STABILITY OF ULTRAVIOLET-CUTOFF QUANTUM ELECTRODYNAMICS WITH NON-RELATIVISTIC MATTER

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Abstract We prove that the quantum-mechanical ground state energy of a system consisting of an arbitrary number, M, of static nuclei of atomic number $\leq Z$ and of an arbitrary number, N, of Pauli electrons interacting with the quantized, ultraviolet-cutoff radiation field is bounded below by $-K \cdot M$, where K is a finite constant depending on Z, on the finestructure constant α and on the ultraviolet cutoff Λ, with $K \leq K'\Lambda$, as $\Lambda \to \infty$, and K' independent of Λ.

1 Introduction and Survey of Results

In this paper we prove that the quantum electrodynamics (QED) of non-relativistic quantum-mechanical matter interacting with the quantized radiation field is *stable* (more precisely, H-stable), provided an ultraviolet cutoff is imposed on the quantized electromagnetic vector potential. A typical physical system described by this theory consists of an arbitrary number, N, of non-relativistic electrons with electric charge $-e$, bare mass $m > 0$, spin $1/2$ and a bare gyro-magnetic factor $g = 2$, an arbitrary number, M, of nuclei of nuclear charge $\leq Ze$, for some positive integer $Z < \infty$ (e.g. $Z < 150$), and an arbitrary, variable number of photons; (see refs. [1] - [6]).

H-stability is the statement that, in the ground state of the system, the *energy per charged particle* (electron or nucleus) remains *finite*, as N and/or M tend to ∞; see [7].

Since the masses of nuclei are much larger than the electron mass m, we shall treat the nuclei as *static*. This would yield a lower bound on the ground state energy of the system if the gyro-magnetic factors of nuclei were less than or equal to 2, [1]. However, there are plenty of nuclei (including the proton) with a gyro-magnetic factor > 2. For systems containing such nuclei, H-stability will *not* hold, *unless* the interactions between the nuclear magnetic moments and the quantized radiation field are neglected or regularized by a hard- or soft-core form factor of nuclei. However, for a size of nuclei much smaller than the Bohr radius of an atom, the contribution of the nuclear Zeeman energies to the ground state energy of the system is much smaller than typical atomic energies, provided an ultraviolet cutoff at an energy at least as large as the rest energy of an electron is imposed on the quantized radiation field. It is then justified to treat nuclei as static point particles in estimates of the ground state energies of atomic and molecular systems. This approximation is made throughout our paper.

Much of atomic, molecular and condensed matter physics is the study of physical properties of the systems just described.

Throughout this paper, we impose the *Coulomb* (or radiation) *gauge condition* on the electromagnetic potentials. In this gauge, electrons and nuclei interact through instantaneous Coulomb two-body potentials, and the electrons are coupled to the transverse degrees of freedom of the radiation field by minimal substitution (i.e., by replacing ordinary derivatives by covariant ones). Treating the nuclei as static implies that they do not couple to the transverse degrees of freedom of the radiation field.

The field quanta of the transverse degrees of freedom of the electromagnetic field are the *photons*. A typical electron energy in an atom is of order $-mc^2(Z\alpha)^2$, where c is the velocity of light, $\alpha = e^2/4\pi\hbar c \approx 1/137$ is the dimensionless finestructure constant, and $\hbar$ is Planck's constant. Interactions between photons with energy *large* compared to typical atomic electron energies and the electrons are turned off by means of an *ultraviolet cutoff* imposed on the electromagnetic vector potential.

The Hilbert space of pure state vectors of a system of N-electrons and arbitrarily many photons is given by

$$\mathcal{H} \;=\; (\mathcal{H}_1)^{\wedge N} \;\otimes\; \mathcal{F}, \tag{1.1}$$

where $\mathcal{H}_1 = L^2(\mathbb{E}^3, d^3x) \otimes \mathbb{C}^2$ is the one-electron Hilbert space, Λ denotes an antisymmetric tensor product, and $\mathcal{F}$ is the bosonic Fock space over the one-photon Hilbert space $L^2(\mathbb{R}^3, d^3k) \otimes \mathbb{C}^2$, i.e., $\mathcal{F}$ is the symmetric tensor algebra over $L^2(\mathbb{R}^3, d^3k) \otimes \mathbb{C}^2$. The factors $\mathbb{C}^2$ describe the spin states of an electron and the helicities of photons, respectively. The choice of an antisymmetric tensor product in $(\mathcal{H}_1)^{\wedge N}$, on the r.s. of (1.1), corresponds to the *Pauli principle*, i.e., to the Fermi statistics of electrons. Photons are bosons, and therefore symmetric tensor products are used in the definition of $\mathcal{F}$.

Next, we describe the Hamiltonian that generates the dynamics of a system of N electrons, M nuclei and arbitrarily many photons. We work in units where $\hbar = c = 1$, and we impose the Coulomb gauge condition on the electromagnetic potentials, as announced. Then the Hamiltonian of the system is given by

$$\widetilde{H} \;=\; \widetilde{H}_{el} \;+\; \mathbb{I} \,\otimes\, \widetilde{H}_{ph}, \tag{1.2}$$

where

$$\widetilde{H}_{el} \;=\; \sum_{j=1}^{N} \frac{1}{2m} \left[\boldsymbol{\sigma}^{(j)} \cdot \left(-i\boldsymbol{\nabla}_j + e\tilde{\mathbf{A}}^{(\Lambda)}\left(\mathbf{x}_j\right) \right) \right]^2 \;+\; \widetilde{V}_C, \tag{1.3}$$

and

$$\begin{aligned} \widetilde{V}_C \;&=\; \sum_{1 \le i < j \le N} \frac{\alpha}{|\mathbf{x}_i - \mathbf{x}_j|} \;-\; \sum_{i=1}^{N}\sum_{l=1}^{M} \frac{\alpha\, Z_l}{|\mathbf{x}_i - \mathbf{y}_l|} \\ &+\; \sum_{1 \le k < l \le M} \frac{\alpha\, Z_k Z_l}{|\mathbf{y}_l - \mathbf{y}_k|} \;, \end{aligned} \tag{1.4}$$

with $Z_l \le Z < \infty$, for all $l = 1, \cdots, M$ and arbitrary M.

We write $\sigma_\beta^{(j)}$ for $\mathbb{I} \otimes \cdots \otimes \mathbb{I} \otimes \sigma_\beta \otimes \mathbb{I} \otimes \cdots \otimes \mathbb{I}$ on spin space $(\mathbb{C}^2)^{\otimes N}$, where σ_1, σ_2 and σ_3 are the three Pauli matrices, and the factor σ_β appears in the j^{th} factor of the tensor product. An explicit matrix representation of the Pauli matrices is given by

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

The point $\mathbf{x}_j \in \mathbb{E}^3$ denotes the position of the j^{th} electron, $-i\boldsymbol{\nabla}_j$ is its momentum operator (in the Schrödinger representation), and $\mathbf{y}_\mathbf{l} \in \mathbb{E}^\mathbf{3}$ denotes the position of the l^{th} nucleus; $\{\mathbf{y}_1, \cdots, \mathbf{y}_M\}$ describes an *arbitrary*, but fixed configuration of nuclei of nuclear charges $Z_1 e, \cdots, Z_M e$. Furthermore, $\widetilde{V}_C$ is the electro-static Coulomb potential.

The quantized electromagnetic vector potential, $\tilde{\mathbf{A}}(\mathbf{x})$, in the Coulomb gauge is given by the following operator-valued distributions on Fock space.

$$\tilde{\mathbf{A}}(\mathbf{x}) \;=\; \tilde{\mathbf{A}}_-(\mathbf{x}) + \tilde{\mathbf{A}}_+(\mathbf{x}), \quad \tilde{\mathbf{A}}_+(\mathbf{x}) \;=\; \Big(\tilde{\mathbf{A}}_-(\mathbf{x})\Big)^*, \tag{1.5}$$

where

$$\tilde{\mathbf{A}}_-(\mathbf{x}) \;=\; \frac{1}{(2\pi)^{3/2}} \int \frac{d^3k}{\sqrt{2|\mathbf{k}|}} \sum_{\lambda=\pm} c_\lambda(\mathbf{k})\, \boldsymbol{\varepsilon}_\lambda(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}}. \tag{1.6}$$

The integral on the r.s. of (1.6) may be understood as a weak integral on $\mathcal{F} \times \mathcal{F}$. In these formulae, the direction of propagation, $\hat{k} = \frac{\mathbf{k}}{|\mathbf{k}|}$ where $\mathbf{k}$ denotes a wave vector, and the polarization vectors $\boldsymbol{\varepsilon}_+(\mathbf{k}), \boldsymbol{\varepsilon}_-(\mathbf{k})$ form an orthonormal basis of $\mathbb{R}^3 \otimes \mathbb{C}$. For concreteness, we identify $\boldsymbol{\varepsilon}_+$ and $\boldsymbol{\varepsilon}_-$ with right- and left circular polarization, respectively. Furthermore, the operators $c_\lambda(\mathbf{k})^*$ and $c_\lambda(\mathbf{k})$ are standard creation- and annihilation operators on $\mathcal{F}$ satisfying *canonical commutation relations* :

$$\begin{aligned} \Big[c_\lambda(\mathbf{k})^\#,\; c_{\lambda'}(\mathbf{k}')^\#\Big] \;&=\; 0, \\ [c_\lambda(\mathbf{k}),\; c_{\lambda'}(\mathbf{k})^*] \;&=\; \delta_{\lambda\lambda'}\; \delta^{(3)}(\mathbf{k}-\mathbf{k}'). \end{aligned} \tag{1.7}$$

Here $c_\lambda(\mathbf{k})^\# = c_\lambda(\mathbf{k})$ or $c_\lambda(\mathbf{k})^*$, and $c_\lambda(\mathbf{k})^*$ is the adjoint (operator-valued distribution) of $c_\lambda(\mathbf{k})$. Fock space $\mathcal{F}$ contains a vector Ω (unique, up to a complex phase), the *vacuum*, with the property that

$$c_\lambda(\mathbf{k})\, \Omega \;=\; 0\ , \tag{1.8}$$

for all $\lambda = \pm$, $\mathbf{k} \in \mathbb{R}^3$. The vector Ω is cyclic for the algebra of polynomials in c_λ and c_λ^* (smeared out with test functions). From this fact and eqs. (1.7) and (1.8), it follows that

$$\mathcal{F} \cong \bigoplus_{n=0}^{\infty} \left(L^2(\mathbb{R}^3) \otimes \mathbb{C}^2\right)^{\otimes_s n}, \tag{1.9}$$

where $\otimes_s$ denotes a symmetric tensor product, (as claimed above). See e.g. [8, 9] for back ground material on Fock space.

