{2\pi} \iint_{\mathbb{R}^3\times\mathbb{R}^+} \Omega_{zR} \frac{dzdR}{R^5} \tag{2.2}$$

Let $\psi \in L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N})$ be antisymmetric with norm 1, and let $A(x) = (A_\mu(x))_{\mu=1,2,3}$ be a vector potential. If $Q \subset \mathbb{R}^3$ is a cube of side δ, then we define

$$T(\psi, A, Q) = \sum_{k=1}^N \int_{\mathbb{R}^{3N}} |(i\nabla_{x_k} - A(x_k))\psi|^2 \chi_Q(x_k)\, dx_1 \ldots dx_N \text{ , and}$$

$$PE(\psi, Q) \;=\; \left\langle \tfrac{1}{2\pi} \sum_{y_k \in Q} \quad \iint\limits_{\substack{B(z,R) \ni y_k \\ R < \frac{1}{10}\delta}} \frac{\Omega_{zR}}{M_{zR}} \; \frac{dz dR}{R^5} \; \psi, \psi \right\rangle .$$

We call $T(\psi, A, Q)$ the (Schrödinger) kinetic energy of Q.

We write $\sigma \cdot (i\nabla - A)$ for the Dirac operator with vector potential A, and $\sigma^{(k)} \cdot (i\nabla_{x_k} - A(x_k))$ for the tensor product

$$I \otimes \ldots \otimes I \otimes [\sigma \cdot (i\nabla - A)] \otimes I \otimes \ldots \otimes I, \quad \text{acting on}$$

$$\bigotimes^N L^2(\mathbb{R}^3, \mathbb{C}^2) \;=\; L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N}).$$

Here, I denotes the identity operator, and the Dirac operator occurs as the $k^{\underline{\text{th}}}$ factor in the tensor product. If ψ, A, Q are as above, then we define

$$T_{\text{Pauli}}(\psi, A, Q) \;=\; \sum_{k=1}^{N} \int\limits_{\mathbb{R}^{3N}} |\sigma^{(k)} \cdot (i\nabla_{x_k} - A(x_k))\, \psi|^2 \, \chi_Q(x_k)\, dx_1 \ldots dx_N .$$

We call $T_{\text{Pauli}}(\psi, A, Q)$ the Pauli kinetic energy of Q.

If $Q \subset \mathbb{R}^3$ is a cube of side δ with center x_0, then for $C > 0$ we write CQ for the cube with center x_0 and sides of length $C\delta$, parallel to the sides of Q. We write Q^* for $2Q$ and Q^{**} for $4Q$.

3 Comparison of Kinetic Energies

We begin with the following trivial estimate, comparing the Schrödinger and Pauli kinetic energies.

Comparison Lemma: *Let $Q \subset \mathbb{R}^3$ be a cube of side δ, and let $A(x)$ be a vector potential. Set $B(x) = \mathrm{curl} A$, and assume that $|B(x)| \leq C B_0\, \delta^{-2}$ on Q^*. Then, for any antisymmetric $\psi \in L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N})$ of norm 1, we have*

$$T_{\text{Pauli}}(\psi, A, Q^*) \;\geq\; \frac{1}{2}\, T\left(\psi, A, \frac{3}{2} Q\right) \;-\; C' B_0\, \delta^{-2}\, \langle \mathcal{N}_{Q^*} \psi, \psi \rangle . \tag{3.1}$$

Proof: Recall the standard identity

$$(3.2)\qquad \int_{\mathbb{R}^3} |\sigma\cdot(i\nabla - A)\,\varphi|^2\,dx = \int_{\mathbb{R}^3} |(i\nabla - A)\,\varphi|^2\,dx \pm \int_{\mathbb{R}^3} [(\sigma\cdot B)\varphi]\cdot\bar{\varphi}\,dx,$$

for $\varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2)$. Introduce a cutoff function $\theta \in C_0^\infty(Q^*)$, with $0 \le \theta \le 1$ and $|\nabla\theta| \le C'\,\delta^{-1}$ everywhere, and with $\theta = 1$ on $\frac{3}{2}Q$. Applying (3.2) with $\theta\varphi$ in place of φ, and noting that

$|\theta\sigma\cdot(i\nabla - A)\,\varphi|^2 \ge \frac{1}{2}\,|\sigma\cdot(i\nabla - A)\,(\theta\,\varphi)|^2 - |\nabla\,\theta|^2\,|\varphi|^2$, we obtain the estimate

$$(3.3)\qquad \int_{Q^*} |\sigma\cdot(i\nabla - A)\,\varphi|^2\,dx \ge \frac{1}{2}\int_{\frac{3}{2}Q} |(i\nabla - A)\,\varphi|^2\,dx - C' B_0 \delta^{-2}\int_{Q^*} |\varphi|^2\,dx,$$

since $|B(x)| \le CB_0\delta^{-2}$. The desired estimate (3.1) follows from (3.3) by separation of variables. ■

4 One Electron in a Constant Magnetic Field

Suppose $A(x) = (A_1(x), A_2(x), A_3(x))$ $(x = (x_1, x_2, x_3) \in \mathbb{R}^3)$ is a vector potential, that satisfies

$$(4.1)\qquad A_3 \equiv 0;\ \frac{\partial A_\nu}{\partial x_3} = 0 \text{ for } \nu = 1, 2;\ \text{ and}$$

$$(4.2)\qquad |\nabla A(x)| \le CB_0$$

Then, for $\varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2)$, integration by parts yields the standard identities

$$(4.3)\qquad \int_{\mathbb{R}^3} |\sigma\cdot(i\nabla - A)\,\varphi|^2\,dx = \int_{\mathbb{R}^3} |(i\nabla - A)\,\varphi|^2\,dx \pm \int_{\mathbb{R}^3} [(\sigma\cdot \operatorname{curl} A)\,\varphi]\cdot\bar{\varphi}\,dx \ \text{ and}$$

$$\int_{\mathbb{R}^3} |\sigma \cdot (i\nabla - A)\,\varphi|^2\,dx = \int_{\mathbb{R}^3} |\frac{\partial \varphi}{\partial x_3}|^2\,dx + \int_{\mathbb{R}^3} |\sum_{\nu=1,2} \sigma_\nu (i\frac{\partial}{\partial x_\nu} - A_\nu(x))\,\varphi|^2\,dx \tag{4.4}$$

Let $Q \subset \mathbb{R}^3$ be a cube of side 1, with sides not necessarily parallel to the axes. We can cover Q by closed rectangular tubes $T_\alpha = I_{\alpha 1} \times I_{\alpha 2} \times I_{\alpha 3} \subset \frac{3}{2}Q$, where $I_{\alpha\nu}$ is an interval, with length

$$|I_{\alpha 1}| = |I_{\alpha 2}| = B_0^{-1/2}, \ \frac{1}{10} < |I_{\alpha 3}| < 10. \tag{4.5}$$

We may suppose that the T_α have pairwise disjoint interiors, and that the number of distinct T_α is at most CB_0. (To construct the T_α, we first cover the projection of Q onto the (x_1, x_2)-plane by a grid of squares $I_{\alpha 1} \times I_{\alpha 2}$ of side $B_0^{-1/2}$, and then introduce appropriate $I_{\alpha 3}$.)

Let $\mathcal{T} = \bigcup_\alpha T_\alpha$, and let $\theta \in C_0^\infty(Q^*)$ be a cutoff function, with $0 \le \theta \le 1$, $|\nabla\theta| \le C'$, and $\theta|_{\mathcal{T}} \equiv 1$. Applying (4.4) with $\theta\varphi$ in place of φ, and noting that

$$|\theta\sigma \cdot (i\nabla - A)\,\varphi|^2 \ge \frac{1}{2}|\sigma \cdot (i\nabla - A)\,(\theta\varphi)|^2 - |\nabla\theta|^2\,|\varphi|^2, \ \text{we obtain} \tag{4.6}$$

$$\int_{Q^*} |\sigma \cdot (i\nabla - A)\,\varphi|^2\,dx \ge \frac{1}{2}\sum_\alpha \int_{T_\alpha} |\frac{\partial\varphi}{\partial x_3}|^2\,dx - C' \int_{Q^*} |\varphi|^2\,dx. \tag{4.7}$$

Similarly, (4.3) with $\theta\varphi$ in place of φ yields

$$\begin{aligned} \int_{Q^*} |\sigma \cdot (i\nabla - A)\,\varphi|^2\,dx &\ge \frac{1}{2}\sum_\alpha \int_{T_\alpha} |(i\nabla - A)\,\varphi|^2\,dx - C' \int_{Q^*} |\varphi|^2\,dx \\ &\quad - \int_{Q^*} |\mathrm{curl}\,A|\,|\varphi|^2\,dx \\ &\ge \tfrac{1}{2}\sum_\alpha \int_{T_\alpha} |(i\nabla - A)\,\varphi|^2\,dx - C' B_0 \int_{Q^*} |\varphi|^2\,dx, \end{aligned} \tag{4.8}$$

thanks to (4.2) and (4.6).

Let $A^\alpha = (A_1^\alpha, A_2^\alpha, A_3^\alpha)$ be the value of A at the center of T_α. Then (4.1) , (4.2), (4.5) show that $|A(x) - A^\alpha| \leq C' B_0^{1/2}$ for $x \in T_\alpha$.

Hence, $\int\limits_{T_\alpha} |(i\nabla - A)\,\varphi|^2\,dx \geq \frac{1}{2}\int\limits_{T_\alpha} |(i\nabla - A^\alpha)\,\varphi|^2\,dx - \int\limits_{T_\alpha} |A - A^\alpha|^2\,|\varphi|^2\,dx$

$\geq \frac{1}{2}\int\limits_{T_\alpha} |(i\nabla - A^\alpha)\,\varphi|^2\,dx - C' B_0 \int\limits_{T_\alpha} |\varphi|^2\,dx$, so that (4.8) implies

$$\int\limits_{Q^*} |\sigma\cdot(i\nabla - A)\,\varphi|^2\,dx \geq \frac{1}{4}\sum_\alpha \int\limits_{T_\alpha} |(i\nabla - A^\alpha)\,\varphi|^2\,dx - C' B_0 \int\limits_{Q^*} |\varphi|^2\,dx. \tag{4.9}$$

Multiplying (4.9) by B_0^{-1} and combining the result with (4.7), we obtain the basic estimate

$$\int\limits_{Q^*} |\sigma\cdot(i\nabla - A)\varphi|^2\,dx \geq c\sum_\alpha \int\limits_{T_\alpha} \left\{\left|\frac{\partial\varphi}{\partial x_3}\right|^2 + B_0^{-1}\sum_{\nu=1,2}\left|\left(i\frac{\partial}{\partial x_\nu} - A_\nu^\alpha\right)\varphi\right|^2\right\} dx$$
$$-C'\int\limits_{Q^*} |\varphi|^2\,dx. \tag{4.10}$$

We want to strengthen (4.10) to provide a lower bound for

$$\int\limits_{Q^*} |\sigma\cdot(i\nabla - A)\,\varphi|^2\,dx - \int\limits_{Q} V\,|\varphi|^2\,dx, \tag{4.11}$$

for small potentials V. We assume that V is supported on Q and satisfies

$$\int\limits_{Q^*} |V|^3\,dx \leq K^{-1}\,B_0^{-1}. \tag{4.12}$$

To control (4.11), we use the Sobolev and Hölder inequalities to write

$$\text{(4.13)} \qquad \int_{Q_0} |W|\,|\varphi|^2\,dx \le \left(\int_{Q_0} |W|^3\,dx\right)^{1/3} \left(\int_{Q_0} |\varphi|^3\,dx\right)^{2/3} \le$$

$$C' \left(\int_{Q_0} |W|^3\,dx\right)^{1/3} \left\{\int_{Q_0} |\nabla\varphi|^2\,dx + \int_{Q_0} |\varphi|^2\,dx\right\},$$

where Q_0 is the unit cube. Rescaling and applying a gauge transformation, we obtain

$$\text{(4.14)} \int_{T_\alpha} |V|\,|\varphi|^2\,dx \le$$

$$C'(B_0 \int_{T_\alpha} |V|^3\,dx)^{1/3} \cdot \int_{T_\alpha} \left\{ |\frac{\partial\varphi}{\partial x_3}|^2 + B_0^{-1} \sum_{\nu=1,2} \left|(i\frac{\partial}{\partial x_\nu} - A_\nu^\alpha)\,\varphi\right|^2 + |\varphi|^2 \right\} dx.$$

If V satisfies (4.12), then $(B_0 \int_{T_\alpha} |V|^3 dx)^{1/3} \le K^{-1/3}$, so (4.14) and (4.10) imply

$$\text{(4.15)} \qquad \int_{Q^*} |\sigma \cdot (i\nabla - A)\,\varphi|^2\,dx - \int_{Q} V\,|\varphi|^2\,dx \ge$$

$$c \sum_\alpha \int_{T_\alpha} \left\{ |\frac{\partial\varphi}{\partial x_3}|^2 + B_0^{-1} \sum_{\nu=1,2} |(i\frac{\partial}{\partial x_\nu} - A_\nu^\alpha)\,\varphi|^2 \right\} dx - C' \int_{Q^*} |\varphi|^2\,dx,$$

since K is large. (See the discussion of K in Section 2.)

In view of (4.5), the quadratic form

$\mathcal{Q}_\alpha(\varphi) = \int_{T_\alpha} \left\{ |\frac{\partial\varphi}{\partial x_3}|^2 + B_0^{-1} \sum_{\nu=1,2} |(i\frac{\partial}{\partial x_\nu} - A_\nu^\alpha)\varphi|^2 \right\} dx$ is equivalent to $\int_{Q_0} |\nabla\varphi|^2 dx$ (Q_0 = unit cube) by a rescaling and a gauge transformation. Hence it follows easily from the standard eigenvalue asymptotics of the Neumann Laplacian on Q_0 that $\mathcal{Q}_\alpha(\varphi)$ has at most $CK^{3/2}$ eigenvalues less than K, when $\mathcal{Q}_\alpha(\varphi)$ is diagonalized against $\int_{T_\alpha} |\varphi|^2 dx$.

Setting

$\mathcal{Q}(\varphi) = c\sum_\alpha \mathcal{Q}_\alpha(\varphi)$, and recalling that there are at most CB distinct T_α, we draw from (4.15) the following conclusions.

(4.16) $$\mathcal{Q}(\varphi) \text{ is a quadratic form on } L^2(\mathcal{T},\mathbb{C}^2).$$

(4.17)

When $\mathcal{Q}$ (φ) is diagonalized against $\int\limits_{\mathcal{T}} |\varphi|^2 dx$, there are at most $C'K^{3/2}B_0$ eigenvalues less than cK.

(4.18) $$\text{We have} \int\limits_{Q^*} |\sigma\cdot(i\nabla - A)\varphi|^2 dx - \int\limits_{Q} V|\varphi|^2 dx \geq \mathcal{Q}(\varphi|\mathcal{T}) - C' \int\limits_{Q^*} |\varphi|^2 dx,$$

whenever V satisfies (4.12).

We have proven (4.16), (4.17), (4.18) under the assumptions (4.1), (4.2). However, if instead of (4.1) , (4.2) we assume

(4.19) $$B = \operatorname{curl} A(\mathrm{x}) \text{ is independent of x, and}$$

(4.20) $$|B| \leq CB_0,$$

then we may reduce matters to the case in which (4.1), (4.2) hold, by making a rotation and a gauge transformation. Hence, we have proven the following.

One-electron Lemma: *Let Q be a cube of side 1, and let $A(x)$ be a vector potential whose magnetic field B = curl $A(x)$ is independent of x. Assume that $|B| \leq CB_0$.*

Then there exist an open set $\mathcal{T}$, with $Q \subset \mathcal{T} \subset Q^*$, and a quadratic form $\mathcal{Q}$ on $L^2(\mathcal{T},\mathbb{C}^2)$, having the following properties.

(A) *If V is any potential satisfying* $\int\limits_Q |V|^3 dx \le K^{-1} B_0^{-1}$, *then for every* $\varphi \in L^2(Q^*, \mathbb{C}^2)$ *we have*

$$\int\limits_{Q^*} |\sigma \cdot (i\nabla - A)\,\varphi|^2 dx - \int\limits_Q V|\varphi|^2 dx \ge \mathcal{Q}(\varphi|\mathcal{T}) - C' \int\limits_{Q^*} |\varphi|^2 dx.$$

(B) *When* $\mathcal{Q}(\varphi)$ *is diagonalized with respect to* $\|\varphi\|^2_{L^2(\mathcal{T},\mathbb{C}^2)}$ *then there are at most* $C'K^{3/2}B_0$ *eigenvalues less than* cK.

5 Variable Magnetic Fields

In this section, we extend the One-Electron Lemma to variable magnetic fields, and then use that result to study N electrons.

We begin with an elementary result.

(5.1)

VECTOR POTENTIAL SPLITTING LEMMA:
Let Q be the unit cube in $\mathbb{R}^3$, let $A(x)$ be a vector potential on Q^{**}, and let $B(x) = curl\, A$. Assume that

$$\int\limits_{Q^{**}} |B(x)|^2 dx \le CB_0^2, \quad \text{and} \tag{5.2}$$

$$\int\limits_{Q^{**}} |B(x) - Av_{Q^{**}} B|^2\, dx \le CK^{-2} B_0^{-1/3}. \tag{5.3}$$

Then on Q^* we may express A in the form

$$A = \tilde{A} + A^{\#} + \nabla f, \quad \text{where} \tag{5.4}$$

(5.5) $$\tilde{A} \text{ is linear (i.e., } \tilde{A}_\nu = \sum_{\mu=1}^{3} \tilde{A}_{\mu\nu}\, x_\mu \text{ for constants } \tilde{A}_{\mu\nu}\text{)},$$

(5.6) $$|\nabla \tilde{A}| \leq C' B_0, \quad \text{and}$$

(5.7) $$\int_{Q^*} |A^\#|^6\, dx \leq C'\, K^{-6}\, B_0^{-1}.$$

Proof: Set $\tilde{B}(x) = B(x) - Av_{Q^{**}} B$. Let e_ν be the $\nu^{\underline{\text{th}}}$ coordinate vector in $\mathbb{R}^3$. By separation of variables, we may solve the following boundary-value problem.

(5.8) $$-\triangle F_\nu = \tilde{B}_\nu \text{ on } Q^{**}, \text{ where } \tilde{B}_\nu \text{ is the } \nu^{\underline{\text{th}}} \text{ component of } \tilde{B}(x).$$

(5.9) $$\frac{\partial}{\partial x_\nu} F_\nu = 0 \text{ on the faces of } \partial Q^{**} \text{ that are perpendicular to } e_\nu.$$

(5.10) $$F_\nu = 0 \text{ on the faces of } \partial Q^{**} \text{ that are parallel to } e_\nu.$$

Set $F(x) = (F_\nu(x))_{\nu=1,2,3}$. Separation of variables let us check that

(5.11) $$\|F_\nu\|_{L^2(Q_\nu^{**})} \leq C' \|\tilde{B}_\nu\|_{L^2(Q_\nu^{**})} \leq C'\, K^{-1}\, B_0^{-1/6}, \text{ by (5.3)}.$$

Hence, the standard elliptic estimate

$$\|\nabla F_\nu\|_{L^2(Q^*)} + \|\nabla^2 F_\nu\|_{L^2(Q^*)} \leq C' \|\triangle F_\nu\|_{L^2(Q^{**})} + C' \|F_\nu\|_{L^2(Q^{**})}$$

implies

$$\|\nabla F\|_{L^2(Q^*)} + \|\nabla^2 F\|_{L^2(Q^*)} \leq C' K^{-1} B_0^{-1/6}, \quad \text{and therefore}$$

(5.12) $$\int_{Q^*} |\nabla F|^6\, dx \leq C' K^{-6} B_0^{-1},$$

by the Sobolev inequality.

¿From the boundary conditions (5.9), (5.10), we see that div $F = 0$ on ∂Q^{**}. Equation (5.8) shows that div$F$ is harmonic on Q^{**}. Hence, div $F = 0$ on Q^{**}. Another application of (5.8) therefore gives

$\tilde{B} = -\triangle F = \operatorname{curl}(\operatorname{curl} F) \pm \triangledown(\operatorname{div} F) = \operatorname{curl} A^{\#}$, with $A^{\#} = \operatorname{curl} F$. Thus,

$$\operatorname{curl} A^{\#} = \tilde{B}, \text{ with} \tag{5.13}$$

$$\int_{Q^*} |A^{\#}|^6 \, dx \leq C' K^{-6} B_0^{-1}, \text{ by (5.12).} \tag{5.14}$$

On the other hand, $Av_{Q^{**}} B$ is a constant vector of magnitude at most $C' B_0$, by virtue of (5.2). Hence, we can easily find a linear vector potential $\tilde{A}$ satisfying

$$\operatorname{curl} \tilde{A} = Av_{Q^{**}} B, \text{ and} \tag{5.15}$$

$$|\triangledown \tilde{A}| \leq C' B_0. \tag{5.16}$$

Since curl $(A - \tilde{A} - A^{\#}) = B(x) - Av_{Q^{**}} B - \tilde{B}(x) = 0$, we have

$$A - \tilde{A} - A^{\#} = \triangledown f, \text{ for a scalar function } f. \tag{5.17}$$

The conclusions of the lemma are contained in (5.17), (5.16), (5.14), since $\tilde{A}$ is linear. ■

To apply the above lemma, we write $A = A_c + A^{\#}$, with $A_c = \tilde{A} + \triangledown f$. Thus, A_c has constant magnetic field $B_c = \operatorname{curl} A_c$, and B_c satisfies

$$|B_c| \leq C' B_0. \tag{5.18}$$

We write $|\sigma \cdot (i\nabla - A)\varphi|^2 \geq \frac{1}{2}|\sigma \cdot (i\nabla - A_c)\varphi|^2 - |A^{\#}|^2|\varphi|^2$, set $W_1(x) = |A^{\#}(x)|^2$ on Q^*, and apply the ONE-ELECTRON LEMMA to the vector potential A_c. This yields the following result.

(5.19)

Lemma: *Let Q and A be as in Lemma (5.1). Then there exist an open set $\mathcal{T}$, with $Q \subset \mathcal{T} \subset Q^*$, a quadratic form $\mathcal{Q}$ on $L^2(\mathcal{T}, \mathbb{C}^2)$, and a potential W_1 supported in Q^*, having the following properties.*

(5.20)

If V is any potential satisfying $\int_Q |V|^3\,dx \leq cK^{-1}B_0^{-1}$, then for any $\varphi \in L^2(Q^*, \mathbb{C}^2)$, we have

$$\int_{Q^*} |\sigma \cdot (i\nabla - A)\varphi|^2\,dx - \int_Q V|\varphi|^2\,dx \geq \mathcal{Q}(\varphi|\mathcal{T}) - C'\int_{Q^*}|\varphi|^2\,dx - \int_{Q^*} W_1|\varphi|^2\,dx.$$

(5.21)

When $\mathcal{Q}(\varphi)$ is diagonalized with respect to $\|\varphi\|^2_{L^2(\mathcal{T},\mathbb{C}^2)}$, then there are at most $C'K^{3/2}B_0$ eigenvalues less than cK.

(5.22)
$$\int_{Q^*} |W_1|^3\,dx \leq C'K^{-6}B_0^{-1}.$$

Now let $\psi \in L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N})$ be antisymmetric, with norm 1. From Lemma (5.19) and separation of variables, we obtain the following estimate whenever V is as in (5.20).

$$T_{\text{Pauli}}(\psi, A, Q^*) - \left\langle \sum_{k=1}^{N} V(x_k)\,\psi, \psi \right\rangle \geq$$
$$\left\langle cK(\mathcal{N}_Q - C'K^{3/2}B_0)_+\psi, \psi \right\rangle - C'\left\langle \mathcal{N}_{Q^*}\psi, \psi\right\rangle - \left\langle \sum_{k=1}^{N} W_1(x_k)\,\psi, \psi \right\rangle.$$

(Here, $t_+ = \max(t,0)$ for $t \in \mathbb{R}$.) In particular,

$$T_{\text{Pauli}}(\psi, A, Q^*) - \left\langle \sum_{k=1}^{N} V(x_k)\,\psi, \psi \right\rangle \geq$$
$$cK\,\langle \mathcal{N}_Q\,\psi, \psi\rangle - C'\,K^{5/2} B_0 - C'\,\langle \mathcal{N}_{Q^*}\,\psi, \psi\rangle - \left\langle \sum_{k=1}^{N} W_1(x_k)\,\psi, \psi \right\rangle .$$

Rescaling from the unit cube Q to a cube of side δ, we obtain the following result.

(5.23)

N-Electron Lemma: *Let $A(x)$ be a vector potential, and let $Q \subset \mathbb{R}^3$ be a cube of side δ. Assume that $B(x) = \text{curl } A$ satisfies*

(5.24) $$\int_{Q^{**}} |B(x)|^2\,dx \leq C\,B_0^2\,\delta^{-1}, \text{ and}$$

(5.25) $$\int_{Q^{**}} |B(x) - Av_{Q^{**}}\,B|^2\,dx \leq C\,K^{-2}\,B_0^{-1/3}\,\delta^{-1}.$$

Then there exists a potential $W_1(x)$, supported on Q^*, with the following properties.

(5.26) $$\int_{Q^*} |W_1|^3\,dx \leq C'\,K^{-6}\,B_0^{-1}.$$

(5.27)

Suppose $\psi \in L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N})$ is antisymmetric with norm 1; and suppose that $V(x)$ is any potential, supported on Q, that satisfies

(5.28) $$\int_{Q} |V|^3\,dx \leq cK^{-1}\,B_0^{-1}.$$

Then we have

(5.29)
$$\delta \cdot T_{\text{Pauli}}(\psi, A, Q^*) - \left\langle \sum_{k=1}^{N} V(x_k)\,\psi, \psi \right\rangle \geq$$
$$\frac{cK}{\delta}\,\langle \mathcal{N}_Q\,\psi, \psi\rangle - \frac{C'}{\delta}\,\langle \mathcal{N}_{Q^*}\,\psi, \psi\rangle$$
$$-\frac{C'\,K^{5/2}}{\delta}\,B_0 - \left\langle \sum_{k=1}^{N} W_1(x_k)\,\psi, \psi \right\rangle .$$

6 Local Stability of Matter

The first main result of this section is as follows:

(6.1)

<u>Local Stability of Matter</u> (see [Min] and [FL]): Let $\psi \in L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N})$ be antisymmetric, with norm 1. Let A be a <u>constant</u> vector potential, and let $Q \subset \mathbb{R}^3$ be a cube of side δ. Then we have

(6.2)
$$Z\delta \cdot T(\psi, A, Q^*) + PE(\psi, Q) \geq -\frac{CZ}{\delta}\,\mathcal{M}_Q - \frac{CZ}{\delta}\,\langle \mathcal{N}_{Q^*}\,\psi, \psi\rangle .$$

<u>Proof:</u> By performing a suitable gauge transformation and rescaling, we may assume without loss of generality that $A \equiv 0$ and $\delta = 1$. We use the following elementary results from [FL].

(6.3)

<u>Lemma:</u> *If $f \in L^2(\mathbb{R}^3)$, then*

$$\left\langle (-\triangle)^{1/2} f, f \right\rangle = c \iint\limits_{\mathbb{R}^3 \times \mathbb{R}^+} \int\limits_{B(z,R)} |f(x) - Av_{B(z,R)}\, f|^2\, dx\, \frac{dz\,dR}{R^5}.$$

(6.4)

Lemma: *Let $R \longmapsto B(R)$ be a one-parameter family of balls in $\mathbb{R}^3$. Suppose*

$$B(R) \text{ has radius } R, \text{and} \tag{6.5}$$

$$\text{If } R_1 < R_2, \text{ then } B(R_1) \subset B(R_2). \tag{6.6}$$

Then there exist universal constants $\kappa_0, e_0 > 0$, such that, for any $R_0 > 0$ and any $u \in L^2(\mathbb{R}^3)$, we have the estimate

$$\kappa_0 \int_0^{R_0} \int_{B(R)} |u - Av_{B(R)}\, u|^2 \, dx \, \frac{dR}{R^2} - 2 \int_0^{R_0} \int_{B(R)} |u|^2 \, dx \, \frac{dR}{R^2} \geq \frac{-e_0}{R_0} \int_{B(R_0)} |u|^2 \, dx. \tag{6.7}$$

In our proof of (6.1), we will carry along a large constant $\kappa > 0$, to be picked later. We let c, C, etc. denote constants independent of Z and κ, we write $C(\kappa)$ for a constant depending on κ but not Z, and we assume that Z is greater than a large enough constant $C(\kappa)$. Eventually, we will take κ to be a large enough universal constant. Our usual constants K, B_0 will play no role in the proof of (6.1).