Let $\Lambda(\mathbf{k})$ be a function satisfying

$$|\Lambda(\mathbf{k})| \le 1, \quad \text{supp}\ \Lambda \subseteq \{\mathbf{k} \in \mathbb{R}^3 \;\big|\; |\mathbf{k}| \le \Lambda\}, \tag{1.10}$$

for some constant $\Lambda < \infty$ (the ultraviolet cutoff). The electromagnetic vector potential with ultraviolet cutoff Λ, $\tilde{\mathbf{A}}^{(\Lambda)}(\mathbf{x})$, is given by

$$\tilde{\mathbf{A}}^{(\Lambda)}(\mathbf{x}) \;=\; \tilde{\mathbf{A}}_{+}^{(\Lambda)}(\mathbf{x}) \;+\; \tilde{\mathbf{A}}_{-}^{(\Lambda)}(\mathbf{x}), \quad \tilde{\mathbf{A}}_{+}^{(\Lambda)}(\mathbf{x}) \;=\; \left(\tilde{\mathbf{A}}_{-}^{(\Lambda)}(\mathbf{x})\right)^{*},$$

where

$$\tilde{\mathbf{A}}_{-}^{(\Lambda)}(\mathbf{x}) \;=\; \frac{1}{(2\pi)^{3/2}} \int \frac{d^3k}{\sqrt{2|\mathbf{k}|}}\, \Lambda(\mathbf{k}) \sum_{\lambda=\pm} c_\lambda(\mathbf{k})\, \boldsymbol{\varepsilon}_\lambda(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}}. \tag{1.11}$$

It is well known (and easy to prove) that, for $\Lambda < \infty$, $\tilde{A}_{\beta}^{(\Lambda)}(\mathbf{x})\,, \beta = 1, 2, 3,$ are three commuting selfadjoint operators on $\mathcal{F}$, for all $\mathbf{x} \in \mathbb{E}^3$, which are smooth in $\mathbf{x}$; (see Proposition 1, Sect. 3).

Finally, we define the free photon Hamiltonian $\tilde{H}_{ph}$

$$\tilde{H}_{ph} \;=\; \sum_{\lambda=\pm} \int d^3k\; c_\lambda(\mathbf{k})^{*} |\mathbf{k}| c_\lambda(\mathbf{k}). \tag{1.12}$$

This operator is positive and selfadjoint on its dense domain of definition. Its spectrum is absolutely continuous, except for a single, simple eigenvalue at 0. The corresponding eigenvector is the vacuum Ω.

The main results proven in this paper are Theorems 1 and 2. Theorem 1 is stated below, while Theorem 2 is stated in Sect. 4 and proven in Sect. 5 and in [12]. Theorem 2 and arguments first described in [6] are the basic ingredients used in the proof of Theorem 1; but Theorem 2 is of independent interest.

Theorem 1

(1) For an arbitrary number, N, of electrons, an arbitrary number, M, of nuclei of charges $\leq Ze$, for arbitrary values of Z and of the finestructure constant α, and for an arbitrary ultraviolet cutoff Λ (see (1.10)), there exists a finite constant $E(\alpha, Z)$ (only depending on α and Z) such that

$$\widetilde{H} \;\geq\; -\, E(\alpha, Z)\; \Lambda \;\cdot\; M.$$

(2) For arbitrary N, M, and Z (as above), for an ultraviolet cutoff

$$\Lambda \;\leq\; 2\, m\, Z^2\, \alpha^{5/4}, \tag{1.13}$$

and for sufficiently small values of αZ and $\alpha^{5/2} Z^3$, there exists a finite constant $\varepsilon(Z) \leq$ const. $Z^{3/2}$ independent of α, m, N and M such that

$$\widetilde{H} \;\geq\; -\,\varepsilon(Z)\; m(\alpha Z)^2 \;\cdot\; M. \tag{1.14}$$

Remarks

(i) Part (1) says that the ground state energy of a system of M static nuclei and N non-relativistic electrons interacting with the quantized radiation field cutoff at an energy Λ tends to $-\infty$ no worse than linearly in M and in Λ, as $M \to \infty$, or $\Lambda \to \infty$. The dependence on Λ of our estimate on the ground state energy is related to the fact that we are studying the *unrenormalized* Hamiltonian of quantum electrodynamics with non-relativistic matter; (see the discussion at the end of ref. [6]). One expects that the ground state energy of the correctly renormalized Hamiltonian grows linearly in M, but is *independent* of Λ, (for α and Z small enough). However, at present, there is no proof in sight of this conjecture.

(ii) As remarked before, typical electron energies in a system of the kind we are considering are of order $-m(Z\alpha)^2$. Thus the bound imposed on the ultraviolet cutoff Λ in (1.13) is physically acceptable, since, in nature, $\alpha = 1/137 \ll 1$. Furthermore, our estimate on ground state energies in part (2), inequality (1.14), has the right asymptotic behavior in α, as $\alpha \to 0$.

(iii) It is shown in [6], by methods relying on [5], that, for Λ as in (1.13), $\alpha \leq 1/132$ and $Z \leq 6$, there is a finite constant ε such that

$$\widetilde{H} \;\geq\; -\,\varepsilon\; m\; \alpha^2\; (N + M).$$

2 Dimensionless variables and natural units

Before we start with the proof of our main results we choose natural, *dimensionless* variables that will simplify our formulae. We set

$$\mathbf{x}_j \;=\; \beta\; \boldsymbol{\xi}_j,\; \mathbf{y}_l \;=\; \beta\; \boldsymbol{\eta}_l, \quad \text{and } \mathbf{k} = \;\mu\; \boldsymbol{\kappa}, \tag{2.1}$$

with $0 < \beta, \mu < \infty$, and β and μ^{-1} have the dimension of length. Then $\boldsymbol{\xi}_j, j = 1, \cdots, N$, $\boldsymbol{\eta}_l, l = 1, \cdots, M$, and the rescaled wave vectors $\boldsymbol{\kappa}$ are dimensionless variables. We introduce rescaled creation- and annihilation operators

$$a_\lambda(\boldsymbol{\kappa})^{\#} \;:=\; \mu^{2/3}\; c_\lambda(\mathbf{k})^{\#} \tag{2.2}$$

and note that

$$\begin{aligned} \left[a_\lambda(\boldsymbol{\kappa})^{\#}\;,\; a_{\lambda'}(\boldsymbol{\kappa})^{\#}\right] \;&=\; 0, \\ \left[a_\lambda(\boldsymbol{\kappa}),\; a_{\lambda'}(\boldsymbol{\kappa}')^{*}\right] \;&=\; \delta_{\lambda\lambda'}\; \delta^{(3)}(\boldsymbol{\kappa} - \boldsymbol{\kappa}'). \end{aligned} \tag{2.3}$$

It is easy to verify that there exist unitary operators $U(\mu)$ on $\mathcal{F}$, corresponding to a dilatation of photon wave vectors by a factor $\mu > 0$, such that $U(\mu)\; U(\mu') = U(\mu \cdot \mu')$ and

$$a_\lambda(\boldsymbol{\kappa})^\# \;=\; U(\mu)\; c_\lambda(\boldsymbol{\kappa})^\#\; U(\mu)^{-1},$$

and hence the commutation relations (1.7) and (2.3) are equivalent.

One now checks that

$$\begin{aligned} \widetilde{H}_{ph} &= \mu \sum_{\lambda=\pm} \int d^3\kappa\; a_\lambda(\boldsymbol{\kappa})^* |\boldsymbol{\kappa}|\; a_\lambda(\boldsymbol{\kappa}) \\ &=: \mu\; H_{ph}, \end{aligned} \tag{2.4}$$

where $H_{ph} = U(\mu)\; \widetilde{H}_{ph}\; U(\mu)^{-1}$.