As a consequence of (6.3), we have

$$\int_{Q^*} |\nabla u|^2 \, dx \geq \frac{\kappa}{2\pi} \iint\limits_{\substack{B(z,R) \cap Q \neq \phi \\ R < \frac{1}{10}}} \int_{B(z,R)} |u(x) - Av_{B(z,R)}\, u|^2 \, dx \, \frac{dz dR}{R^5} - C(\kappa) \int_{Q^*} |u|^2 \, dx \tag{6.8}$$

for $u \in L^2(Q^*)$.

To prove (6.8), we take a cutoff function $\theta \in C_0^\infty(Q^*)$, with $0 \leq \theta \leq 1$ and $|\nabla \theta| \leq C$ everywhere, and with $\theta|_{B(z,R)} \equiv 1$ whenever $B(z,R) \cap Q \neq \phi$ and $R < \frac{1}{10}$. (Recall that Q has side 1.)

Applying (6.3) to $f = \theta u$, and noting that $-\triangle \geq \frac{\kappa}{C}(-\triangle)^{1/2} - C(\kappa)$, we find that

$$\int_{\mathbb{R}^3} |\nabla(\theta u)|^2 \, dx \;\geq\; \frac{\kappa}{\pi} \iint_{\substack{B(z,R)\cap Q\neq\phi \\ R<\frac{1}{10}}} \int_{B(z,R)} |u(x) \,-\, Av_{B(z,R)}\, u|^2 \, dx \, \frac{dzdR}{R^5} - C(\kappa) \int_{\mathbb{R}^3} |\theta u|^2 \, dx,$$

which easily implies (6.8), since $|\theta \nabla u|^2 \,\geq\, \frac{1}{2}|\nabla(\theta u)|^2 \,-\, |\nabla\theta|^2\, |u|^2$.

Next, we pass to N electrons. Let $\psi \in L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N})$, and define

$$T(z,R) \,=\, \sum_{j=1}^{N} \int_{\mathbb{R}^{3N}} |\psi \,-\, \psi_{jzR}|^2 \, \chi_{B(z,R)}(x_j)\, dx_1 \,\ldots\, dx_N, \text{ where} \tag{6.9}$$

$$\psi_{jzR}\,(x_1 \,\ldots\, x_n) \,=\, Av_{\tilde{x}\in B(z,R)}\, \psi(x_1 \,\ldots\, x_{j-1}\, \tilde{x}\, x_{j+1} \,\ldots\, x_N). \tag{6.10}$$

Then (6.8) and separation of variables imply

$$T(\psi, A, Q^*) \,\geq\, \frac{\kappa}{2\pi} \iint_{\substack{B(z,R)\cap Q\neq\phi \\ R<\frac{1}{10}}} T(z,R)\, \frac{dzdR}{R^5} \,-\, C(\kappa)\, \langle \mathcal{N}_{Q^*}\, \psi, \psi\rangle\, . \tag{6.11}$$

(Recall that $A \,\equiv\, 0$.)

Moreover, if ψ is antisymmetric, then another application of separation of variables yields

$$T(z,R) \,\geq\, \langle (N_{zR} - 2)_+\, \psi, \psi\rangle \,+\, \tilde{T}(z,R), \text{ where} \tag{6.12}$$

$$\tilde{T}(z,R) \,=\, \sum_{j=1}^{N} \int_{\mathbb{R}^{3N}} |\psi \,-\, \psi_{jzR}|^2 \, \chi_{B(z,R)}\,(x_j)\, \chi_{N_{zR}\leq 2}\, dx_1 \,\ldots\, dx_N. \tag{6.13}$$

Putting (6.12) into (6.11), we obtain

$$T(\psi, A, Q^*) \;\;\geq\;\; \frac{1}{2\pi} \sum_{y_k\in Q} \iint_{\substack{B(z,R)\ni y_k \\ R<\frac{1}{10}}} \left\langle \frac{\kappa(N_{zR}-2)_+}{M_{zR}}\, \psi, \psi \right\rangle \frac{dzdR}{R^5}$$

$$+ \frac{1}{2\pi} \sum_{y_k \in Q} \iint_{\substack{B(z,R) \ni y_k \\ R < \frac{1}{10}}} \frac{\kappa \tilde{T}(z,R)}{M_{zR}} \frac{dz dR}{R^5} - C(\kappa) \langle \mathcal{N}_{Q^*} \psi, \psi \rangle .$$

Together with the definition of $PE(\psi, Q)$ in Section 2, this gives

$$(6.14) \qquad Z\, T(\psi, A, Q^*) + PE(\psi, Q) \geq$$

$$\frac{1}{2\pi} \sum_{y_k \in Q} \iint_{\substack{B(z,R) \ni y_k \\ R < \frac{1}{10}}} \left\{ \left\langle \frac{\Omega^{\#}_{zR}}{M_{zR}} \psi, \psi \right\rangle + \frac{\kappa Z \tilde{T}(z,R)}{M_{zR}} \right\} \frac{dz dR}{R^5} - Z C(\kappa) \langle \mathcal{N}_{Q^*} \psi, \psi \rangle$$

where we set

$$(6.15) \quad \Omega^{\#}_{zR} = \kappa Z\, (N_{zR} - 2)_+ + N_{zR}(N_{zR} - 1) + Z^2 M_{zR}(M_{zR} - 1) - 2 Z N_{zR} M_{zR}.$$

If we take κ large enough and $Z > C(\kappa)$, then for any integers $N_{zR} \geq 0$, $M_{zR} \geq 1$, we have

$$(6.16) \qquad \left(\frac{\Omega^{\#}_{zR}}{M_{zR}} \right) \geq \frac{\kappa Z}{20} \chi_{N_{zR} \geq 3} + [Z^2 (M_{zR} - 1) - 2 Z N_{zR}]\, \chi_{N_{zR} \leq 2}.$$

We check (6.16) by cases.

- If $N_{zR} \leq 2$, then (6.16) is immediate from (6.15).
- If $N_{zR} \geq 3$ and $M_{zR} = 1$, then $\Omega^{\#}_{zR} \geq \kappa Z (N_{zR} - 2)_+ - 2 Z N_{zR} \geq \frac{\kappa}{20} Z$, so (6.16) holds.
- If $N_{zR} \geq 3$, $M_{zR} \geq 2$, and $N_{zR} \leq \frac{1}{10} Z M_{zR}$, then
  $\Omega^{\#}_{zR} = \kappa Z (N_{zR} - 2)_+ + (N_{zR} - Z M_{zR})^2 - N_{zR} - Z^2 M_{zR} \geq$
  $\{\kappa Z\, (N_{zR} - 2) - N_{zR}\} + \left(\frac{9}{10} Z M_{zR}\right)^2 - Z^2 M_{zR} \geq$
  $\left\{\frac{\kappa Z}{3} N_{zR} - N_{zR}\right\} + \frac{81}{100} Z^2 M_{zR}^2 - Z^2 M_{zR} \geq$
  $\frac{81}{50} Z^2 M_{zR} - Z^2 M_{zR} = \frac{31}{50} Z^2 M_{zR} \geq \frac{\kappa}{20} Z\, M_{zR}$, so again (6.16) holds.

- If $N_{zR} \geq 3$, $M_{zR} \geq 2$ and $N_{zR} \geq \frac{1}{10} Z\, M_{zR}$, then
  $\Omega^{\#}_{zR} = \kappa Z\,(N_{zR} - 2)_+ + (N_{zR} - Z\, M_{zR})^2 - N_{zR} - Z^2\, M_{zR} \geq$
  $\frac{99}{100}\,\kappa Z\, N_{zR} - N_{zR} - Z^2\, M_{zR} \geq \frac{9}{10}\,\kappa Z\, N_{zR} - Z^2\, M_{zR} \geq$
  $\frac{8}{10}\,\kappa Z\, N_{zR} + \left\{\frac{\kappa}{10}\, Z\, N_{zR} - Z^2\, M_{zR}\right\} \geq \frac{8}{10}\,\kappa Z\, N_{zR} \geq \frac{8}{100}\,\kappa Z^2\, M_{zR}$, so again (6.16) holds.

Thus, (6.16) holds in all cases.

Putting (6.16) into (6.14), we find that

$$ZT(\psi, A, Q^*) + PE(\psi, Q) \geq -C(\kappa) Z\,\langle \mathcal{N}_{Q^*}\psi, \psi\rangle + \frac{1}{2\pi} \sum_{y_k \in Q} En(y_k), \tag{6.17}$$

where

$$En(y_k) = \iint\limits_{\substack{B(z,R)\ni y_k \\ R< \frac{1}{10}}} \left\{ \left\langle \left[\frac{\kappa Z}{20}\, \chi_{N_{zR}\geq 3} + (Z^2(M_{zR} - 1) - 2ZN_{zR})\, \chi_{N_{zR}\leq 2}\right] \psi, \psi \right\rangle \right.$$
$$\left. + \frac{\kappa Z \tilde{T}(z, R)}{M_{zR}} \right\} \frac{dz dR}{R^5}. \tag{6.18}$$

Fix a particular y_k. We make a change of variable in (6.18) from (z, R) to (ω, R), where

$$\omega = (z - y_k)/R, \text{ i.e., } z = y_k + R\omega. \tag{6.19}$$

With ω and z related by (6.19), we set

$$B_\omega(R) = B(z, R), N_\omega(R) = N_{zR}, M_\omega(R) = M_{zR}, \psi^{j\omega R} = \psi_{jzR}, \tilde{T}_\omega(R) = \tilde{T}(z, R). \tag{6.20}$$

Note that $B(z, R) \ni y_k$ if and only if $|\omega| < 1$, and that $\frac{dzdR}{R^5} = \frac{d\omega dR}{R^2}$. Also, note that $R_1 < R_2$ implies $B_\omega(R_1) \subset B_\omega(R_2)$, provided $|\omega| < 1$. Therefore, we may rewrite (6.18) in the form

$$En(y_k) = \int\limits_{|\omega|<1} En(y_k, \omega)\, d\omega, \text{ where} \tag{6.21}$$

(6.22) $$En(y_k, \omega) = \int_0^{1/10} \left\{ \left\langle \left[\frac{\kappa Z}{20} \chi_{N_\omega(R) \geq 3} + (Z^2(M_\omega(R) - 1) - 2ZN_\omega(R))\chi_{N_\omega(R) \leq 2} \right] \psi, \psi \right\rangle + \frac{\kappa Z \tilde{T}_\omega(R)}{M_\omega(R)} \right\} \frac{dR}{R^2}.$$

Fix both y_k and ω ($|\omega| < 1$). We make the following definitions. For $(x_1, \dots, x_N) \in \mathbb{R}^{3N}$, let

$R_*(x_1 \dots x_N) = \sup\{R \in (0, \frac{1}{10}] :$ At most two of the x_j lie in $B_\omega(R)\}$

$S_*(x_1 \dots x_N) = \{j : x_j$ is in the interior of $B_\omega(R_*)$, where $R_* = R_*(x_1 \dots x_N)\}$.

For $S \subset \{1, 2, \dots, N\}$, set $x_S = (x_j)_{j \in S}$ and $x'_S = (x_j)_{j \notin S}$.

We write dx_S for $\prod_{j \in S} dx_j$, and dx'_S for $\prod_{j \notin S} dx_j$.

Define also

$R_0(x'_S) = \sup\{R \in (0, 1/10] :$ None of the x_j ($j \notin S$) belongs to $B_\omega(R)\}$, and set

$$E(S) = \begin{cases} \{(x'_S) \in (\mathbb{R}^3)^{N-|S|} : R_0(x'_S) = 1/10\} & \text{if} \quad |S| = 0 \text{ or } 1 \\ (\mathbb{R}^3)^{N-2} & \text{if} \quad |S| = 2 \\ \phi & \text{for} \quad |S| \geq 3 \end{cases}$$

Then the reader can verify the following result without difficulty.

(6.23)

Lemma: *For every $S \subset \{1, 2, \dots, N\}$, and for almost every $(x_1, \dots, x_N) \in \mathbb{R}^{3N}$, we have $S_*(x_1 \dots x_N) = S$ if and only if $[x'_S \in E(S)$ and $x_j \in B_\omega(R_0(x'_S))$ for all $j \in S]$.*

Moreover, suppose $S_*(x_1 \dots x_N) = S$. Then the following hold.

(6.24) $$R_*(x_1 \dots x_N) = R_0(x'_S)$$

(6.25) For all $R \in (0, 1/10]$, we have $N_\omega(R) \le 2$ if and only if $R \le R_0(x'_S)$.

(6.26) For all $R < R_0(x'_S)$, we have $x_j \notin B_\omega(R)$ for $j \notin S$, hence

$$N_\omega(R) = \sum_{j \in S} \chi_{B_\omega(R)}(x_j).$$

In the integrals (6.13) and

$$\int_{\mathbb{R}^{3N}} \left[\frac{\kappa Z}{20} \chi_{N_\omega(R) \ge 3} + (Z^2(M_\omega(R) - 1) - 2Z\, N_\omega(R))\, \chi_{N_\omega(R) \le 2} \right] |\psi|^2\, dx_1 \ldots dx_N,$$

we insert a factor $1 = \sum_S \chi_{S_*(x_1 \ldots x_N) = S}$ into the integrand, and bring the sum outside the integral. Using Lemma (6.23) to control the characteristic functions in (6.13) and (6.22), we may rewrite (6.22) as follows.

$$En(y_k, \omega) = \sum_{|S| \le 2} \int_{x'_S \in E(S)} En(y_k, \omega, S, x'_S)\, dx'_S, \quad \text{where} \tag{6.27}$$

$$En(y_k, \omega, S, x'_S) = \tag{6.28}$$

$$\kappa\, Z \sum_{j \in S} \int_0^{R_0} \int_{(B_\omega(R_0))^{|S|}} |\psi - \psi^{j\omega R}|^2\, \chi_{B_\omega(R)}(x_j)\, dx_S\, \frac{dR}{M_\omega(R) R^2} +$$

$$\left[\frac{\kappa Z}{20} \int_{R_0}^{1/10} \frac{dR}{R^2} + \int_0^{R_0} Z^2(M_\omega(R) - 1)\, \frac{dR}{R^2} \right] \int_{(B_\omega(R_0))^{|S|}} |\psi|^2\, dx_S$$

$$-2Z \sum_{j \in S} \int_0^{R_0} \int_{(B_\omega(R_0))^{|S|}} \chi_{B_\omega(R)}(x_j)\, |\psi|^2\, dx_S\, \frac{dR}{R^2}\,;$$

we have set

$$R_0 \;=\; R_0\left(x'_S\right) \;\leq\; 1/10 \;\text{ in } (6.28). \tag{6.29}$$

We prepare to apply Lemma (6.4). Note that the balls $B_\omega(R)$ satisfy (6.5) and (6.6). For any $u \in L^2(B_\omega(R_0))$, we have

$$\left[\int_0^{R_0} Z^2(M_\omega(R)-1)\,\frac{dR}{R^2}\right] \int_{B_\omega(R_0)} |u|^2\,dx \;\geq$$

$$\int_0^{R_0} Z^2(M_\omega(R)-1) \int_{B_\omega(R)} |u|^2\,dx\,\frac{dR}{R^2}. \text{ Hence,}$$

$$\kappa Z \int_0^{R_0} \int_{B_\omega(R)} |u - Av_{B_\omega(R)}\,u|^2\,dx\,\frac{dR}{M_\omega(R)R^2} \;+\; \left[\int_0^{R_0} Z^2\,\frac{(M_\omega(R)-1)}{2}\,\frac{dR}{R^2}\right] \int_{B_\omega(R_0)} |u|^2\,dx$$

$$\geq \int_0^{R_0} \left\{\frac{\kappa Z}{M_\omega(R)} \;+\; Z^2\,\frac{(M_\omega(R)-1)}{2}\right\} \int_{B_\omega(R)} |u - Av_{B_\omega(R)}\,u|^2\,dx\,\frac{dR}{R^2}$$

$$\geq\; \kappa_0 Z \int_0^{R_0} \int_{B_\omega(R)} |u - Av_{B_\omega(R)}\,u|^2\,dx\,\frac{dR}{R^2} \quad \text{(with } \kappa_0 \text{ as in (6.7)),}$$

provided κ exceeds a universal constant determined by κ_0.

Therefore, (6.7) implies the following inequality.

$$\begin{aligned}
&\kappa Z \int_0^{R_0} \int_{B_\omega(R)} |u - Av_{B_\omega(R)}\,u|^2\,dx\,\frac{dR}{M_\omega(R)R^2} + \\
&\left[\frac{\kappa Z}{40} \int_{R_0}^{1/10} \frac{dR}{R^2} + \int_0^{R_0} \frac{Z^2(M_\omega(R)-1)}{2}\,\frac{dR}{R^2}\right] \int_{B_\omega(R)} |u|^2\,dx \\
&-2Z \int_0^{R_0} \int_{B_\omega(R)} |u|^2\,dx\,\frac{dR}{R^2} \;\geq
\end{aligned} \tag{6.30}$$

$$\left\{ \frac{\kappa Z}{40} \left(R_0^{-1} - 10 \right) - e_0 Z \, R_0^{-1} \right\} \int\limits_{B_\omega(R_0)} |u|^2 \, dx \ \geq$$

$$-\frac{\kappa Z}{4} \int\limits_{B_\omega(R_0)} |u|^2 \, dx \quad \text{(we may assume } \frac{\kappa}{40} \geq e_0\text{)}.$$

We apply (6.30) to $u(x_j) = (\psi(x_1 \ldots x_N))_{\mu_1 \ldots \mu_N}$ for $j \in S$. (Recall that $\psi(x_1 \ldots x_N) \in (\mathbb{C}^2)^{\otimes N}$; its components are $(\psi(x_1 \ldots x_N))_{\mu_1 \ldots \mu_N}$ for $\mu_j = 1$ or 2.)

Summing and integrating (6.30), and comparing the result with (6.28), we find that

$$En(y_k, \omega, S, x'_S) \geq -\frac{\kappa Z}{2} \int\limits_{(B_\omega(R_0))^{|S|}} |\psi|^2 \, dx_S \quad \text{for } |S| \leq 2.$$

Substituting this into (6.27), and using (6.29) and Lemma (6.23), we obtain the estimates

$$En(y_k, \omega) \geq -\frac{\kappa Z}{2} \sum_{|S| \leq 2} \int\limits_{\mathbb{R}^{3N}} \chi_{E(S)}(x'_S) \prod_{j \in S} \chi_{B_\omega(R_0(x'_S))}(x_j) |\psi|^2 \, dx_1 \ldots dx_N$$

$$= -\frac{\kappa Z}{2} \sum_{|S| \leq 2} \int\limits_{\mathbb{R}^{3N}} \chi_{S_*(x_1 \ldots x_N) = S} |\psi|^2 \, dx_1 \ldots dx_N$$

$$= -\frac{\kappa Z}{2} \int\limits_{\mathbb{R}^{3N}} |\psi|^2 \, dx_1 \ldots dx_N = -\frac{\kappa Z}{2}.$$

Hence, (6.21) yields $En(y_k) \geq -C\kappa Z$.

Taking κ to be a universal constant, large enough to make the preceding arguments work, we conclude that

$$En(y_k) \geq -CZ. \tag{6.31}$$

The desired estimate (6.2) then follows at once from (6.17), since we are taking $\delta = 1$ and κ = universal constant. ■

We will need a refinement of local stability of matter, based on the following elementary result.

(6.32)

Lemma: *For any $x_1, \ldots, x_N \in \mathbb{R}^3$, and for any cube $Q \subset \mathbb{R}^3$ of side δ, we have*

$$\sum_{y_k \in Q} \iint_{\substack{B(z,R) \ni y_k \\ \frac{\delta}{20} < R < \frac{\delta}{10}}} \frac{\Omega_{zR}}{M_{zR}} \frac{dz dR}{R^5} \geq -\frac{CZ^2}{\delta} \mathcal{M}_Q + \frac{cZ^2}{\delta} \mathcal{M}_Q^2 \, \chi_{\mathcal{M}_Q > \frac{C}{Z} \mathcal{N}_{Q^*} + C}$$

Proof: If $\mathcal{M}_Q \leq \frac{C}{Z} \mathcal{N}_{Q^*} + C$, then the right side of (6.32) is simply $-\frac{CZ^2}{\delta} \mathcal{M}_Q$, and (6.32) follows trivially from (2.1). Hence, we may assume that $\mathcal{M}_Q > \frac{C}{Z} \mathcal{N}_{Q^*} + C$. We subdivide Q into subcubes $\{Q_\nu\}$ of side $\frac{\delta}{100}$. By the pigeonhole principle, there is some Q_{ν_0} for which

$$\mathcal{M}_{Q_{\nu_0}} \geq 10^{-6} \mathcal{M}_Q \geq (10^{-6} C) Z^{-1} \mathcal{N}_{Q^*} + (10^{-6} C). \tag{6.33}$$

If $B(z, R)$ satisfies $Q_{\nu_0} \subset B(z, R) \subset Q^*$, then (6.33) implies $M_{zR} \geq (10^{-6}C) Z^{-1} N_{zR} + (10^{-6}C)$. If C is large, then it follows that $\Omega_{zR} \geq \frac{1}{2} Z^2 M_{zR}^2 - 2Z \, N_{zR} \, M_{zR} \geq \frac{1}{4} Z^2 \, M_{zR}^2$, so that

$$\frac{\Omega_{zR}}{M_{zR}} \geq \frac{1}{4} Z^2 \, M_{zR} \geq c \, Z^2 \, \mathcal{M}_Q, \text{ by another application of (6.33).} \tag{6.34}$$

Using (6.34) when $Q_{\nu_0} \subset B(z, R) \subset Q^*$, and (2.1) otherwise, we obtain easily that

$$\iint_{\substack{B(z,R) \ni y_k \\ \frac{\delta}{20} < R < \frac{\delta}{10}}} \frac{\Omega_{zR}}{M_{zR}} \frac{dz dR}{R^5} \geq \left[\begin{array}{ll} c \frac{Z^2}{\delta} \mathcal{M}_Q - \frac{CZ^2}{\delta} & \text{if } \; y_k \in Q_{\nu_0} \\ - \frac{CZ^2}{\delta} & \text{if } \; y_k \notin Q_{\nu_0} \end{array} \right.$$

Therefore,

$$\sum_{y_k \in Q} \iint_{\substack{B(z,R) \ni y_k \\ \frac{\delta}{20} < R < \frac{\delta}{10}}} \frac{\Omega_{zR}}{M_{zR}} \frac{dzdR}{R^5} \geq -\frac{CZ^2}{\delta} \mathcal{M}_Q + \frac{cZ^2}{\delta} \mathcal{M}_Q \mathcal{M}_{Q_{\nu_0}}.$$

This implies the conclusion of (6.32), by virtue of (6.33). ■

We are ready to give the second main result of this section.

(6.35)

Local Stability with Bounded Magnetic Field: Let $A(x)$ be a vector potential, and let $Q \subset \mathbb{R}^3$ be a cube of side δ.

Assume that

(6.36) $$|\nabla A(x)| \leq C B_0 \, \delta^{-2} \quad \text{on } Q^*.$$

Then for every antisymmetric $\psi \in L^2(\mathbb{R}^{3N}, (\mathbb{C})^{\otimes N})$ of norm 1, we have

(6.37) $$C' B_0^{-1/2} Z\delta \cdot T(\psi, A, \frac{3}{2} Q) + PE(\psi, Q) \geq$$

$$-\frac{C'Z}{\delta} B_0^{1/2} \langle \mathcal{N}_{Q^*}\psi, \psi\rangle - \frac{C'Z^2}{\delta} B_0^{1/2} \mathcal{M}_Q + \frac{cZ^2}{\delta} \mathcal{M}_Q^2 \left\langle \chi_{\mathcal{M}_Q > \frac{C}{Z} \mathcal{N}_{Q^*} + C} \, \psi, \psi \right\rangle$$

Proof: Subdivide Q into subcubes $\{Q_\nu\}$ of side $\tilde{\delta}$, where

(6.38) $$\frac{1}{2} B_0^{-1/2} \delta \leq \tilde{\delta} \leq B_0^{-1/2} \delta.$$

Let x_ν be the center of Q_ν, and let $A^\nu = A(x_\nu)$. Then (6.36) and (6.38) yield

$|A(x) - A^\nu| \leq C' B_0 \, \delta^{-2} \, \tilde{\delta} \leq C' B_0^{1/2} \delta^{-1}$ for $x \in Q_\nu^*$. Hence, for $x_k \in Q_\nu^*$, we have

$|(i\nabla_{x_k} - A(x_k)) \psi|^2 \geq \frac{1}{2} |(i\nabla_{x_k} - A^\nu) \psi|^2 - C' B_0 \, \delta^{-2} |\psi|^2.$

Integrating over all $(x_1 \ldots x_N) \in \mathbb{R}^{3N}$ with $x_k \in Q_\nu^*$, and then summing on k, we obtain

$$(6.39) \qquad T(\psi, A, Q_\nu^*) \geq \frac{1}{2} T(\psi, A^\nu, Q_\nu^*) - C' B_0 \, \delta^{-2} \left\langle \mathcal{N}_{Q_\nu^*} \psi, \psi \right\rangle .$$

Summing on ν, and noting that $T(\psi, A, \frac{3}{2} Q) \geq c \sum_\nu T(\psi, A, Q_\nu^*)$, we find that

$$(6.40) \quad C' B_0^{-1/2} Z\delta \cdot T(\psi, A, \frac{3}{2} Q) \geq \sum_\nu Z\tilde{\delta} \cdot T(\psi, A^\nu, Q_\nu^*) - \frac{C'Z}{\delta} B_0^{1/2} \langle \mathcal{N}_{Q^*} \psi, \psi \rangle .$$

We turn to the potential energy. Lemma (6.32) and (2.1) show that

$$\begin{aligned} PE(\psi, Q) &= \sum_\nu PE(\psi, Q_\nu) + \left\langle \frac{1}{2\pi} \sum_{y_k \in Q} \iint_{\substack{B(z,R) \ni y_k \\ \frac{\tilde{\delta}}{10} < R < \frac{\delta}{10}}} \frac{\Omega_{zR}}{M_{zR}} \frac{dz dR}{R^5} \psi, \psi \right\rangle \\ &\geq \sum_\nu PE(\psi, Q_\nu) - \frac{C'Z^2}{\delta} B_0^{1/2} \mathcal{M}_Q + \frac{cZ^2}{\delta} \mathcal{M}_Q^2 \left\langle \chi_{\mathcal{M}_Q > \frac{C}{Z} \mathcal{N}_{Q^*} + C} \psi, \psi \right\rangle . \end{aligned}$$

Combining this with (6.40), we obtain

$$\begin{aligned} (6.41) \quad & C' B_0^{-1/2} Z\delta \cdot T(\psi, A, \frac{3}{2} Q) + PE(\psi, Q) \geq \\ & \sum_\nu \{ Z\tilde{\delta} \cdot T(\psi, A^\nu, Q_\nu^*) + PE(\psi, Q_\nu) \} \\ & - \frac{C'}{\delta} Z B_0^{1/2} \langle \mathcal{N}_{Q^*} \psi, \psi \rangle - \frac{C'}{\delta} Z^2 B_0^{1/2} \mathcal{M}_Q + \frac{cZ^2}{\delta} \mathcal{M}_Q^2 \left\langle \chi_{\mathcal{M}_Q > \frac{C}{Z} \mathcal{N}_{Q^*} + C} \psi, \psi \right\rangle . \end{aligned}$$

Local Stability of Matter (6.1) shows that

$$\sum_\nu \{ Z \tilde{\delta} \cdot T(\psi, A^\nu, Q_\nu^*) + PE(\psi, Q_\nu) \} \geq$$

$$- C' \sum_{\nu} \left\{ \frac{Z}{\delta} B_0^{1/2} \mathcal{M}_{Q_\nu} + \frac{Z}{\delta} B_0^{1/2} \left\langle \mathcal{N}_{Q_\nu^*} \psi, \psi \right\rangle \right\} \quad \text{(see (6.38))}$$

$$\geq - \frac{C'Z}{\delta} B_0^{1/2} \mathcal{M}_Q - \frac{C'Z}{\delta} B_0^{1/2} \left\langle \mathcal{N}_{Q^*} \psi, \psi \right\rangle .$$

Putting this into the right-hand side of (6.41), we obtain the desired conclusion (6.37). ■

7 Local Pauli Stability

In this section, we prove a version of Local Stability of Matter, in which the Pauli kinetic energy appears in place of the Schrödinger kinetic energy.