Furthermore

$$\begin{aligned} \tilde{\mathbf{A}}_-^{(\Lambda)}(\mathbf{x}) &= \frac{1}{(2\pi)^{3/2}} \int \frac{d^3\, k}{\sqrt{2|\mathbf{k}|}}\; \Lambda(\mathbf{k}) \sum_{\lambda=\pm} c_\lambda(\mathbf{k})\; \boldsymbol{\varepsilon}_\lambda(\mathbf{k})\; e^{i\mathbf{k}\cdot\mathbf{x}} \\ &= \frac{\mu}{(2\pi)^{3/2}} \int \frac{d^3\, \kappa}{\sqrt{2|\boldsymbol{\kappa}|}}\; \Lambda(\mu\boldsymbol{\kappa}) \sum_{\lambda=\pm} a_\lambda(\boldsymbol{\kappa})\; \boldsymbol{\varepsilon}_\lambda(\mu\boldsymbol{\kappa})\; e^{i\boldsymbol{\kappa}\,\cdot(\mu\mathbf{x})} \\ &=: \mu\; \mathbf{A}_-^{(\Lambda_\mu)}\,(\mu\mathbf{x}), \end{aligned} \tag{2.5}$$

where $\Lambda_\mu(\boldsymbol{\kappa}) = \Lambda(\mu\boldsymbol{\kappa})$, with Λ as in eq. (1.10). Note that, for our choice of polarization vectors $\boldsymbol{\varepsilon}_\pm(\cdot)$, we have that $\boldsymbol{\varepsilon}_\pm(\mu\boldsymbol{\kappa}) = \boldsymbol{\varepsilon}_\pm(\boldsymbol{\kappa})$. We set

$$\mathbf{A}_+^{(\Lambda_\mu)}(\mathbf{x}) \;=\; \left(\mathbf{A}_-^{(\Lambda_\mu)}(\mathbf{x})\right)^*,$$

and

$$\mathbf{A}^{(\Lambda_\mu)}(\mathbf{x}) \;=\; \mathbf{A}_+^{(\Lambda_\mu)}(\mathbf{x}) \;+\; \mathbf{A}_-^{(\Lambda_\mu)}(\mathbf{x}).$$

We conclude that, in dimensionless variables $\boldsymbol{\xi}_j, \boldsymbol{\eta}_l, \boldsymbol{\kappa}$, the Hamiltonian $\widetilde{H}$ is given by

$$\begin{aligned} \widetilde{H} &= \sum_{j=1}^{N} \frac{1}{2m\beta^2} \left[\boldsymbol{\sigma}^{(j)} \cdot \left(-i\boldsymbol{\nabla}_j + \beta\mu\; e\mathbf{A}^{(\Lambda_\mu)}\left(\beta\mu\boldsymbol{\xi}_j\right)\right)\right]^2 \\ &+ \frac{\alpha}{\beta}\; V_C \otimes \mathbf{I} \;+\; \mu\; \mathbf{I} \otimes H_{ph}, \end{aligned} \tag{2.6}$$

where

$$\begin{aligned} V_C &= \sum_{1\le i<j\le N} \frac{1}{|\boldsymbol{\xi}_i - \boldsymbol{\xi}_j|} - \sum_{i=1}^{N}\sum_{l=1}^{M} \frac{Z_l}{|\boldsymbol{\xi}_i - \boldsymbol{\eta}_l|} \\ &+ \sum_{1\le l<k\le M} \frac{Z_l\; Z_k}{|\boldsymbol{\eta}_l - \boldsymbol{\eta}_k|} \end{aligned} \tag{2.7}$$

Equations (2.4), (2.6) and (2.7) suggest to choose β and μ as follows.

$$\left(2m\beta^2\right)^{-1} \;=\; \alpha\,\beta^{-1} \;=\; \mu\;, \tag{2.8}$$

i.e.,

$$\beta = (2m\alpha)^{-1} , \; \mu = 2m\alpha^2 , \tag{2.9}$$

and hence

$$\beta\mu = \alpha , \;\; \beta\mu e = 2\sqrt{\pi}\, \alpha^{3/2} . \tag{2.10}$$

We set

$$H := \frac{1}{\mu} \widetilde{H} = \frac{1}{2m\alpha^2} \widetilde{H} , \tag{2.11}$$

so that energy eigenvalues of H are given in units where the ground state energy (1 Rydberg) of a hydrogen atom is $= -4$. See [10] for further details.

In what follows, we rename variables:

$$\boldsymbol{\xi}_j \to \mathbf{x}_j, \; \boldsymbol{\eta}_l \to \mathbf{y}_l, \; \boldsymbol{\kappa} \to \mathbf{k} \text{ and } \Lambda_\mu \to \Lambda ,$$

with $|\Lambda(\mathbf{k})| \leq 1$, and

$$\text{supp}\, \Lambda \subseteq \left\{ \mathbf{k} \,\middle|\, |\mathbf{k}| \leq (2m\alpha^2)^{-1}\Lambda \right\} . \tag{2.12}$$

We find that

$$H = H_{el}(\alpha) + \mathbf{I} \otimes H_{ph}, \tag{2.13}$$

where

$$H_{el}(\alpha) = \sum_{j=1}^{N} \left[\boldsymbol{\sigma}^{(j)} \cdot \left(-i\, \boldsymbol{\nabla}_j + 2\sqrt{\pi}\, \alpha^{3/2}\, \mathbf{A}^{(\Lambda)}\, (\alpha \mathbf{x}_j) \right) \right]^2 + V_C \otimes \mathbf{I} . \tag{2.14}$$

In the following, it will be convenient to make use of field variables $\boldsymbol{\mathcal{A}}$ and $\boldsymbol{\mathcal{B}}$ given by

$$\begin{aligned} \boldsymbol{\mathcal{A}}(\mathbf{x}) &:= 2\sqrt{\pi}\, \alpha^{3/2}\, \mathbf{A}^{(\Lambda)}(\alpha \mathbf{x}) \\ \boldsymbol{\mathcal{B}}(\mathbf{x}) &:= \text{curl}\, \boldsymbol{\mathcal{A}}(\mathbf{x}) . \end{aligned} \tag{2.15}$$

Then, for an arbitrary function $h(\mathbf{x})$,

$$\int |\boldsymbol{\mathcal{B}}(\mathbf{x})|^2 h(\mathbf{x}) d^3x = 4\pi\alpha^2 \int |\text{curl}\, \mathbf{A}^{(\Lambda)}(\mathbf{x})|^2\, h\left(\frac{\mathbf{x}}{\alpha}\right)\, d^3x , \tag{2.16}$$

and

$$\begin{aligned} &\int |(\boldsymbol{\nabla} \otimes \boldsymbol{\mathcal{B}})(\mathbf{x})|^2\, h(\mathbf{x})\, d^3x = \\ &\qquad 4\pi\, \alpha^4 \int |\boldsymbol{\nabla} \otimes (\text{curl}\, \mathbf{A}^{(\Lambda)})(\mathbf{x})|^2\, h\left(\frac{\mathbf{x}}{\alpha}\right)\, d^3x . \end{aligned} \tag{2.17}$$

3 The Schrödinger representation of Fock space

In the proof of our main result it is convenient to make use of the *Schrödinger representation* of Fock space $\mathcal{F}$, which we briefly review next; (see also [9]).

We define the Sobolev space $\mathcal{H}_{-1/2}$ as the complex, linear space of measurable functions, h, on $\mathbb{E}^3$ whose Fourier transforms, $\hat{h}$, have the property that

$$\int \frac{d^3k}{|\mathbf{k}|} \, |\hat{h}(\mathbf{k})|^2 \ < \ \infty \ . \tag{3.1}$$

For $h \in \mathcal{H}_{-1/2}$ and $\beta = 1, 2, 3$, we define

$$\begin{aligned} A_\beta(h) \quad := \quad \int \frac{d^3k}{\sqrt{2|\mathbf{k}|}} \sum_{\lambda=\pm} \Big\{ & a_\lambda(\mathbf{k}) \ \varepsilon_{\lambda,\beta}(\mathbf{k}) \ \hat{h}(\mathbf{k}) \\ & + a_\lambda(\mathbf{k})^* \ \overline{\varepsilon_{\lambda,\beta}(\mathbf{k})} \ \hat{h}(-\mathbf{k}) \Big\} \ , \end{aligned} \tag{3.2}$$

where $\varepsilon_{\lambda,\beta}$ is the $\beta^{\rm th}$ component of $\boldsymbol{\varepsilon}_\lambda$, and $\bar{z}$ denotes the complex conjugate of z. If h is real then

$$\hat{h}(-\mathbf{k}) \ = \ \overline{\hat{h}(\mathbf{k})} \ ,$$

and hence $A_\beta(h)$ is a densely defined, *symmetric* operator on $\mathcal{F}$, (see, e.g., [8, 9]). Actually, much more is true: Let

$$N \ = \ \int d^3k \sum_{\lambda=\pm} a_\lambda(\mathbf{k})^* \ a_\lambda(\mathbf{k}) \tag{3.3}$$

denote the photon number operator on $\mathcal{F}$. This is a positive, selfadjoint operator on $\mathcal{F}$, and its spectrum consists of all non-negative integers. The eigenspace of N corresponding to a non-negative integer n is the subspace $\left(L^2\left(\mathbb{R}^3\right) \otimes \mathbb{C}^2\right)^{\otimes_s n}$ of $\mathcal{F}$ in the representation of $\mathcal{F}$ given in eq. (1.9).

We recall the following well known result.

Proposition 1, [8, 9, 11]

(1) For $h \in \mathcal{H}_{-1/2}$, h real, $\beta = 1, 2, 3$, the operator $A_\beta(h)$ defined in (3.2) is essentially selfadjoint on any core for N.

(2) The operators

$$\left\langle \exp i\mathbf{A}(\mathbf{h}) \ \middle| \ \mathbf{A}(\mathbf{h}) \ := \ \sum_{\beta=1}^{3} A_\beta(h_\beta), h_\beta \in \mathcal{H}_{-1/2}, \ h_\beta \text{ real}, \ \forall \ \beta \ = \ 1,2,3 \right\rangle \tag{3.4}$$

generate an *abelian* *algebra of bounded operators on $\mathcal{F}$. The vacuum Ω is a *cyclic* and *separating* vector for this algebra.