Our result is as follows:

(7.1)

<u>Local Pauli Stability:</u> Let $Q \subset \mathbb{R}^3$ be a cube of side δ, and let $A(x)$ be a vector potential. Suppose $B(x) = \operatorname{curl} A$ satisfies

$$\int_{Q^{**}} |B(x)|^2 \, dx \leq C \, B_0^2 \, \delta^{-1}, \text{ and} \tag{7.2}$$

$$\int_{Q^{**}} |B(x) - Av_{Q^{**}} B|^2 \, dx \leq C \, K^{-2} \, B_0^{-1/3} \, \delta^{-1}. \tag{7.3}$$

Then there exists a potential $W_2(x)$, supported in Q^*, with the following properties:

$$\int_{Q^*} |W_2(x)|^3 \, dx \leq C' \, K^{-6} \, B_0^{-1}. \tag{7.4}$$

(7.5)

For any antisymmetric $\psi \in L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N})$ of norm 1, we have

$$C' B_0^{-1/2} Z\delta \cdot T_{\text{Pauli}}(\psi, A, Q^*) + PE(\psi, Q) \geq$$

$$- \frac{C'}{\delta} Z B_0^{1/2} \langle \mathcal{N}_{Q^*} \psi, \psi \rangle - \frac{C''}{\delta} Z^2 B_0^{1/2} \mathcal{M}_Q$$

$$- C' B_0^{-1/2} \left\langle \sum_{k=1}^{N} Z W_2(x_k) \psi, \psi \right\rangle + \frac{c}{\delta} Z^2 \mathcal{M}_Q^2 \left\langle \chi_{\mathcal{M}_Q > \frac{C}{Z} \mathcal{N}_{Q^*} + C} \psi, \psi \right\rangle$$

Proof: We apply the Vector Potential Splitting Lemma (5.1), rescaled from the unit cube to Q. Thus, on Q^* we may express A in the form

$$A = \tilde{A} + A^{\#} + \nabla f, \text{ with } \tilde{A} \text{ linear,} \tag{7.6}$$

$$|\nabla \tilde{A}| \leq C' B_0 \delta^{-2}, \text{ and} \tag{7.7}$$

$$\int_{Q^*} |A^{\#}|^6 \, dx \leq C' K^{-6} B_0^{-1} \delta^{-3}. \tag{7.8}$$

Since $|\sigma^{(k)} \cdot \left(i\nabla_{x_k} - \left[\tilde{A}(x_k) + A^{\#}(x_k)\right]\right) \psi|^2 \geq$

$\frac{1}{2} |\sigma^{(k)} \cdot \left(i\nabla_{x_k} - \tilde{A}(x_k)\right) \psi|^2 - |A^{\#}(x_k)|^2 |\psi|^2$, we have

$$T_{\text{Pauli}}(\psi, \tilde{A} + A^{\#}, Q^*) \geq \frac{1}{2} T_{\text{Pauli}}(\psi, \tilde{A}, Q^*) - \left\langle \sum_{k=1}^{N} |A^{\#}(x_k)|^2 \chi_{Q^*}(x_k) \psi, \psi \right\rangle. \tag{7.9}$$

In view of (7.7), we may apply the Comparison Lemma (3.1), to conclude that

$$T_{\text{Pauli}}(\psi, \tilde{A}, Q^*) \geq \frac{1}{2} T\left(\psi, \tilde{A}, \frac{3}{2} Q\right) - C' B_0 \delta^{-2} \langle \mathcal{N}_{Q^*} \psi, \psi \rangle.$$

Combining this with (7.9), and setting

$$W_2(x) \;=\; |A^{\#}(x)|^2\, \chi_{Q^*}(x)\;\cdot\;\delta, \;\;\text{we obtain} \tag{7.10}$$

$$\begin{aligned} C''\, B_0^{-1/2}\, Z\delta\;\cdot\; T_{\text{Pauli}}\,(\psi, \tilde{A}\;+\;A^{\#}, Q^*) \;\;&\geq\;\; C'\, B_0^{-1/2}\, Z\delta\;\cdot\; T\,(\psi, \tilde{A}, \frac{3}{2}Q) \\ &-\;\; \frac{C''}{\delta}\, B_0^{1/2}\, Z\,\langle \mathcal{N}_{Q^*}\,\psi, \psi\rangle \\ &-\;\; C'\, B_0^{-1/2}\, Z\left\langle \sum_{k=1}^{N} W_2(x_k)\,\psi, \psi\right\rangle. \end{aligned} \tag{7.11}$$

In view of (7.7), we may apply Local Stability of Matter with Bounded Magnetic Fields (6.35) to the vector potential $\tilde{A}$. Thus,

$$\begin{aligned} &C'\, B_0^{-1/2}\, Z\delta\cdot T(\psi, \tilde{A}, \frac{3}{2}Q) \;+\; PE\,(\psi, Q)\;\geq \\ &\quad -\frac{C'}{\delta}\, ZB_0^{1/2}\;\langle \mathcal{N}_{Q^*}\,\psi, \psi\rangle \;-\; \frac{C'}{\delta}\, Z^2\, B_0^{1/2}\, \mathcal{M}_Q \;+\; \frac{c}{\delta}\, Z^2\, \mathcal{M}_Q^2\,\left\langle \chi_{\mathcal{M}_Q > \frac{C}{Z}\mathcal{N}_{Q^*}+C}\,\psi, \psi\right\rangle. \end{aligned}$$

Combining this with (7.11), we find that

$$\begin{aligned} &C''\, B_0^{-1/2}\, Z\delta\;\cdot\; T_{\text{Pauli}}\,(\psi, \tilde{A}\;+\;A^{\#}, Q^*)\;+\;PE\,(\psi, Q)\;\geq \\ &\quad -\frac{C'}{\delta}\, Z\, B_0^{1/2}\;\langle \mathcal{N}_{Q^*}\,\psi, \psi\rangle \;-\; \frac{C'}{\delta}\, Z^2\, B_0^{1/2}\, \mathcal{M}_Q \\ &\quad -C'\, B_0^{-1/2}\, Z\,\left\langle \sum_{k=1}^{N} W_2(x_k)\psi, \psi\right\rangle \;+\; \frac{c}{\delta}\, Z^2\, \mathcal{M}_Q^2\,\left\langle \chi_{\mathcal{M}_Q > \frac{C}{Z}\mathcal{N}_{Q^*}+C}\,\psi, \psi\right\rangle. \end{aligned} \tag{7.12}$$

Since $\tilde{A}+A^{\#}$ is gauge-equivalent to A (see (7.6)), estimate (7.12) is equivalent to conclusion (7.5) of Local Pauli Stability. It remains to check (7.4). However, (7.4) follows at once from (7.8) and (7.10). ■

8 The Calderón-Zygmund Decomposition

In this section, we decompose $\mathbb{R}^3$ into cubes $\{Q_\nu\}$ in a manner determined by the magnetic field $B(x)$, and we relate the geometry of the cubes to the energy and smoothness of the field. We start by subdividing $\mathbb{R}^3$ into a grid of cubes $\{Q_\alpha^0\}$ of length L. Here, $L > 0$ is given. We define

$$B_L^\#(x) = \left(\sum_{4Q_\alpha^0 \ni x} |B(x) - Av_{4Q_\alpha^0} B|^2 \right)^{1/2} . \tag{8.1}$$

We say that a cube $Q \subset \mathbb{R}^3$ of side δ is <u>tame</u> if it satisfies

$$\int_{C_1 Q} \left\{ |B(x)|^2 + K^2 B_0^{7/3} |B_L^\#(x)|^2 \right\} dx \leq B_0^2 \delta^{-1}. \tag{8.2}$$

Here, C_1 is a large constant, to be picked later. Our cubes $\{Q_\nu\}$ are constructed as follows. We start with the $\{Q_\alpha^0\}$. We retain each of the tame Q_α^0; and we subdivide each Q_α^0 that is not tame into subcubes of length $L/2$. Thus, we obtain a family $\{Q_\alpha^1\}$ of cubes of side $L/2$. We retain each of the tame $\{Q_\alpha^1\}$; and we subdivide each Q_α^1 that is not tame into subcubes of side $L/4$. Thus, we obtain a family $\{Q_\alpha^2\}$ of cubes of side $L/4$. We retain each of the tame Q_α^2; and we subdivide each Q_α^2 that is not tame. We continue in this way, obtaining at stage m a family $\{Q_\alpha^m\}$ of cubes of side $L/2^m$. Our Calderón-Zygmund family $\{Q_\nu\}$ consists of all the cubes retained at all stages of the above construction. We say that a cube Q is <u>dyadic</u> if it arises from a Q_α^0 by successive bisections. Thus, all the Q_ν are dyadic.

Let δ_ν be the side of Q_ν. We can immediately draw some simple conclusions about the Q_ν. First of all, Q_ν is tame, so we have

$$\int_{C_1 Q_\nu} \left\{ |B(x)|^2 + K^2 B_0^{7/3} |B_L^\#(x)|^2 \right\} dx \leq B_0^2 \delta_\nu^{-1}. \tag{8.3}$$

In particular,

(8.4) $$\int_{Q_\nu^{**}} |B(x)|^2\, dx \;\le\; B_0^2\, \delta_\nu^{-1}.$$

Also, Q_ν is contained in some Q_α^0, for which we have

$Q_\nu^{**} \;=\; 4Q_\nu \,\subset\, 4Q_\alpha^0$, and therefore $|B(x) \,-\, Av_{4Q_\alpha^0}\, B| \;\le\; B_L^{\#}(x)$

for $x \in Q_\nu^{**}$. It follows that

$K^2\, B_0^{7/3} \int_{Q_\nu^{**}} |B(x) \,-\, Av_{4Q_\alpha^0}\, B|^2\, dx \;\le\; B_0^2\, \delta_\nu^{-1}$, by (8.3). Hence,

(8.5) $$\int_{Q_\nu^{**}} |B(x) \,-\, Av_{Q_\nu^{**}}\, B|^2\, dx \;\le\; \int_{Q_\nu^{**}} |B(x) \,-\, Av_{4Q_\alpha^0}\, B|^2\, dx \;\le\; K^{-2}\, B_0^{-1/3}\, \delta_\nu^{-1}.$$

Suppose $\delta_\nu \,<\, L$. Then Q_ν arises by subdividing a "dyadic parent" cube Q_ν^+ of side $2\delta_\nu$. Since Q_ν^+ is subdivided, it is not tame. Therefore, since $Q_\nu^+ \subset 3Q_\nu$, we have

(8.6) $$\int_{3C_1 Q_\nu} \left\{|B(x)|^2 \,+\, K^2\, B_0^{7/3} |B_L^{\#}(x)|^2\right\}\, dx \;\ge\; \frac{1}{2} B_0^2\, \delta_\nu^{-1}, \;\text{ if }\; \delta_\nu < L.$$

Next, we check that the $\{Q_\nu\}$ form a decomposition of $\mathbb{R}^3$. It is clear that distinct Q_ν are pairwise disjoint. We check that the union of the Q_ν is all of $\mathbb{R}^3$. In fact, we have the following stronger result.

(8.7)

Each of the Q_α^0 (of side L) is a union of finitely many of the Q_ν.

To see this, we just note that any cube $Q \subset Q_\alpha^0$, whose side δ is so small that

$$\int_{C_1 Q_\alpha^0} \left\{|B(x)|^2 \,+\, K^2\, B_0^{7/3}\, |B_L^{\#}(x)|^2\right\}\, dx \;\le\; B_0^2\, \delta^{-1},$$

is automatically tame.

We want to understand the geometry of the $Q_{\nu'}$, near a given Q_ν.

(8.8)

Lemma: *If C_1 in (8.2) is taken larger than some universal constant, then $Q^*_\nu \cap Q^*_{\nu'} \neq \phi$ implies $\frac{1}{2}\,\delta_\nu \leq \delta_{\nu'} \leq 2\delta_\nu$.*

Proof: Suppose not. After possibly interchanging ν and ν', we may assume that $\delta_\nu < \frac{1}{2}\,\delta_{\nu'}$. Since δ_ν, $\delta_{\nu'}$ have the form $2^{-m}L$, it follows that $\delta_\nu \leq \frac{1}{4}\,\delta_{\nu'}$. In particular, $\delta_\nu < L$, so Q_ν arises by subdividing a dyadic parent Q^+_ν. Thus, we have

$$(Q^+_\nu)^* \cap Q^*_{\nu'} \neq \phi, \text{ and side } (Q^+_\nu) \leq \frac{1}{2} \text{ side } (Q_{\nu'}). \tag{8.9}$$

If C_1 exceeds a large universal constant, then (8.9) implies $C_1\,Q^+_\nu \subset C_1 Q_{\nu'}$. Therefore, Q^+_ν is tame, since $Q_{\nu'}$ is tame.

The tameness of Q^+_ν contradicts the fact that we subdivide it to produce Q_ν. ■

¿From now on, we fix C_1 to be a universal constant, large enough so that Lemma (8.8) applies. An immediate consequence of Lemma (8.8) is as follows.

(8.10)

Corollary: *If $Q_{\nu'}$ meets $3C_1Q_\nu$, then $\delta_{\nu'} \leq C_2\delta_\nu$ for a universal constant C_2.*

Proof: Suppose not. If we take C_2 large enough, then

$Q_{\nu'} \cap 3C_1Q_\nu \neq \phi$ and $\delta_{\nu'} > C_2\delta_\nu$ imply $Q_\nu \subset Q^*_{\nu'}$.

Hence, $Q^*_\nu \cap Q^*_{\nu'} \neq \phi$ with $\delta_{\nu'} > C_2\delta_\nu$, contradicting Lemma (8.8). ■

Note that $3C_1Q_\nu$ may meet $Q_{\nu'}$ with $\delta_{\nu'} \ll \delta_\nu$.

We now bring in the nuclei $y_1, y_2 \ldots y_M \in \mathbb{R}^3$. For $x \in \mathbb{R}^3$, we set

$$D(x) = \min\{|x - y_k| : 1 \leq k \leq M\}, \text{ and define} \tag{8.11}$$

(8.12)
$$\theta_\nu = \max\left\{\exp\left(-\frac{D(x)}{L}\right) : x \in Q_\nu\right\}.$$

Since the Q_ν have sides $\delta_\nu \leq L$, it follows that

(8.13)
$$c\theta_\nu \leq \exp\left(-\frac{D(x)}{L}\right) \leq \theta_\nu \text{ for all } x \in Q_\nu, \text{ and}$$

(8.14) $CQ^*_\nu \cap CQ^*_{\nu'} \neq \phi$ implies $c'\theta_\nu \leq \theta_{\nu'} \leq C'\theta_\nu$, with c', C' depending only on C.

A second consequence of Lemma (8.8) is as follows.

Corollary: *We have*

(8.15)
$$\sum_\nu \theta_\nu\, \delta_\nu\, \chi_{Q^*_\nu} \leq C \sum_\nu \theta_\nu\, \delta_\nu\, \chi_{Q_\nu}, \text{ and}$$

(8.16)
$$\sum_\nu \theta_\nu\, \delta_\nu^{-1}\, \chi_{Q^*_\nu} \leq C \sum_\nu \theta_\nu\, \delta_\nu^{-1}\, \chi_{Q_\nu}.$$

These estimates are immediate from (8.8) and (8.14).

We shall need an upper bound for $\sum_\nu \theta_\nu \delta_\nu^{-1}$. As a first step, we prove the following geometrical result.

(8.17)

Lemma: *Given any Q_ν, there exists a $Q_{\nu'}$ with the properties*

(8.18)
$$C_3\, Q_{\nu'} \subseteq C_3\, Q_\nu, \text{ and}$$

(8.19)
$$\textit{If } Q_{\nu''} \textit{ meets } 3C_1\, Q_{\nu'}, \textit{ then } \delta_{\nu''} \geq \delta_{\nu'}.$$

Proof: Let C_3 be a large enough universal constant, and impose a partial order on the $\{Q_\nu\}$ by saying that $Q_\nu \le Q_{\nu'}$ if $C_3 Q_\nu \subseteq C_3 Q_{\nu'}$. Observation (8.7) rules out infinite descending chains of Q_ν. Hence, there must exist some $Q_{\nu'} \le Q_\nu$ which is minimal, in the sense that $Q_{\nu''} \le Q_{\nu'}$ implies $Q_{\nu''} = Q_{\nu'}$. Evidently, $Q_{\nu'}$ satisfies (8.18). We will check that it also satisfies (8.19). If not, then some $Q_{\nu''}$ would satisfy

(8.20) $$Q_{\nu''} \cap 3C_1 Q_{\nu'} \ne \phi, \quad \delta_{\nu''} \le \frac{1}{2}\delta_{\nu'}.$$

If C_3 is a large enough universal constant, then (8.20) implies $C_3 Q_{\nu''} \subset C_3 Q_{\nu'}$. That is, $Q_{\nu''} \le Q_{\nu'}$. Since $\delta_{\nu''} \le \frac{1}{2}\delta_{\nu'}$, this contradicts the minimality of $Q_{\nu'}$. Thus, (8.19) holds, and the proof of the Lemma is complete. ■

Define

(8.21) $$S = \{\nu : \text{ Any } Q_{\nu'} \text{ that meets } 3C_1 Q_\nu \text{ must satisfy } \delta_\nu \le \delta_{\nu'} \le C_2 \delta_\nu\},$$

and

(8.22) $$\mathcal{S} = \{(\nu, \nu') : C_3 Q_{\nu'} \subseteq C_3 Q_\nu \text{ and } \nu' \in S\}.$$

Lemma (8.17) and Corollary (8.10) imply

(8.23)

For every Q_ν there is some $Q_{\nu'}$ with $(\nu, \nu') \in \mathcal{S}$.

Also, (8.14) implies

(8.24) $$c\theta_\nu \le \theta_{\nu'} \le C\theta_\nu \text{ whenever } (\nu, \nu') \in \mathcal{S}.$$

In addition, for each fixed $\nu' \in \mathcal{S}$, we have

(8.25)
$$\sum_{(\nu,\nu')\in\mathcal{S}} \delta_\nu^{-1} \le \sum_{\substack{Q \text{ dyadic cube} \\ C_3Q\supseteq C_3Q_{\nu'}}} (\text{side } Q)^{-1} \le C\,\delta_{\nu'}^{-1}.$$

¿From (8.23), (8.24), (8.25), we obtain the inequalities

(8.26)
$$\begin{aligned}\sum_\nu \theta_\nu\,\delta_\nu^{-1} &\le \sum_{(\nu,\nu')\in\mathcal{S}} \theta_\nu\,\delta_\nu^{-1} \le C \sum_{(\nu,\nu')\in\mathcal{S}} \theta_{\nu'}\,\delta_\nu^{-1} \\ &= C\sum_{\nu'\in S}\theta_{\nu'}\left[\sum_{(\nu,\nu')\in\mathcal{S}} \delta_\nu^{-1}\right] \le C'\sum_{\nu'\in S}\theta_{\nu'}\,\delta_{\nu'}^{-1}.\end{aligned}$$

Thus, to control $\sum_\nu \theta_\nu\,\delta_\nu^{-1}$, we may restrict the sum to $\nu\in\mathcal{S}$. To bound the right hand side of (8.26), we use the following simple observation.

(8.27)

Lemma: *Suppose $\nu\in S$ and $\delta_\nu < L$. Then, for some $Q_{\nu'}$ that meets $3C_1Q_\nu$, we have*

(8.28)
$$\int_{Q_{\nu'}} \left\{|B(x)|^2 + K^2\,B_0^{7/3}\,|B_L^\#(x)|^2\right\} dx \ge cB_0^2\,\delta_{\nu'}^{-1}.$$

Proof: Since $\delta_\nu < L$, (8.6) yields

(8.29)
$$\sum_{\nu'}\int_{Q_{\nu'}} \left\{|B(x)|^2 + K^2\,B_0^{7/3}|B_L^\#(x)|^2\right\} dx \ge \frac{1}{2}\,B_0^2\,\delta_\nu^{-1}.$$

where the sum is taken over all ν' for which $Q_{\nu'}\cap 3C_1Q_\nu \ne \phi$.

Since $\nu\in S$, we have $\delta_\nu \le \delta_{\nu'} \le C_2\delta_\nu$ for each ν' in (8.29). Hence, there are at most C summands in (8.29), so that, for some $Q_{\nu'}$ that meets $3C_1Q_\nu$, we have

(8.30)
$$\int_{Q_{\nu'}} \left\{|B(x)|^2 + K^2\,B_0^{7/3}\,|B_L^\#(x)|^2\right\} dx \ge cB_0^2\,\delta_\nu^{-1}.$$

Again using the fact that $\delta_\nu \le \delta_{\nu'} \le C_2\delta_\nu$, we see that (8.30) implies (8.28). ∎

Now define

$$P = \left\{\nu : \int\limits_{Q_\nu} \left\{|B(x)|^2 + K^2 B_0^{7/3}|B_L^{\#}(x)|^2\right\} dx \ge cB_0^2\,\delta_\nu^{-1}\right\}, \text{ and set}$$

$$\mathcal{A} = \{(\nu,\nu') : \nu \in S, \delta_\nu < L,\ Q_{\nu'} \cap 3C_1Q_\nu \ne \phi,\ \text{ and } \nu' \in P\}.$$

Then Lemma (8.27) says that for any $\nu \in \mathcal{S}$ with $\delta_\nu < L$, there exists a ν' with $(\nu,\nu') \in \mathcal{A}$. Note also that $(\nu,\nu') \in \mathcal{A}$ implies $c\theta_\nu \le \theta_{\nu'} \le C\theta_\nu$, by (8.14); and $\delta_\nu \le \delta_{\nu'} \le C_2\delta_\nu$, since $\nu \in S$. In particular, given any ν', there are at most C distinct ν for which $(\nu,\nu') \in \mathcal{A}$. These remarks show that

$$\sum_{\substack{\nu\in S\\ \delta_\nu<L}} \theta_\nu\,\delta_\nu^{-1} \le \sum_{(\nu,\nu')\in\mathcal{A}} \theta_\nu\,\delta_\nu^{-1} \le C \sum_{(\nu,\nu')\in\mathcal{A}} \theta_{\nu'}\,\delta_{\nu'}^{-1} \le C' \sum_{\nu'\in P} \theta_{\nu'}\,\delta_{\nu'}^{-1}.$$

Combining this with (8.26), we obtain

$$\sum_{\nu} \theta_\nu\,\delta_\nu^{-1} \le C \sum_{\delta_\nu = L} \theta_\nu\,\delta_\nu^{-1} + C \sum_{\nu\in P} \theta_\nu\delta_\nu^{-1}. \tag{8.31}$$

The sums on the right in (8.31) are easy to control.

In fact, $\nu \in P$ implies

$$\delta_\nu^{-1} \le C\,B_0^{-2} \int\limits_{Q_\nu} |B(x)|^2\,dx + C\,K^2\,B_0^{+1/3} \int\limits_{Q_\nu} |B_L^{\#}(x)|^2\,dx,$$

and (8.13) yields

$$\theta_\nu \le C \min_{x\in Q_\nu} e^{-D(x)/L}. \quad \text{Therefore,}$$

$$\theta_\nu\,\delta_\nu^{-1} \le C\,B_0^{-2} \int\limits_{Q_\nu} e^{-D(x)/L}\,|B(x)|^2\,dx + C\,K^2\,B_0^{1/3} \int\limits_{Q_\nu} e^{-D(x)/L}|B_L^{\#}(x)|^2\,dx.$$

Summing over ν, we obtain

$$(8.32)\quad \sum_{\nu\in P} \theta_\nu\,\delta_\nu^{-1} \,\le\, C\,B_0^{-2}\int_{\mathbb{R}^3} e^{-\frac{D(x)}{L}}\,|B(x)|^2\,dx \,+\, C\,K^2\,B_0^{1/3}\int_{\mathbb{R}^3} e^{-\frac{D(x)}{L}}\,|B_L^{\#}(x)|^2\,dx.$$

On the other hand, when $\delta_\nu = L$, then (8.11) and (8.13) yield

$$\theta_\nu\,\delta_\nu^{-1} \,=\, \theta_\nu L^{-1} \,\le\, C\,L^{-4}\int_{Q_\nu} e^{-\frac{D(x)}{L}}\,dx \,\le\, C\,L^{-4}\int_{Q_\nu}\sum_{k=1}^{M} e^{-|x-y_k|/L}\,dx.$$

Summing over ν, we obtain the estimates

$$(8.33)\qquad \sum_{\delta_\nu=L} \theta_\nu\,\delta_\nu^{-1} \,\le\, C\,L^{-4}\sum_{k=1}^{M}\int_{\mathbb{R}^3} e^{-|x-y_k|/L}\,dx \,\le\, \frac{C'}{L}\,M.$$

Putting (8.32) and (8.33) into (8.31), we find that

$$(8.34)\quad \sum_{\nu} \theta_\nu\,\delta_\nu^{-1} \,\le$$

$$C\,B_0^{-2}\int_{\mathbb{R}^3} e^{-D(x)/L}\,|B(x)|^2\,dx \,+\, C\,K^2\,B_0^{1/3}\int_{\mathbb{R}^3} e^{-D(x)/L}\,|B_L^{\#}(x)|^2\,dx \,+\, \frac{C}{L}\,M.$$

Thus, we have succeeded in estimating $\sum_\nu \theta_\nu\,\delta_\nu^{-1}$. We can tidy up the right-hand side of (8.34) as follows. Note that

$$(8.35)\qquad \int_{\mathbb{R}^3} e^{-D(x)/L}\,|B_L^{\#}(x)|^2\,dx \,=\, \sum_\alpha \int_{4Q_\alpha^0} e^{-D(x)/L}\,|B(x) \,-\, Av_{4Q_\alpha^0}\,B|^2\,dx,$$

by definition (8.1) of $B_L^{\#}$.

For any $x, y \in 4Q_\alpha^0$, we have $e^{-D(x)/L} \,\le\, Ce^{-D(y)/L}$.

Therefore, for any $y \in Q_\alpha^0$, we have

$$\begin{aligned}
(8.36)\qquad & \int_{4Q^0_\alpha} e^{-D(x)/L}\,|B(x)\,-\,Av_{4Q^0_\alpha}\,B|^2\,dx \,\le \\
& C\,e^{-D(y)/L}\int_{4Q^0_\alpha} |B(x)\,-\,Av_{4Q^0_\alpha}\,B|^2\,dx \,\le \\
& C\,e^{-D(y)/L}\int_{4Q^0_\alpha} |B(x)\,-\,Av_{|z-y|<\bar{C}L}\,B(z)|^2\,dx \,\le \\
& C\,e^{-D(y)/L}\int_{|x-y|<\bar{C}L} |B(x)\,-\,Av_{|z-y|<\bar{C}L}\,B(z)|^2\,dx,
\end{aligned}$$

provided we take $\bar{C}$ to be a universal constant, so large that $y \in Q^0_\alpha$ implies $4Q^0_\alpha \subset \{z \in \mathbb{R}^3 : |z-y| < \bar{C}L\}$.

Averaging (8.36) over all $y \in Q^0_\alpha$, we obtain

$$\begin{aligned}
(8.37)\qquad & \int_{4Q^0_\alpha} e^{-D(x)/L}\,|B(x)\,-\,Av_{4Q^0_\alpha}\,B|^2\,dx \,\le \\
& C\int_{Q^0_\alpha} e^{-D(y)/L}\,\{L^{-3}\int_{|x-y|<\bar{C}L} |B(x)\,-\,Av_{|z-y|<\bar{C}L}\,B(z)|^2\,dx\}\,dy.
\end{aligned}$$

Summing (8.37) over α, and substituting in (8.35), we find that

$$\int_{\mathbb{R}^3} e^{-D(x)/L}\,|B^{\#}_L(x)|^2\,dx \,\le\, C\int_{\mathbb{R}^3} e^{-D(y)/L}\left\{L^{-3}\int_{|x-y|<\bar{C}L} |B(x)\,-\,Av_{|z-y|<\bar{C}L}\,B(z)|^2\,dx\right\}dy.$$

Putting this into (8.34), we obtain our basic bound for $\sum_\nu \theta_\nu \, \delta_\nu^{-1}$, namely

$$(8.38)\quad \sum_\nu \theta_\nu \, \delta_\nu^{-1} \le$$

$$\frac{C}{L} M + C\, B_0^{-2} \int_{\mathbb{R}^3} e^{-D(x)/L} \, |B(x)|^2 \, dx$$

$$+ C\, K^2 \, B_0^{1/3} \int_{\mathbb{R}^3} e^{-D(y)/L} \left\{ L^{-3} \int_{|x-y|<\bar{C}L} |B(x) \, - Av_{|z-y|<\bar{C}L} \, B(z)|^2 \, dx \right\} dy.$$

We summarize the results of this section in the following lemma.

(8.39)

Calderón-Zygmund Lemma: *Given a length $L > 0$ and a magnetic field $B(x)$, we can partition $\mathbb{R}^3$ into cubes $\{Q_\nu\}$, with sides δ_ν, so that the following properties hold.*

$$(8.40)\qquad \delta_\nu \le L.$$

$$(8.41)\qquad \int_{Q_\nu^{**}} |B(x)|^2 \, dx \le B_0^2 \, \delta_\nu^{-1}.$$

$$(8.42)\qquad \int_{Q_\nu^{**}} |B(x) \, - Av_{Q_\nu^{**}} \, B|^2 \, dx \le K^{-2} \, B_0^{-1/3} \, \delta_\nu^{-1}.$$

$$(8.43)\qquad \text{If } Q_\nu^* \cap Q_{\nu'}^* \ne \phi, \text{ then } \frac{1}{2} \delta_\nu \le \delta_{\nu'} \le 2\delta_\nu.$$

Moreover, let $y_1, y_2, \ldots, y_M \in \mathbb{R}^3$ be given. Define

$D(x) = \min\{|x - y_k| : 1 \le k \le M\}$ for $x \in \mathbb{R}^3$, and set $\theta_\nu = \max\{e^{-D(x)/L} : x \in Q_\nu\}$.