(3) For real functions h_1, h_2, h_3 in $\mathcal{H}_{-1/2}$ we have that

$$\langle \Omega,\ \exp i\, \mathbf{A}(\mathbf{h})\Omega\rangle_{\mathcal{F}} \; = \; \exp\left[-\frac{1}{2}\, Q(\mathbf{h})\right], \tag{3.5}$$

where

$$Q(\mathbf{h}) \; := \; \sum_{\beta,\gamma=1}^{3} \int \frac{d^3k}{|\mathbf{k}|}\, \overline{h_\beta(k)}\, \left(\delta_{\beta\,\gamma} - \frac{k_\beta\, k_\gamma}{|\mathbf{k}|^2}\right)\, h_\gamma(k). \tag{3.6}$$

Note that the quadratic form Q is positive semi-definite. More precisely, on the space

$$\mathcal{H}^T_{-1/2} \; = \; \left\{\mathbf{h} \; = \; (h_1, h_2, h_3)\, \middle|\, h_\beta \in \mathcal{H}_{-1/2},\ \beta = 1,2,3,\ \nabla \cdot \mathbf{h} \; = \; 0\right\},$$

Q is positive-definite. This implies that

$$\exp\left[-\frac{1}{2}\, Q(\mathbf{h})\right]$$

is the characteristic functional of a Gaussian measure, $d\mu_Q(\mathbf{A})$, of mean 0 and covariance Q with support contained in the Schwartz distribution space of transverse vector potentials,

$$\mathcal{A} \equiv \mathcal{S}^T(\mathbb{R}^3)' \; = \; \left\{\mathbf{A} = (A_1, A_2, A_3)\, \middle|\, A_\beta \in \mathcal{S}(\mathbb{R}^3)',\ \forall\beta = 1,2,3,\ \nabla \cdot \mathbf{A} = 0\right\}, \tag{3.7}$$

(Minlos' theorem; see e.g. [8]).

Remarks concerning the proof of Proposition 1.

The proofs of (1) and (2) can be inferred from [9, 11]. [The proof of the fact that Ω is cyclic for the algebra of operators defined in (3.4) follows from explicit calculations, see [9]; the rest follows from general results in [11].] Part (3) follows from a straightforward calculation. For further discussion and references see [8, 9, 11].

As a corollary of Proposition 1 and Minlos' theorem (see e.g. [8]), we conclude that Fock space $\mathcal{F}$ is isomorphic to the L^2-space $L^2(\mathcal{A}, d\mu_Q)$. In the representation of $\mathcal{F}$ as

$$\mathcal{F} \;\cong\; L^2(\mathcal{A},\ d\mu_Q), \tag{3.8}$$

called *Schrödinger representation* of $\mathcal{F}$, all the operators affiliated with the weak closure of the *algebra defined in (3.4), in particular $\mathbf{A}(\mathbf{h})$, for h_1, h_2 and h_3 functions in $\mathcal{H}_{-1/2}$, are *multiplication operators.* In particular, they are "simultaneously diagonalized", (see [8, 9] for further details).

4 Beginning of the proof of Theorem 1

In this section we reduce the proof of Theorem 1 to a result on H-stability of systems in arbitrary *external* magnetic fields (Theorem 2, below), making use of the Schrödinger representation of Fock space reviewed in the last section. The proof of Theorem 2 is then outlined in Sect. 5; (technical details can be found in [12]). Our strategy and most of the arguments in Sect. 4 follow those in [6].

We define

$$D(\mathbf{x}) \;=\; \min_{1 \le k \le M} \; |\mathbf{x} - \mathbf{y}_k| \; . \tag{4.1}$$

We employ the natural, dimensionless variables introduced in Sect. 2. Thus $\mathbf{x}$ and $\mathbf{y}_k$ are dimensionless, and the Bohr radius of an electron orbit bound to a nucleus of charge Ze is of order Z^{-1}.

We decompose the Hamiltonian H defined in eq. (2.13) into a sum of two terms:

$$H \;=\; H_I \;+\; \mathbf{I} \otimes H_{II} \;,$$

where

$$\begin{aligned} H_I \;&=\; \sum_{j=1}^{N} \Big[\boldsymbol{\sigma}^{(j)} \cdot \Big(-i\, \boldsymbol{\nabla}_j + 2\sqrt{\pi}\, \alpha^{3/2} \mathbf{A}^{(\Lambda)}\,(\alpha \mathbf{x}_j)\Big)\Big]^2 \\ &+\; V_C \otimes \mathbf{1} + \mathbf{1} \otimes \Big\{ 4\pi\alpha^2 \Gamma \int |\text{ curl } \mathbf{A}^{(\Lambda)}(\mathbf{x})|^2 \; e^{-L^{-1}D(\mathbf{x}/\alpha)} d^3x \\ &+\; 4\pi\, \alpha^4 C(\Gamma, Z) L^2 \int |\boldsymbol{\nabla} \otimes (\text{curl } \mathbf{A}^{(\Lambda)})(\mathbf{x})|^2 \; e^{-L^{-1}D(\mathbf{x}/\alpha)} d^3x \Big\} \end{aligned} \tag{4.2}$$

and

$$\begin{aligned} H_{II} \;&=\; H_{ph} - 4\pi\, \alpha^2 \Gamma \int |\text{ curl } \mathbf{A}^{(\Lambda)}(\mathbf{x})|^2 \; e^{-L^{-1}D(\mathbf{x}/\alpha)} d^3x \\ &\qquad -4\pi\, \alpha^4 C(\Gamma, Z) L^2 \int |\boldsymbol{\nabla} \otimes (\text{curl } \mathbf{A}^{(\Lambda)})(\mathbf{x})|^2 \; e^{-L^{-1}D(\mathbf{x}/\alpha)} d^3x \;, \end{aligned} \tag{4.3}$$

where Γ and $C(\Gamma, Z)$ are finite, positive constants yet to be chosen (see Theorem 2 and Sect. 5). On the r.s. of (4.2) we insert the fields $\boldsymbol{\mathcal{A}}$ and $\boldsymbol{\mathcal{B}}$ defined in eq. (2.15). Then we find that

$$\begin{aligned} H_I \;&=\; \sum_{j=1}^{N} \Big[\boldsymbol{\sigma}^{(j)} \cdot (-i\, \boldsymbol{\nabla}_j + \boldsymbol{\mathcal{A}}(\mathbf{x}_j))\Big]^2 \;+\; V_C \otimes \mathbf{I} \\ &+\; \mathbf{I} \otimes \Big\{ \Gamma \int |\boldsymbol{\mathcal{B}}(\mathbf{x})|^2 \; e^{-L^{-1}D(\mathbf{x})} d^3x \\ &\qquad + C(\Gamma, Z)\, L^2 \int |(\boldsymbol{\nabla} \otimes \boldsymbol{\mathcal{B}})(\mathbf{x})|^2 \; e^{-L^{-1}D(\mathbf{x})} d^3x \Big\} \;. \end{aligned} \tag{4.4}$$

It follows from the definition of $\boldsymbol{\mathcal{A}}$ and $\boldsymbol{\mathcal{B}} = \text{curl } \boldsymbol{\mathcal{A}}$, see eq. (2.15), and Proposition 1 of Sect. 3 that the components $\boldsymbol{\mathcal{A}}_\beta(\mathbf{x})$, $\boldsymbol{\mathcal{B}}_\beta(\mathbf{x})$ and $\partial_\alpha \boldsymbol{\mathcal{B}}_\beta(\mathbf{x})$ (with $\partial_\alpha = (\partial/\partial x^\alpha)$, $\alpha, \beta = 1, 2, 3$) are commuting, selfadjoint operators on $\mathcal{F}$, for arbitrary $\mathbf{x}$ and an arbitrary choice of the ultraviolet cutoff $\Lambda < \infty$; (see eq. (2.12)). These operators are multiplication operators in the Schrödinger representation (3.8) of Fock space. We conclude that, in order to prove a lower bound on the Hamiltonian H_I, it is enough to establish a lower bound on the following energy functional, $\mathcal{E}$:

$$\begin{aligned} \mathcal{E}(\psi, \boldsymbol{\mathcal{A}}) \; &:= \; \left\langle \psi, \left\{ \sum_{j=1}^{N} \left[\boldsymbol{\sigma}^{(j)} \cdot (-i\boldsymbol{\nabla}_j + \boldsymbol{\mathcal{A}}(\mathbf{x}_j)) \right]^2 \; + \; V_C \right\} \psi \right\rangle \\ &+ \; \int \left\{ \Gamma |\boldsymbol{\mathcal{B}}(\mathbf{x})|^2 \; + \; C(\Gamma, Z) \, L^2 |(\boldsymbol{\nabla} \otimes \boldsymbol{\mathcal{B}})(\mathbf{x})|^2 \right\} \, e^{-L^{-1} D(\mathbf{x})} d^3 x \; , \end{aligned} \tag{4.5}$$

for $\psi \in (\mathcal{H}_1)^{\wedge N}$, with $\| \psi \| = 1$, (where, recall, $\mathcal{H}_1 = L^2(\mathbb{E}^3, d^3x) \otimes \mathbb{C}^2$ is the one-electron Hilbert space), and for an *arbitrary external* vector potential $\boldsymbol{\mathcal{A}}$ (belonging to a suitable Sobolev space), with $\boldsymbol{\mathcal{B}} = \text{curl } \boldsymbol{\mathcal{A}}$. More precisely,

$$H_I \; \geq \; \left\{ \inf_{\psi : \|\psi\| = 1, \boldsymbol{\mathcal{A}}} \; \mathcal{E}(\psi, \boldsymbol{\mathcal{A}}) \right\} \; \mathbb{1} \; . \tag{4.6}$$

The functional $\mathcal{E}(\psi, \boldsymbol{\mathcal{A}})$ is studied in Sect. 5 and in ref. [12]. Our main result on this functional is described in the following theorem.

Theorem 2.

Given $\Gamma > 0$ and $Z < \infty$, there are finite, positive constants $c(\Gamma, Z)$, $C(\Gamma, Z)$ and $C'(\Gamma, Z)$ such that, for $\mathcal{E}(\psi, \boldsymbol{\mathcal{A}})$ as in (4.5), $\| \psi \| = 1$, and $L \leq c(\Gamma, Z)$,

$$\mathcal{E}(\psi, \boldsymbol{\mathcal{A}}) \; \geq \; - \, C'(\Gamma, Z) \, L^{-1} \, M \; , \tag{4.7}$$

where M is the number of nuclei.

If $\Gamma \geq Z^2$ there are finite, positive constants c and C such that, for

$$\begin{aligned} c(\Gamma, Z) \; = \; c \, Z^{-1}, \quad C(\Gamma, Z) \; = \; C \; Z^2 \; , \\ C'(\Gamma, Z) \; \leq \; C \; Z^2 \; . \end{aligned} \tag{4.8}$$

Remarks

(1) In [12], explicit expressions for $c(\Gamma, Z)$, $C(\Gamma, Z)$ and $C'(\Gamma, Z)$ are derived in the three regimes:

(i) $\Gamma \geq Z^2$, (ii) $Z^2 \geq \Gamma \geq 1$, (iii) $\Gamma \leq 1$.

Below we shall choose $\Gamma = \frac{1}{16\pi\,\alpha^2}$, where α is the finestructure constant. Since $\alpha \cong 1/137$, regime (i) is the one most relevant for atomic physics. We therefore do not present explicit expressions for $c\,(\Gamma, Z)$ and $C'(\Gamma, Z)$ in regimes (ii) and (iii), but refer the reader to [12].

(2) We recall that the results proven in [5, 6] imply that, for $\Gamma = (8\pi\,\alpha^2)^{-1}$, $\alpha \leq 1/132$ and $Z \leq 6$, we have that

$$\begin{aligned} &\left\langle \psi, \left\{ \sum_{j=1}^{N} \left[\boldsymbol{\sigma}^{(j)} \cdot (-i\,\nabla_j + \boldsymbol{\mathcal{A}}\,(\mathbf{x}_j)) \right]^2 \;+\; V_C \right\} \psi \right\rangle \\ &\qquad + \Gamma \int\limits_{\Omega} \left|\, (\nabla \otimes \boldsymbol{\mathcal{A}})(\mathbf{x}) \,\right|^2 d^3x \;\geq\; -\,CZ^2(N+M), \end{aligned} \tag{4.9}$$

for a finite constant C. Here

$$\Omega \;=\; \left\{ \mathbf{x} \in \mathbb{E}^3 \;\middle|\; |\mathbf{x} - \mathbf{y}_l| \;\leq\; (Z+1)^{-1}, \;\; \text{for some} \;\; l = 1, \cdots, M \right\} \;.$$

As shown in [6], this implies part (2) of Theorem 1, (for $Z \leq 6$).

Our next task is to prove a lower bound on the operator H_{II}, and here we follow arguments described in Sect. 3 of [6].

Recall that

$$\begin{aligned} \mathbf{A}_{-}^{(\Lambda)}(\mathbf{x}) \;&=\; \frac{1}{(2\pi)^{3/2}} \int \frac{d^3k}{\sqrt{2|\mathbf{k}|}}\, \Lambda(\mathbf{k}) \left\{ \sum_{\lambda=\pm} a_\lambda(\mathbf{k})\, \boldsymbol{\varepsilon}_\lambda(\mathbf{k})\; e^{i\,\mathbf{k}\cdot\mathbf{x}} \right\}, \\ \mathbf{A}_{+}^{(\Lambda)}(\mathbf{x}) \;&=\; \left(\mathbf{A}_{-}^{(\Lambda)}(\mathbf{x}) \right)^*, \quad \mathbf{A}^{(\Lambda)}(\mathbf{x}) \;=\; \mathbf{A}_{+}^{(\Lambda)}(\mathbf{x}) \;+\; \mathbf{A}_{-}^{(\Lambda)}(\mathbf{x}), \end{aligned} \tag{4.10}$$

and $\Lambda(\mathbf{k})$ is a (smooth) function, with

$$|\Lambda(\mathbf{k})| \;\leq\; 1 \quad \text{and} \quad \text{supp}\,\Lambda \;\subseteq\; \left\{ \mathbf{k} \;\middle|\; |\mathbf{k}| \;\leq\; (2m\,\alpha^2)^{-1}\,\Lambda \right\} \;;$$

see eq. (2.12). We set

$$\mathbf{B}^{\pm}(\mathbf{x}) \;:=\; \text{curl}\; \mathbf{A}_{\pm}^{(\Lambda)}(\mathbf{x}), \quad \Pi^{\pm}(\mathbf{x}) \;=\; \nabla \otimes \mathbf{B}^{\pm}(\mathbf{x}) \;. \tag{4.11}$$

Clearly

$$B_\beta^{+}(\mathbf{x}) \;=\; \left(B_\beta^{-}(\mathbf{x}) \right)^*, \quad \Pi_{\beta\delta}^{+}(\mathbf{x}) \;=\; \left(\Pi_{\beta\delta}^{-}(\mathbf{x}) \right)^* \;. \tag{4.12}$$

We define

$$F^{\pm}(\mathbf{x}) \;=\; \begin{cases} B_\beta^{\pm}\,(\mathbf{x}), & \text{or} \\ \Pi_{\beta\delta}^{\pm}\,(\mathbf{x}), & \end{cases} \tag{4.13}$$

$\beta, \delta = 1, 2, 3$, and $F(\mathbf{x}) = F^+(\mathbf{x}) + F^-(\mathbf{x})$.

Let $f(\mathbf{x})$ be a positive function on $\mathbb{E}^3$. Then

$$\begin{aligned} f(\mathbf{x})\, F(\mathbf{x})^2 &= f(\mathbf{x}) \left[F^+(\mathbf{x})\, F^-(\mathbf{x}) \,+\, F^-(\mathbf{x})\, F^+(\mathbf{x}) \,+\, F^+(\mathbf{x})^2 \,+\, F^-(\mathbf{x})^2 \right] \\ &\leq 2f\,(\mathbf{x}) \left[F^+(\mathbf{x})\, F^-(\mathbf{x}) \,+\, F^-(\mathbf{x})\, F^+(\mathbf{x}) \right] \\ &= 4f\,(\mathbf{x}) \left[F^+(\mathbf{x})\, F^-(\mathbf{x}) \,+\, \frac{1}{2} \,\parallel F^+(\mathbf{x})\,\Omega \parallel^2 \right] , \end{aligned} \tag{4.14}$$

where Ω is the vacuum vector in $\mathcal{F}$. To prove (4.14), we use the general inequality

$$\begin{aligned} \left| \, \langle \psi, T^2 \psi \rangle \, \right| &\leq \parallel T^* \psi \parallel \, \parallel T \psi \parallel \\ &\leq \frac{1}{2} \, \langle \psi, (T\,T^* \,+\, T^*\,T)\; \psi \rangle , \end{aligned}$$

for an arbitrary operator T and ψ in the intersection of the domain of T and the domain of T^*. We apply this inequality to the special choice of $T = F^{\pm}(\mathbf{x})$. Next, we note that

$$\begin{aligned} F^-(\mathbf{x})\, F^+(\mathbf{x}) &= F^+(\mathbf{x})\, F^-(\mathbf{x}) \,+\, \left[F^-(\mathbf{x}), F^+(\mathbf{x}) \right] \\ &= F^+(\mathbf{x})\, F^-(\mathbf{x}) \,+\, \langle \Omega, F^-(\mathbf{x})\, F^+(\mathbf{x}) \Omega \rangle \\ &= F^+(\mathbf{x})\, F^-(\mathbf{x}) \,+\, \parallel F^+(\mathbf{x})\, \Omega \parallel^2 , \end{aligned}$$

which is a simple consequence of eqs. (4.10)-(4.13); (recall the commutation relations (2.3) and use that $a_\lambda(\mathbf{k})\Omega = 0$, for $\lambda = \pm$ and all $\mathbf{k} \in \mathbb{R}^3$, where Ω is the vacuum vector in $\mathcal{F}$). It is obvious that $\parallel F^+(\mathbf{x})\Omega \parallel^2$ is independent of $\mathbf{x}$. Thus inequality (4.14) yields the bound

$$\int f(\mathbf{x})\, F(\mathbf{x})^2 \; d^3x \;\leq\; 4 \parallel f \parallel_\infty \int F^+(\mathbf{x})\, F^-(\mathbf{x}) \; d^3x \;+\; 2 \parallel f \parallel_1 \, \parallel F^+(0)\Omega \parallel^2 . \tag{4.15}$$