Then we have

$$\sum_\nu \theta_\nu\, \delta_\nu\, \chi_{Q_\nu^*} \;\le\; C \sum_\nu \theta_\nu\, \delta_\nu\, \chi_{Q_\nu}, \tag{8.44}$$

$$\sum_\nu \theta_\nu\, \delta_\nu^{-1}\, \chi_{Q_\nu^*} \;\le\; C \sum_\nu \theta_\nu\, \delta_\nu^{-1}\, \chi_{Q_\nu}, \;\text{ and} \tag{8.45}$$

$$\begin{aligned} \sum_\nu \theta_\nu\, \delta_\nu^{-1} \;\le\; & \\ & C\, M\, L^{-1} \,+\, C\, B_0^{-2} \int_{\mathbb{R}^3} e^{-D(x)/L}\, |B(x)|^2\, dx \\ & + C\, K^2\, B_0^{1/3} \int_{\mathbb{R}^3} e^{-D(x)/L} \left\{ L^{-3} \int_{B(x,\bar{C}L)} |B(y) \,-\, Av_{B(x,\bar{C}L)}\, B|^2\, dy \right\} dx. \end{aligned} \tag{8.46}$$

9 Proof of the Main Theorem

Let $y_1, \ldots, y_M \in \mathbb{R}^3$ be the positions of nuclei of charge Z, let $A(x)$ be a vector potential with magnetic field $B(x) = \operatorname{curl} A$, and let $\psi \in L^2(\mathbb{R}^{3N}, (\mathbb{C}^2)^{\otimes N})$ be antisymmetric with norm 1.

Fix $L > 0$, and let $\{Q_\nu\}$, with sides $\{\delta_\nu\}$, be the cubes given by the Calderón-Zygmund lemma (8.39). Conclusions (8.41) and (8.42) of the Calderón-Zygmund lemma show that we may apply Local Pauli Stability (7.1) and the N-Electron Lemma (5.23) to the cubes Q_ν. Thus, we have the following results.

There exists a potential $W_{1,\nu}(x)$, supported on Q_ν^*, satisfying:

$$\int_{Q_\nu^*} |W_{1,\nu}|^3\, dx \;\le\; C\, K^{-6}\, B_0^{-1}. \tag{9.1}$$

(9.2) If V_ν is any potential, supported on Q_ν, that satisfies

$$\int_{Q_\nu} |V_\nu|^3 \, dx \;\le\; cK^{-1} B_0^{-1}, \quad \text{then} \tag{9.3}$$

$$\begin{aligned} Z B_0^{1/2} \delta_\nu \cdot T_{\text{Pauli}}(\psi, A, Q_\nu^*) \;-\; Z B_0^{1/2} \left\langle \sum_{k=1}^N V_\nu(x_k)\, \psi, \psi \right\rangle \;\ge \\ \frac{cK}{\delta_\nu} Z B_0^{1/2} \langle \mathcal{N}_{Q_\nu} \psi, \psi \rangle \;-\; \frac{C'}{\delta_\nu} Z B_0^{1/2} \left\langle \mathcal{N}_{Q_\nu^*} \psi, \psi \right\rangle \\ -\frac{C'}{\delta_\nu} K^{5/2} B_0^{3/2} Z \;-\; Z B_0^{1/2} \left\langle \sum_{k=1}^N W_{1,\nu}(x_k)\, \psi, \psi \right\rangle. \end{aligned} \tag{9.4}$$

There exists a potential $W_{2,\nu}(x)$, supported on Q_ν^*, satisfying:

$$\int_{Q_\nu^*} |W_{2,\nu}|^3 \, dx \;\le\; C\, K^{-6} B_0^{-1}. \tag{9.5}$$

$$\begin{aligned} C\, Z\, B_0^{-1/2} \delta_\nu \cdot T_{\text{Pauli}}(\psi, A, Q_\nu^*) \;+\; PE(\psi, Q_\nu) \;\ge \\ -\frac{C'}{\delta_\nu} Z B_0^{1/2} \left\langle \mathcal{N}_{Q_\nu^*} \psi, \psi \right\rangle - \frac{C'}{\delta_\nu} Z^2 B_0^{1/2} \mathcal{M}_Q \\ -C' B_0^{-1/2} Z \left\langle \sum_{k=1}^N W_{2,\nu}(x_k)\, \psi, \psi \right\rangle \;+\; \frac{c}{\delta_\nu} Z^2 \mathcal{M}_{Q_\nu}^2 \left\langle \chi_{\mathcal{M}_{Q_\nu} \ge \frac{C}{Z} \mathcal{N}_{Q_\nu^*} + C}\, \psi, \psi \right\rangle. \end{aligned} \tag{9.6}$$

Set $W_\nu(x) = W_{1,\nu}(x) \,+\, C' B_0^{-1} W_{2,\nu}(x)$. Thus, (9.1) and (9.5) yield

$$\int_{Q_\nu^*} |W_\nu|^3 \, dx \;\le\; C' K^{-6} B_0^{-1}, \tag{9.7}$$

and of course W_ν is supported on Q_ν^*.

If V_ν is supported on Q_ν and satisfies (9.3), then by adding (9.4) and (9.6), we obtain the estimate

$$(9.8) \qquad C\,Z\,B_0^{1/2}\,\delta_\nu\,\cdot\,T_{\mathrm{Pauli}}\,(\psi, A, Q_\nu^*)\;+\;PE\,(\psi, Q_\nu)\;-\;Z\,B_0^{1/2}\,\left\langle\sum_{k=1}^{N} V_\nu\,(x_k)\,\psi, \psi\right\rangle\;\geq$$

$$\frac{cK}{\delta_\nu}\,Z\,B_0^{1/2}\,\langle\mathcal{N}_{Q_\nu}\psi, \psi\rangle\;-\;\frac{C'}{\delta_\nu}\,Z\,B_0^{1/2}\,\left\langle\mathcal{N}_{Q_\nu^*}\,\psi, \psi\right\rangle$$

$$-\;\frac{C'}{\delta_\nu}\,Z^2\,B_0^{1/2}\,\mathcal{M}_{Q_\nu}\;-\;\frac{C'}{\delta_\nu}\,K^{5/2}\,B_0^{3/2}\,Z\;-\;Z\,B_0^{1/2}\left\langle\sum_{k=1}^{N}\,W_\nu\,(x_k)\,\psi,\;\psi\right\rangle$$

$$+\;\frac{c}{\delta_\nu}\,Z^2\,\mathcal{M}_{Q_\nu}^2\;\left\langle\chi_{\mathcal{M}_{Q_\nu}\,\geq\frac{C}{Z}\,\mathcal{N}_{Q_\nu^*}\,+C}\,\psi, \psi\right\rangle.$$

Our plan is to multiply (9.8) by θ_ν (from the Calderón-Zygmund lemma), and sum over ν. We have

$$(9.9) \quad C\,Z\,B_0^{1/2}\,\sum_\nu\,\theta_\nu\,\delta_\nu\,\cdot\,T_{\mathrm{Pauli}}\,(\psi, A, Q_\nu^*)\;\leq$$

$$C'\,Z\,B_0^{1/2}\,\sum_\nu\,\theta_\nu\,\delta_\nu\,\cdot\,T_{\mathrm{Pauli}}\,(\psi, A, Q_\nu)\;\;\text{(by (8.44))}$$

$$\leq\;C'\,Z\,B_0^{1/2}\,L\,\cdot\,\sum_\nu\,T_{\mathrm{Pauli}}\,(\psi, A, Q_\nu)\;\;\text{(by (8.40) and the fact that } \theta_\nu \leq 1\text{)}$$

$$=\;C'\,Z\,B_0^{1/2}\,L\,\cdot\,\sum_{k=1}^{N}\,\|\sigma^{(k)}\,\cdot\,(i\nabla_{x_k}\,-\,A(x_k))\,\psi\,\|^2.$$

To control the potential energy, we deduce from (2.1), (2.2) that

$$(9.10) \qquad \langle V_{\mathrm{Coulomb}}\,\psi,\;\psi\rangle\;\geq\;\left\langle\sum_{y_k}\,\frac{1}{2\pi}\,\iint_{B(z,R)\ni y_k}\,\left(\frac{\Omega_{zR}}{M_{zR}}\right)\,\frac{dzdR}{R^5}\,\psi, \psi\right\rangle$$

$$\text{(since } \Omega_{zR}\,\geq\,0\,\text{ if }\,M_{zR}\,=\,0\text{)}$$

$$=\;\sum_\nu\,\left\langle\frac{1}{2\pi}\,\sum_{y_k\in Q_\nu}\,\iint_{B(z,R)\ni y_k}\,\frac{\Omega_{zR}}{M_{zR}}\,\frac{dzdR}{R^5}\,\psi,\;\psi\right\rangle$$

$$\geq \sum_\nu \left\{ \left\langle \frac{1}{2\pi} \sum_{y_k \in Q_\nu} \iint_{\substack{B(z,R)\ni y_k \\ R<\frac{1}{10}\delta_\nu}} \frac{\Omega_{zR}}{M_{zR}} \frac{dz dR}{R^5} \psi, \psi \right\rangle - \frac{CZ^2}{\delta_\nu} \mathcal{M}_{Q_\nu} \right\}$$

$$= \sum_\nu PE(\psi, Q_\nu) - C Z^2 \sum_\nu \delta_\nu^{-1} \mathcal{M}_{Q_\nu}.$$

If $\mathcal{M}_{Q_\nu} \neq 0$, then $\theta_\nu = 1$ by definition. On the other hand, if $\mathcal{M}_{Q_\nu} = 0$, then $PE(\psi, Q_\nu) = 0$ by definition. It follows that (9.10) may be rewritten in the form

$$\langle V_{\text{Coulomb}} \psi, \psi \rangle \geq \sum_\nu \theta_\nu PE(\psi, Q_\nu) - C Z^2 \sum_\nu \theta_\nu \delta_\nu^{-1} \mathcal{M}_{Q_\nu}. \tag{9.11}$$

Multiplying (9.8) by θ_ν, summing on ν, and applying (9.9) and (9.11), we obtain the following inequality.

$$\begin{aligned} &C' Z B_0^{1/2} L \cdot \sum_{k=1}^N \|\sigma^{(k)} \cdot (i\nabla_{x_k} - A(x_k)) \psi\|^2 + \langle V_{\text{Coulomb}} \psi, \psi \rangle \\ &- Z B_0^{1/2} \left\langle \sum_{k=1}^N \left\{ \sum_\nu \theta_\nu V_\nu(x_k) \right\} \psi, \psi \right\rangle \geq \\ &cK Z B_0^{1/2} \left\langle \sum_\nu \theta_\nu \delta_\nu^{-1} \mathcal{N}_{Q_\nu} \psi, \psi \right\rangle - C' Z B_0^{1/2} \left\langle \sum_\nu \theta_\nu \delta_\nu^{-1} \mathcal{N}_{Q_\nu^*} \psi, \psi \right\rangle \\ &- C' Z^2 B_0^{1/2} \sum_\nu \theta_\nu \delta_\nu^{-1} \mathcal{M}_{Q_\nu} - C' K^{5/2} B_0^{3/2} Z \cdot \sum_\nu \theta_\nu \delta_\nu^{-1} \\ &- Z B_0^{1/2} \left\langle \sum_{k=1}^N \left\{ \sum_\nu \theta_\nu W_\nu(x_k) \right\} \psi, \psi \right\rangle \\ &+ cZ^2 \left\langle \sum_\nu \theta_\nu \delta_\nu^{-1} \mathcal{M}_{Q_\nu}^2 \chi_{\mathcal{M}_{Q_\nu} \geq \frac{C}{Z} \mathcal{N}_{Q_\nu^*} + C} \psi, \psi \right\rangle. \end{aligned} \tag{9.12}$$

On the right-hand side of (9.12), we want to get rid of the term $C' Z^2 B_0^{1/2} \sum_\nu \theta_\nu \delta_\nu^{-1} \mathcal{M}_{Q_\nu}$. To do so, we note that, with constants c, C, C' as in (9.12), we have

$$C'\,Z^2\,B_0^{1/2}\,\mathcal{M}_{Q_\nu}\;\le\;C''\,Z\,B_0^{1/2}\,\mathcal{N}_{Q_\nu^*}\;+\;C''\,Z^2\,B_0\;+\;cZ^2\,\mathcal{M}_{Q_\nu}^2\,\chi_{\mathcal{M}_{Q_\nu}\ge\frac{C}{Z}\mathcal{N}_{Q_\nu^*}+C}. \tag{9.13}$$

Let us verify (9.13). We distinguish three cases.

- If $\mathcal{M}_{Q_\nu}\;\le\;C'''\,B_0^{1/2}$ (with C''' a universal constant to be picked in a moment) then $C'\,Z^2\,B_0^{1/2}\,\mathcal{M}_{Q_\nu}\;\le\;C''\,Z^2\,B_0$ for $C''\;\ge\;C'\,C'''$, and (9.13) holds.
- If $\mathcal{M}_{Q_\nu}\le\frac{C}{Z}\mathcal{N}_{Q_\nu^*}+C$, then $C'\,Z^2\,B_0^{1/2}\,\mathcal{M}_{Q_\nu}\;\le\;C''\,Z\,B_0^{1/2}\,\mathcal{N}_{Q_\nu^*}+C''\,Z^2\,B_0^{1/2}$ for $C''\;\ge\;CC'$, and again (9.13) holds.
- If $\mathcal{M}_{Q_\nu}\;\ge\;\frac{C}{Z}\,\mathcal{N}_{Q_\nu^*}\;+\;C$ and $\mathcal{M}_{Q_\nu}\;\ge\;C'''\,B_0^{1/2}$, then $C'Z^2\,B_0^{1/2}\,\mathcal{M}_{Q_\nu}\;\le\;C'\,Z^2\,(\mathcal{M}_{Q_\nu}/C''')\,\mathcal{M}_{Q_\nu}\;\le\;c\,Z^2\,\mathcal{M}_{Q_\nu}^2\;\;=\;\;c\,Z^2\,\mathcal{M}_{Q_\nu}^2\,\chi_{\mathcal{M}_{Q_\nu}\ge\frac{C}{Z}\mathcal{N}_{Q_\nu^*}+C}$ for $C'''=C'/c$, and again (9.13) holds.