We apply inequality (4.15) to the examples in (4.13) and sum over $\beta, \delta = 1, 2, 3$. This yields

$$\begin{aligned} &\int f(\mathbf{x}) \,\left|\, \mathrm{curl}\ \mathbf{A}^{(\Lambda)}(\mathbf{x}) \,\right|^2 \; d^3x \\ &\quad \leq\; 2 \parallel f \parallel_\infty \int d^3k \,\left|\, \Lambda(\mathbf{k}) \,\right|^2 \left\{ \sum_{\lambda=\pm} a_\lambda^*(\mathbf{k}) |\mathbf{k}| a_\lambda(\mathbf{k}) \right\} \\ &\quad\quad + 2 \parallel f \parallel_1 \; C_\Lambda , \end{aligned} \tag{4.16}$$

where

$$C_\Lambda \;=\; \sum_{\beta=1}^{3} \parallel B_\beta^+(0)\, \Omega \parallel^2 , \tag{4.17}$$

and

$$\begin{aligned} &\int f(\mathbf{x}) \,\left|\, \boldsymbol{\nabla} \otimes \left(\mathrm{curl}\ \mathbf{A}^{(\Lambda)} \right) (\mathbf{x}) \,\right|^2 \; d^3x \\ &\quad \leq\; 2 \parallel f \parallel_\infty \int d^3k \,\left|\, \Lambda(\mathbf{k}) \,\right|^2 \left\{ \sum_{\lambda=\pm} a_\lambda^*(\mathbf{k}) |\mathbf{k}|^3 a_\lambda(\mathbf{k}) \right\} \\ &\quad\quad + 2 \parallel f \parallel_1 \; D_\Lambda , \end{aligned} \tag{4.18}$$

where

$$D_\Lambda \;=\; \sum_{\beta,\delta=1}^{3} \parallel \Pi^{+}_{\beta\,\delta}\;(0)\;\Omega \parallel^2 \;\; . \tag{4.19}$$

Comparing these expressions with eq. (2.4) and using the definition of $\Lambda(\mathbf{k})$, eq. (2.12), we find that

$$\int f(\mathbf{x}) \mid \mathrm{curl}\; \mathbf{A}^{(\Lambda)}(\mathbf{x}) \mid^2 d^3x \;\leq\; 2 \parallel f \parallel_\infty H_{ph} \;+\; 2 \parallel f \parallel_1 C_\Lambda, \tag{4.20}$$

and

$$\begin{aligned} &\int f(\mathbf{x}) \mid \boldsymbol{\nabla} \otimes \left(\mathrm{curl}\; \mathbf{A}^{(\Lambda)}\right) (\mathbf{x}) \mid^2 d^3x \\ &\quad\leq\; 2 \parallel f \parallel_\infty (2m\,\alpha^2)^{-2} \Lambda^2 H_{ph} \;+\; 2 \parallel f \parallel_1 D_\Lambda \;. \end{aligned} \tag{4.21}$$

We are now prepared to prove a lower bound on the operator H_{II} defined in (4.3). We choose

$$f(\mathbf{x}) \;=\; \exp\;\left(-L^{-1} D(\mathbf{x}/\alpha)\right) \;, \tag{4.22}$$

so that

$$\parallel f \parallel_\infty =\; 1, \quad \parallel f \parallel_1 \leq\; 8\pi\,\alpha^3\, L^3\, M \;. \tag{4.23}$$

We choose Γ and L so small that

$$8\pi\,\alpha^2\,\Gamma \;+\; 8\pi\, C(\Gamma, Z)\, L^2 \left(\frac{\Lambda}{2m}\right)^2 \;\leq\; 1 \;. \tag{4.24}$$

Then

$$H_{II} \;\geq\; -\, 64\pi^2\, \alpha^5\, L^3\, M\; \left(\Gamma\, C_\Lambda \,+\, \alpha^2\, C(\Gamma, Z)\, L^2\, D_\Lambda\right) \;. \tag{4.25}$$

Next, we calculate the constants C_Λ and D_Λ. The result is that

$$C_\Lambda \;\leq\; \frac{1}{2} \int\limits_{B_\Lambda} d^3k|\mathbf{k}| \;=\; \frac{\pi}{2} \left(\frac{\Lambda}{2m\,\alpha^2}\right)^4 \;, \tag{4.26}$$

and

$$D_\Lambda \;\leq\; \frac{1}{2} \int\limits_{B_\Lambda} d^3k|\mathbf{k}|^3 \;=\; \frac{\pi}{3} \left(\frac{\Lambda}{2m\,\alpha^2}\right)^6 \;, \tag{4.27}$$

where B_Λ is the ball of radius $(2m\,\alpha^2)^{-1}\Lambda$ centered at the origin of $\mathbb{R}^3$; (confer to eq. (2.12)). Plugging (4.26) and (4.27) into the r.s. of (4.25) and using (4.24), we obtain the bound

$$H_{II} \;\geq\; -\,4\pi^2\, \alpha^{-5}\, L^3 \left(\frac{\Lambda}{2m}\right)^4 \; M \;. \tag{4.28}$$

Choosing

$$L \;\leq\; \min\;\left(c\,(\Gamma, Z),\, \left(16\pi\, C(\Gamma, Z) \left(\frac{\Lambda}{2m}\right)^{2} \right)^{-1/2} \right) \;, \tag{4.29}$$

see Theorem 2 and (4.24), and combining inequalities (4.7) and (4.28), we find that

$$H \;\geq\; -\left(4\pi\;\alpha^{-5}\;L^{3}\;\left(\frac{\Lambda}{2m}\right)^{4} \;+\; \frac{C'(\Gamma, Z)}{L} \right)\; M \;. \tag{4.30}$$

This bound enables us to complete the proof of part (1) of Theorem 1: By (4.24) and (4.29), we can choose

$$\Gamma \;=\; \left(16\pi\,\alpha^{2}\right)^{-1} \;,\;\; L \;=\; C''(\alpha, Z)\;\frac{2m}{\Lambda}\;, \tag{4.31}$$

for some finite constant $C''(\alpha, Z)$. Then inequality (4.30) shows that there is a finite constant $\varepsilon(\alpha, Z)$ depending on α and Z, but *independent* of Λ, such that

$$H \;\geq\; -\,\varepsilon(\alpha, Z)\;\frac{\Lambda}{2m}\;\cdot\; M\;. \tag{4.32}$$

Hence, since $\widetilde{H} = 2m\,\alpha^{2} H$, part (1) of Theorem 1 is proven.

In order to prove part (2) of Theorem 2, we set $\Gamma = (16\pi\,\alpha^{2})^{-1}$ and assume that $\Gamma \geq Z^{2}$, i.e., $16\pi(\alpha Z)^{2} \;\leq 1$. Furthermore we make the following choices:

$$L \;=\; c'\,Z^{-3/2},\;\; \text{for some } c' \;\leq\; c, \tag{4.33}$$

$$\Lambda \;=\; 2m\,Z^{2}\,\alpha^{5/4}\;. \tag{4.34}$$

For these choices

$$L \;\leq\; c\,(\Gamma, Z) \;=\; c\,Z^{-1}\;,\;\; \text{for } Z \;\geq\; 1\;,$$

so that Theorem 2 applies, and

$$8\pi\,C(\Gamma, Z)\,L^{2}\;\left(\frac{\Lambda}{2m}\right)^{2} \;=\; C'''\,Z^{-1}\left(Z^{2}\,\alpha^{5/4}\right)^{2} \;<\; \frac{1}{2} \tag{4.35}$$

for $Z^{3}\,\alpha^{5/2}$ small enough, so that inequality (4.24) holds. Then inequality (4.30) implies that

$$H \;\geq\; -\,\varepsilon\;Z^{7/2}\;\cdot\; M\;, \tag{4.36}$$

for some constant ε independent of α and Z. Since $\widetilde{H} = 2m\,\alpha^{2}\,H$, part (2) of Theorem 1 follows from (4.36).

It remains to prove Theorem 2. This is the task of Section 5, (see also [12]).

5 Outline of proof of Theorem 2

Before beginning with the proof of Theorem 2 we briefly recall its statement. Let $\boldsymbol{\mathcal{A}}(\mathbf{x})$ denote a vector potential on $\mathbb{E}^3$, and let $\boldsymbol{\mathcal{B}}(\mathbf{x}) = \mathrm{curl}\ \boldsymbol{\mathcal{A}}(\mathbf{x})$. We fix a configuration of nuclei at positions $\mathbf{y}_1, \cdots, \mathbf{y}_M$ in $\mathbb{E}^3$ and with atomic numbers $Z_1, \cdots, Z_M$. We assume that $\max_{1 \leq l \leq M} Z_l \leq Z$, for an arbitrary, but fixed $Z < \infty$.

Let

$$H_{\text{Pauli}} = \sum_{j=1}^{N} \left[\boldsymbol{\sigma}^{(j)} \cdot (i\, \boldsymbol{\nabla}_j - \boldsymbol{\mathcal{A}}(\mathbf{x}_j)) \right]^2 + V_C \ ,$$

with V_C as in (2.7). For a smooth, bounded vector potential $\boldsymbol{\mathcal{A}}$, H_{Pauli} is a densely defined, selfadjoint operator on $(\mathcal{H}_1)^{\wedge N}$, with $\mathcal{H} = L^2(\mathbb{E}^3, d^3x) \otimes \mathbb{C}^2$ (see Sect. 1) whose spectrum is bounded below. In Sect. 4, the following result, Theorem 2, has been stated.

Theorem

Given positive constants Γ and Z, there are finite, positive constants $c(\Gamma, Z)$, $C(\Gamma, Z)$ and $C'(\Gamma, Z) \leq C(\Gamma, Z)$ such that, for $L \leq c(\Gamma, Z)$,

$$\begin{aligned} \langle \psi, H_{\text{Pauli}}\, \psi \rangle \ + \ \Gamma \int |\boldsymbol{\mathcal{B}}(\mathbf{x})|^2\ e^{-D(\mathbf{x})/L}\ d^3x & \\ + \ C(\Gamma, Z) \int L^2 |(\boldsymbol{\nabla} \otimes \boldsymbol{\mathcal{B}})(\mathbf{x})|^2\ e^{-D(\mathbf{x})/L}\ d^3x \ & \geq \ -\frac{C'(\Gamma, Z)}{L}\ M \ , \end{aligned}$$

for any $\psi \in (\mathcal{H}_1)^{\wedge N}$ of norm 1.

Remark: The constants $c(\Gamma, Z)$, $C(\Gamma, Z)$ and $C'(\Gamma, Z)$ only depend on Γ and Z. If we are not interested in optimal estimates we can set $C(\Gamma, Z) = C'(\Gamma, Z)$. In [12] it is shown that, for $\Gamma \geq Z^2$, there are finite, positive constants c and C such that

$$c(\Gamma, Z) \ = \ c\, Z^{-1}, \ C(\Gamma, Z) \ = \ C\, Z^2, \ C'(\Gamma, Z) \ \leq \ C\, Z^2 \ .$$

We sketch the proof of the above theorem. Our goal is to convey the spirit of the proof, sacrificing technical accuracy for the sake of simplicity. A complete proof of the theorem appears in [12].

The proof combines tricks from [13] and [14] with a new lower bound for the Pauli kinetic energy. We explain first the old tricks, then the new kinetic energy bound, and finally how to mix the ingredients and prove the theorem. Without sacrificing any ideas, we just treat the case $Z_1 = \cdots = Z_M = 1$, but see [12].

To explain the old tricks, we first note that one can associate local kinetic and potential energies to a cube $Q \subset \mathbb{E}^3$. If $\boldsymbol{\mathcal{A}}$ is a vector potential and $\psi \in (\mathcal{H}_1)^{\wedge N}$, then we write

$$T_{\text{Pauli}}(\psi, \boldsymbol{\mathcal{A}}, Q) \;=\; \sum_{k=1}^{N} \int\limits_{\mathbb{E}^{3N}} \left| \boldsymbol{\sigma}^{(\mathbf{k})} \cdot (i\, \boldsymbol{\nabla}_{\mathbf{x}_k} \;-\; \boldsymbol{\mathcal{A}}(\mathbf{x}_k))\, \psi \right|^2 \chi_Q\,(\mathbf{x}_k)\, d^3x_1 \cdots d^3x_N \tag{5.1}$$

and

$$T(\psi, \boldsymbol{\mathcal{A}}, Q) \;=\; \sum_{k=1}^{N} \int\limits_{\mathbb{E}^{3N}} \left| (i\, \boldsymbol{\nabla}_{\mathbf{x}_k} \;-\; \boldsymbol{\mathcal{A}}(\mathbf{x}_k))\, \psi \right|^2 \; \chi_Q(\mathbf{x}_k)\, d^3x_1 \cdots d^3x_N \;, \tag{5.2}$$

where χ_Q denotes the characteristic function of Q. To localize the potential energy to Q, we use the following identity from [13].

$$V_C \;=\; \frac{1}{2\pi} \iint\limits_{\mathbb{E}^3 \times \mathbb{R}^+} \Omega_{z\,R}\, \frac{d^3z\, dR}{R^5}\;, \quad \text{where} \tag{5.3}$$

$$\Omega_{z\,R} \;=\; N_{z\,R}(N_{z\,R} - 1) \;+\; M_{z\,R}(M_{z\,R} - 1) - 2\, N_{z\,R}\, M_{z\,R}\;, \text{ with} \tag{5.4}$$

$$N_{z\,R} \;=\; \text{ number of electrons in the ball } B(z, R), \text{ and} \tag{5.5}$$

$$M_{z\,R} \;=\; \text{ number of nuclei in } B(z, R)\;. \tag{5.6}$$

Here, $B(z, R)$ denotes the ball in $\mathbb{E}^3$ with center at z and radius R. Identity (5.3) lets us define the localized potential energy as follows. If $Q \subset \mathbb{E}^3$ is a cube of side δ, then we set

$$PE(\psi, Q) \;=\; \sum_{y_k\, \in\, Q} \left\langle \frac{1}{2\pi} \iint\limits_{\substack{B(z,R)\; \ni\; y_k \\ R\; <\; \frac{1}{10}\,\delta}} \frac{\Omega_{zR}}{M_{zR}}\, \frac{d^3z\, dR}{R^5}\, \psi,\; \psi \right\rangle . \tag{5.7}$$

Since $\Omega_{zR} \;\geq\; -CM_{zR}$ always, and, in particular, $\Omega_{zR} \;\geq\; 0$ when $M_{zR} = 0$, the following remarks are trivial consequences of the above definitions.

(i) If $\mathbb{E}^3$ is partitioned into cubes $\{Q_\nu\}$ of sides $\{\delta_\nu\}$, then

$$\left\langle \sum_{k=1}^{N} \left[\boldsymbol{\sigma}^{(k)} \cdot (i\, \boldsymbol{\nabla}_{\mathbf{x}_k} - \boldsymbol{\mathcal{A}}(\mathbf{x}_k)) \right]^2 \psi, \psi \right\rangle \;=\; \sum_{\nu} T_{\text{Pauli}}\;(\psi, \boldsymbol{\mathcal{A}}, Q), \text{ and} \tag{5.8}$$

$$\langle V_C\; \psi, \psi \rangle \;\geq\; \sum_{\nu} PE(\psi, Q_\nu) \;-\; C \sum_{\nu} \mathcal{M}_{Q_\nu}\; \delta_\nu^{-1}\;. \tag{5.9}$$

In (5.9) and throughout our discussion, $\mathcal{N}_Q$ denotes the number of electrons and $\mathcal{M}_Q$ the number of nuclei in Q. Similarly:

(ii) If Q is partitioned into subcubes $\{Q_\nu\}$ with sides $\{\delta_\nu\}$, then

$$T(\psi, \boldsymbol{\mathcal{A}}, Q) \;=\; \sum_\nu T(\psi, \boldsymbol{\mathcal{A}}, Q_\nu) \;, \tag{5.10}$$

$$T_{\text{Pauli}}(\psi, \boldsymbol{\mathcal{A}}, Q) \;=\; \sum_\nu T_{\text{Pauli}}(\psi, \boldsymbol{\mathcal{A}}, Q_\nu) \;, \text{ and} \tag{5.11}$$

$$PE(\psi, Q) \;\geq\; \sum_\nu PE(\psi, Q_\nu) \;-\; C \sum_\nu \delta_\nu^{-1} \, \mathcal{M}_{Q_\nu} \;. \tag{5.12}$$

The standard integration by parts, $\int_{\mathbb{E}^3} |\sigma \cdot (i\boldsymbol{\nabla} - \boldsymbol{\mathcal{A}})\varphi|^2 d^3x = \int_{\mathbb{E}^3} |(i\boldsymbol{\nabla} - \boldsymbol{\mathcal{A}})\varphi|^2 d^3x \pm \int_{\mathbb{E}^3} (\sigma \cdot B)\varphi \cdot \bar{\varphi}\, d^3x$ trivially implies the following; (we write Q^* for the double of Q).

KE **Comparison Lemma**:
Let Q be a cube of side δ. Suppose the magnetic field $\boldsymbol{\mathcal{B}}$ is constant on Q^*. Then

$$T_{\text{Pauli}}(\psi, \boldsymbol{\mathcal{A}}, Q^*) \;\geq\; c\, T(\psi, \boldsymbol{\mathcal{A}}, Q) - C\,\{|\boldsymbol{\mathcal{B}}| + \delta^{-2}\}\langle \mathcal{N}_{Q^*}\psi, \psi\rangle \;. \tag{5.13}$$

One of the main technical results in [14], proven also in [12], is as follows.

Local Stability of Matter:
Let Q be a cube of side δ. Suppose the magnetic field $\boldsymbol{\mathcal{B}}$ satisfies $|\boldsymbol{\mathcal{B}}| \leq C\,\delta^{-2}$ on Q^*. Then

$$\delta \cdot T(\psi, \boldsymbol{\mathcal{A}}, Q^*) \;+\; PE(\psi, Q) \;\geq\; -\,C\,\delta^{-1}\langle \mathcal{N}_{Q^*}\psi, \psi\rangle \;. \tag{5.14}$$

Here, we have oversimplified slightly the statement of local stability. We will also oversimplify below by neglecting the distinction between Q and Q^*, and by supposing where necessary that $\mathcal{N}_Q$ and $\mathcal{M}_Q$ are of the same order of magnitude. (If not, then Q is far from electrically neutral, so that $PE(\psi, Q)$ will be large positive, and whatever lower bounds we claim for the energy will therefore be trivial.) The new ingredient in the proof of our theorem is the following estimate.