Thus, (9.13) holds in all cases. From (9.13) we obtain

$$\begin{aligned}
&-C'\,Z^2\,B_0^{1/2}\,\sum_\nu\,\theta_\nu\,\delta_\nu^{-1}\,\mathcal{M}_{Q_\nu}\;\ge\\
&\quad-C''\,Z\,B_0^{1/2}\,\left\langle\sum_\nu\,\theta_\nu\,\delta_\nu^{-1}\,\mathcal{N}_{Q_\nu^*}\,\psi,\,\psi\right\rangle-C''\,Z^2\,B_0\,\sum_\nu\,\theta_\nu\,\delta_\nu^{-1}\\
&\quad-c\,Z^2\,\left\langle\sum_\nu\,\theta_\nu\,\delta_\nu^{-1}\,\mathcal{M}_{Q_\nu}^2\,\chi_{\mathcal{M}_{Q_\nu}\ge\frac{C}{Z}\mathcal{N}_{Q_\nu^*}+C}\,\psi,\,\psi\right\rangle.
\end{aligned} \tag{9.14}$$

(To derive (9.14), we simply multiply (9.13) by $\theta_\nu\delta_\nu^{-1}$, sum on ν, and take the expectation with respect to ψ.)

Combining (9.14) with (9.12), we find that

$$(9.15)\quad C' \, Z \, B_0^{1/2} \, L \cdot \sum_{k=1}^{N} \| \sigma^{(k)} \cdot (i \nabla_{x_k} - A(x_k)) \, \psi \|^2 + \langle V_{\text{Coulomb}} \, \psi, \psi \rangle$$

$$- Z \, B_0^{1/2} \left\langle \sum_{k=1}^{N} \left\{ \sum_{\nu} \theta_\nu \, V_\nu \, (x_k) \right\} \psi, \, \psi \right\rangle \geq$$

$$\left\{ c \, K \, Z \, B_0^{1/2} \left\langle \sum_{\nu} \theta_\nu \, \delta_\nu^{-1} \, \mathcal{N}_{Q_\nu} \, \psi, \, \psi \right\rangle - C' \, Z \, B_0^{1/2} \left\langle \sum_{\nu} \theta_\nu \, \delta_\nu^{-1} \, \mathcal{N}_{Q_\nu^*} \, \psi, \, \psi \right\rangle \right\}$$

$$- C'' \, (K^{5/2} \, B_0^{3/2} \, Z + B_0 \, Z^2) \cdot \sum_{\nu} \theta_\nu \, \delta_\nu^{-1}$$

$$- Z \, B_0^{1/2} \left\langle \sum_{k=1}^{N} \left\{ \sum_{\nu} \theta_\nu \, W_\nu \, (x_k) \right\} \psi, \, \psi \right\rangle .$$

¿From (8.45) we conclude that $\sum_{\nu} \theta_\nu \, \delta_\nu^{-1} \mathcal{N}_{Q_\nu^*} \leq C \sum_{\nu} \theta_\nu \, \delta_\nu^{-1} \, \mathcal{N}_{Q_\nu}$.

Therefore, if K exceeds a large universal constant, then the first expression in curly brackets on the right-hand side of (9.15) in non-negative. Hence, (9.15) implies

$$(9.16)\quad C' \, Z \, B_0^{1/2} \, L \cdot \sum_{k=1}^{N} \| \sigma^{(k)} \cdot (i \nabla_{x_k} - A(x_k)) \, \psi \|^2 + \langle V_{\text{Coulomb}} \, \psi, \psi \rangle$$

$$- Z \, B_0^{1/2} \left\langle \sum_{k=1}^{N} \left\{ \sum_{\nu} \theta_\nu \, V_\nu \, (x_k) \right\} \psi, \psi \right\rangle \geq$$

$$- C'' \, (K^{5/2} \, B_0^{3/2} \, Z + B_0 \, Z^2) \cdot \sum_{\nu} \theta_\nu \, \delta_\nu^{-1}$$

$$- Z \, B_0^{1/2} \left\langle \sum_{k=1}^{N} \left\{ \sum_{\nu} \theta_\nu \, W_\nu (x_k) \right\} \psi, \psi \right\rangle .$$

Recall that $W_\nu(x)$ is supported in Q_ν^* and satisfies (9.7); and that (9.16) holds for arbitrary V_ν, supported in Q_ν and satisfying (9.3). We will now pick the potentials V_ν.

For $x \in Q_\nu$, we define

$$V_\nu(x) \;=\; \frac{1}{\theta_\nu} \cdot \sum_{\nu'} \theta_{\nu'}\, W_{\nu'}(x). \tag{9.17}$$

For $x \notin Q_\nu$, we set $V_\nu(x) = 0$.

Clearly, (9.17) implies

$$\sum_\nu \theta_\nu\, V_\nu(x) \;=\; \sum_\nu \theta_\nu W_\nu(x) \;\text{ for all }\; x \in \mathbb{R}^3, \tag{9.18}$$

with V_ν supported in Q_ν. To estimate $V_\nu(x)$, we note that the sum in (9.17) may be restricted to those ν' for which $Q_\nu \cap Q^*_{\nu'} \neq \phi$. There are at most C such ν', by (8.43), and they satisfy $\theta_{\nu'} \leq C\theta_\nu$. Therefore, with $P(\nu) = \{\nu' : Q_\nu \cap Q^*_{\nu'} \neq \phi\}$, we have

$$|V_\nu(x)| \;\leq\; C \sum_{\nu' \in P(\nu)} |W_{\nu'}(x)|, \;\text{ hence}$$

$$|V_\nu(x)|^3 \;\leq\; C' \sum_{\nu' \in P(\nu)} |W_{\nu'}(x)|^3 \;\text{ for }\; x \in Q_\nu, \;\text{ and therefore}$$

$$\int_{Q_\nu} |V_\nu(x)|^3\, dx \;\leq\; C' \sum_{\nu' \in P(\nu)} \int_{\mathbb{R}^3} |W_{\nu'}(x)|^3\, dx \;=\; C' \sum_{\nu' \in P(\nu)} \int_{Q^*_{\nu'}} |W_{\nu'}(x)|^3\, dx$$

$$\leq\; C''\, K^{-6}\, B_0^{-1} \;\text{ by (9.7).}$$

Thus, if K exceeds a large enough universal constant, then the V_ν defined by (9.17) satisfy (9.3), hence also (9.16).

On the other hand, (9.18) shows that, with this choice of V_ν, the term involving V_ν in (9.16) cancels the term involving W_ν in (9.16). Consequently, (9.16) implies

$$C'\, Z\, B_0^{1/2}\, L \cdot \sum_{k=1}^{N} \|\sigma^{(k)} \cdot (i\nabla_{x_k} - A(x_k))\, \psi\|^2 \;+\; \langle V_{\text{Coulomb}}\, \psi, \psi\rangle \;\geq \tag{9.19}$$

$$-C''(K^{5/2}\, B_0^{3/2}\, Z \;+\; B_0\, Z^2) \sum_\nu \theta_\nu\, \delta_\nu^{-1}.$$

¿From now on, we pick K, once and for all, to be a universal constant, large enough that the preceding arguments work. We no longer keep track of the dependence of our constants on K. However, we have still not picked B_0. Thus (9.19) becomes

$$C\,Z\,B_0^{1/2}\,L\cdot\sum_{k=1}^{N}\|\sigma^{(k)}\cdot(i\nabla_{x_k}-A(x_k))\,\psi\,\|^2+\langle V_{\text{Coulomb}}\,\psi,\psi\rangle\geq -C\,(B_0^{3/2}\,Z+B_0\,Z^2)\cdot\sum_{\nu}\theta_\nu\,\delta_\nu^{-1}. \tag{9.20}$$

We can estimate the right-hand side of (9.20) by using (8.46). Thus, (9.20) implies

$$\begin{aligned} C\,Z\,B_0^{1/2}\,L\cdot\sum_{k=1}^{N}\|\sigma^{(k)}\cdot(i\nabla_{x_k}-A(x_k))\,\psi\,\|^2+\langle V_{\text{Coulomb}}\,\psi,\,\psi\rangle\geq\\ -\frac{C}{L}\cdot(B_0^{3/2}\,Z+B_0\,Z^2)\,M\\ -C\cdot(B_0^{-1/2}\,Z+B_0^{-1}\,Z^2)\int_{\mathbb{R}^3}e^{-D(x)/L}\,|B(x)|^2\,dx\\ -C\cdot(B_0^{11/6}Z+B_0^{4/3}\,Z^2)\int_{\mathbb{R}^3}e^{-D(x)/L}\left\{L^{-3}\int_{B(x,\bar{C}L)}|B(y)-Av_{B(x,\bar{C}L)}\,B|^2\,dy\right\}dx. \end{aligned}\tag{9.21}$$

Now let $\Gamma>0$ be given. We fix B_0 large enough that the previous arguments work, and large enough that

$$C\cdot(B_0^{-1/2}\,Z+B_0^{-1}\,Z^2)<\Gamma\ \text{ with } C \text{ as in (9.21)}. \tag{9.22}$$

We may take B_0 to depend only on Γ and Z.

With this value of B_0, (9.21) takes the form

$$C\,(\Gamma,Z)\,L\cdot\sum_{k=1}^{N}\|\sigma^{(k)}\cdot(i\nabla_{x_k}-A(x_k))\,\psi\|^2+\langle V_{\text{Coulomb}}\,\psi,\,\psi\rangle\geq \tag{9.23}$$

$$-\,C'\,(\Gamma,Z)\,\frac{M}{L}-\Gamma\int\limits_{\mathbb{R}^3}e^{-D(x)/L}\,|B(x)|^2\,dx$$

$$-C''\,(\Gamma,Z)\int\limits_{\mathbb{R}^3}e^{-D(x)/L}\left\{L^{-3}\int\limits_{B(x,\bar{C}L)}|B(y)-Av_{B(x,\bar{C}L)}\,B|^2\,dy\right\}dx$$

with $C(\Gamma,Z)$, $C'(\Gamma,Z)$, $C''(\Gamma,Z)$ depending only on Γ and Z.

If we take L so small that

$$L\leq 1/C\,(\Gamma,Z),\ \text{ with } C\,(\Gamma,Z)\ \text{ as in (9.23), then (9.23) implies} \tag{9.24}$$

$$< H_{\text{Pauli}}\,\psi,\,\psi> +\,\Gamma\int\limits_{\mathbb{R}^3}e^{-D(x)/L}\,|B(x)|^2\,dx \tag{9.25}$$

$$+\,C''\,(\Gamma,\,Z)\int\limits_{\mathbb{R}^3}e^{-D(x)/L}\left\{L^{-3}\int\limits_{B(x,\bar{C}L)}|B(y)-Av_{B(x,\bar{C}L)}\,B|^2\,dy\right\}dx$$

$$\geq\,-\,C'\,(\Gamma,\,Z)\cdot\frac{M}{L}.$$

Thus, (9.24) implies (9.25). We now apply (9.25), with L replaced by $\tilde{L}=\bar{C}^{-1}L$. Thus,

$$L<\bar{C}/C\,(\Gamma,\,Z)\ \text{ implies} \tag{9.26}$$

$$(9.27)\quad < H_{\text{Pauli}}\,\psi, \psi > \;+ \Gamma \int\limits_{\mathbb{R}^3} e^{-\bar{C}D(x)/L}\,|B(x)|^2\,dx$$

$$+\,\bar{C}^3 \cdot C''(\Gamma,\,Z) \int\limits_{\mathbb{R}^3} e^{-\bar{C}D(x)/L} \left\{ L^{-3} \int\limits_{B(x,L)} |B(y) \,-\, Av_{B(x,L)}\,B|^2\,dy \right\} dx$$

$$\geq\, -\bar{C} \cdot C'(\Gamma,\,Z) \cdot \frac{M}{L}.$$

Since $\bar{C}$ is a large universal constant (in particular $\bar{C} \geq 1$) and

$$\left\{ L^{-3} \int\limits_{B(x,L)} |B(y) \,-\, Av_{B(x,L)}\,B|^2\,dy \right\} \;=\; \tfrac{4\pi}{3}\,(S_L(x))^2$$

(see the statement of the Main Theorem for the definition of $S_L(x)$), estimate (9.27) implies

$$(9.28)\qquad < H_{\text{Pauli}}\,\psi,\,\psi > \;+ \Gamma \int\limits_{\mathbb{R}^3} e^{-D(x)/L}\,|B(x)|^2\,dx \;+\; C_1\,(\Gamma,\,Z) \int\limits_{\mathbb{R}^3} e^{-D(x)/L}\,(S_L(x))^2\,dx$$

$$\geq\, -\,C_2\,(\Gamma,\,Z) \,\cdot\, \frac{M}{L},$$

which is the desired conclusion (1.1). The proof of the Main Theorem is complete. ■

Remark: From (9.21), one can easily keep track of the constants $c(\Gamma, Z)$, $C_1(\Gamma, Z)$, $C_2(\Gamma, Z)$ in the statement of the Main Theorem. Supposing that $Z \geq 1$, and letting c, C denote constants independent of Z and Γ, we obtain the following results.

Case 1: $\Gamma \geq Z^2$. Then take $B_0 = C$. This gives $c\,(\Gamma, Z) = c\,Z^{-1}$, $C_1(\Gamma, Z) = CZ^2$, $C_2(\Gamma, Z) = CZ^2$.

Case 2: $Z^2 \geq \Gamma \geq 1$. Then take $B_0 = C\,Z^2\,\Gamma^{-1}$. We obtain $c\,(\Gamma, Z) = c\,\Gamma^{1/2}\,Z^{-2}$, $C_1\,(\Gamma, Z) = C\,\Gamma^{-4/3}\,Z^{14/3}$, $C_2\,(\Gamma, Z) = C\,\Gamma^{-1}\,Z^4$.

Case 3: $\Gamma \leq 1$. Then take $B_0 = C\,Z^2\,\Gamma^{-2}$. We find that $c\,(\Gamma, Z) = c\,\Gamma\,Z^{-2}$, $C_1\,(\Gamma, Z) = C\,\Gamma^{-11/3}\,Z^{14/3}$, $C_2\,(\Gamma, Z) = C\,\Gamma^{-3}Z^4$.

The argument in Section 1 then immediately yields similar constants in Theorem (0.4). Presumably, these $c(\Gamma, Z)$, $C_1(\Gamma, Z)$, $C_2(\Gamma, Z)$ are artifacts of our proof. On the other hand, the dependence of our results on the length scale L is optimal.

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