KE **Lower Bound**:
Let Q be the unit cube, and suppose the magnetic field $\boldsymbol{\mathcal{B}}$ is constant on Q^*. If $K > 1$, then

$$T_{\text{Pauli}}(\psi, \boldsymbol{\mathcal{A}}, Q^*) \;\geq\; c\,K\langle \mathcal{N}_Q\psi, \psi\rangle - C\,K^{5/2}\{|\boldsymbol{\mathcal{B}}| + 1\} - C\langle \mathcal{N}_{Q^*}\psi, \psi\rangle \;. \tag{5.15}$$

We sketch the proof of the KE Lower Bound, then return to the proof of Theorem 2. The main point in establishing (5.15) is to prove an estimate for one-electron wave functions $\varphi \in \mathcal{H}_1$ from which (5.15) will follow by separation of variables. Without significant loss of generality, we may suppose that the magnetic field $\boldsymbol{\mathcal{B}}$ points parallel to the x_3-axis. In a suitable gauge we then have $\boldsymbol{\mathcal{A}}(\mathbf{x}) = (\boldsymbol{\mathcal{A}}_1(\mathbf{x}), \boldsymbol{\mathcal{A}}_2(\mathbf{x}), 0)$, with $\boldsymbol{\mathcal{A}}_\nu(\mathbf{x})$ independent of x_3, and $|\boldsymbol{\nabla}\boldsymbol{\mathcal{A}}_\nu| \leq C|\boldsymbol{\mathcal{B}}|$.

Integration by parts yields the identities

$$\int\limits_{\mathbb{E}^3} \left| \boldsymbol{\sigma} \cdot (i\boldsymbol{\nabla} - \boldsymbol{\mathcal{A}})\varphi \right|^2 d^3x = \int\limits_{\mathbb{E}^3} \left| (i\boldsymbol{\nabla} - \boldsymbol{\mathcal{A}})\varphi \right|^2 d^3x \pm \int\limits_{\mathbb{E}^3} (\boldsymbol{\sigma} \cdot \boldsymbol{\mathcal{B}})\varphi \cdot \bar{\varphi} d^3x, \tag{5.16}$$

$$\int\limits_{\mathbb{E}^3} \left| \boldsymbol{\sigma} \cdot (i\boldsymbol{\nabla} - \boldsymbol{\mathcal{A}})\varphi \right|^2 d^3x = \int\limits_{\mathbb{E}^3} \left| \frac{\partial}{\partial x_3}\varphi \right|^2 d^3x$$

$$+ \int\limits_{\mathbb{E}^3} \left| \sum_{\nu=1,2} \sigma_\nu \left(i\frac{\partial}{\partial x_\nu} - \mathcal{A}_\nu \right) \varphi \right|^2 d^3x. \tag{5.17}$$

Applying (5.16) and (5.17) with φ replaced by $\theta\varphi$, for a suitable cutoff θ, we derive the estimate

$$\int\limits_{Q^*} \left| \boldsymbol{\sigma} \cdot (i\boldsymbol{\nabla} - \boldsymbol{\mathcal{A}})\varphi \right|^2 d^3x \ \geq$$

$$c \int\limits_{Q} \left\{ \left| \frac{\partial \varphi}{\partial x_3} \right|^2 + (|\boldsymbol{\mathcal{B}}| + 1)^{-1} \sum_{\nu=1,2} \left| \left(i\frac{\partial}{\partial x_\nu} - \mathcal{A}_\nu \right) \varphi \right|^2 \right\} d^3x - C \int\limits_{Q^*} |\varphi|^2 d^3x \ . \tag{5.18}$$

In deriving (5.18), we had to multiply (5.16) by $(|\boldsymbol{\mathcal{B}}| + 1)^{-1}$ to reduce the effect of the error term $\int_{\mathbb{E}^3} (\boldsymbol{\sigma} \cdot \boldsymbol{\mathcal{B}})\varphi \cdot \bar{\varphi} d^3x$. Next, we cut the unit cube Q into thin rectangular tubes $T_\alpha = I_{\alpha 1} \times I_{\alpha 2} \times I_{\alpha 3}$, where $|I_{\alpha 3}| = 1$ and $I_{\alpha 1} \times I_{\alpha 2}$ is a small square of size $\sim (|\boldsymbol{\mathcal{B}}| + 1)^{-1/2}$. Thus the T_α are parallel to the magnetic field. The number of distinct T_α's is $\sim (|\boldsymbol{\mathcal{B}}| + 1)$. Since $|I_{\alpha 1}|, |I_{\alpha 2}| \sim (|\boldsymbol{\mathcal{B}}| + 1)^{-1/2}$, while $|\boldsymbol{\nabla} \mathcal{A}_\nu| \leq C|\boldsymbol{\mathcal{B}}|$ and $\mathcal{A}_\nu(\mathbf{x})$ is independent of x_3, it follows that $|\mathcal{A}_\nu(\mathbf{x}) - \mathcal{A}_\nu^\alpha| \leq C(|\boldsymbol{\mathcal{B}}| + 1)^{-1/2}$, for $x \in T_\alpha$, where $\mathcal{A}_\nu^\alpha$ is the value of $\mathcal{A}_\nu$ at the center of T_α. Hence, for $x \in T_\alpha$, we have

$$\left| \left(i\frac{\partial}{\partial x_\nu} - \mathcal{A}_\nu(\mathbf{x}) \right) \varphi \right|^2 \geq \frac{1}{2} \left| \left(i\frac{\partial}{\partial x_\nu} - \mathcal{A}_\nu^\alpha \right) \varphi \right|^2 - C(|\boldsymbol{\mathcal{B}}| + 1)|\varphi|^2,$$

and therefore (5.18) implies that

$$\int_{Q^*} |\boldsymbol{\sigma} \cdot (i\boldsymbol{\nabla} - \boldsymbol{\mathcal{A}})\varphi|^2 d^3x \geq c \sum_\alpha \int\limits_{T_\alpha} \left\{ \left| \frac{\partial \varphi}{\partial x_3} \right|^2 \right.$$

$$\left. + (|\boldsymbol{\mathcal{B}}| + 1)^{-1} \sum_{\nu=1,2} \left| \left(i\frac{\partial}{\partial x_\nu} - \mathcal{A}_\nu^\alpha \right) \varphi \right|^2 \right\} d^3x - C \int_{Q^*} |\varphi|^2 d^3x \ . \tag{5.19}$$

This is the basic one-electron estimate in the proof of (5.15). By rescaling and making a gauge transformation, we may regard the r.s. of (5.19) as the kinetic energy of a free particle in $\sim (|\boldsymbol{\mathcal{B}}| + 1)$ copies of the unit cube. Thus, the KE Bound (5.15) follows easily from (5.19) by separation of variables (reflecting the fact that there are $\sim K^{3/2}$ eigenstates of a free particle in the unit cube having energy less than K).

In using (5.15), we will drop the last term $\langle \mathcal{N}_{Q^*}\psi, \psi \rangle$. Roughly speaking, if we neglect the distinction between Q^* and Q, then the error term $\langle \mathcal{N}_{Q^*}\psi, \psi \rangle$ may be absorbed in the main term $cK\langle \mathcal{N}_Q\psi,\psi\rangle$ if K is large. This is of course only a heuristic justification for dropping the last term in (5.15). In the full proof we keep the last term which complicates the analysis.

We can start to combine the above ingredients to prove our theorem. The first main point is to prove the following local stability bound.

Local Pauli Stability (Constant Fields): Let K, B_0 be large constants, to be picked later, and let Q be a cube of side δ. Suppose the magnetic field $\boldsymbol{\mathcal{B}} = \mathrm{curl}\ \boldsymbol{\mathcal{A}}$ is constant on Q, and satisfies there $|\boldsymbol{\mathcal{B}}| \le CB_0\delta^{-2}$. Then

$$CB_0^{1/2}\delta \cdot T_{\mathrm{Pauli}}(\psi,\boldsymbol{\mathcal{A}},Q) + PE(\psi,Q) \ \ge\ -C\,K^{5/2}\,B_0^{3/2}\,\delta^{-1} + c\,\frac{B_0^{1/2}K}{\delta}\langle \mathcal{N}_Q\psi,\psi\rangle. \tag{5.20}$$

An essential point here is that B_0 appears on the right side in (5.20), raised to a power less than 2. To prove (5.20), we subdivide Q into subcubes $\{\hat{Q}_\alpha\}$ of side $\sim B_0^{-1/2}\delta$. Applying local stability of matter (5.14) to the $\hat{Q}_\alpha$, and summing over α using (5.10) and (5.12), we find that

$$C\,B_0^{-1/2}\delta \cdot T(\psi,\boldsymbol{\mathcal{A}},Q) + PE(\psi,\boldsymbol{\mathcal{A}},Q) \ \ge\ -C\,B_0^{1/2}\delta^{-1}\langle \mathcal{N}_Q\psi,\psi\rangle - C\,B_0^{1/2}\delta^{-1}\mathcal{M}_Q. \tag{5.21}$$

We drop the $\mathcal{M}_Q$ term in (5.21) for expository purposes. The rough justification for this is that we may suppose (as explained earlier) that $\mathcal{M}_Q$ and $\mathcal{N}_Q$ are comparable, so that the two terms on the right side in (5.21) are also comparable. In the complete proof of our theorem, we do not drop the $\mathcal{M}_Q$ term from (5.21), and matters become more complicated.

The KE Comparison Lemma yields (roughly speaking)

$$C'B_0^{-1/2}\delta \cdot T_{\mathrm{Pauli}}(\psi,\boldsymbol{\mathcal{A}},Q) \ \ge\ C\,B_0^{-1/2}\delta \cdot T(\psi,\boldsymbol{\mathcal{A}},Q) \ -\ C'B_0^{1/2}\delta^{-1}\langle \mathcal{N}_Q,\psi,\psi\rangle. \tag{5.22}$$

Putting (5.22) into (5.21), we find that

$$C\,B_0^{-1/2}\delta \cdot T_{\mathrm{Pauli}}(\psi,\boldsymbol{\mathcal{A}},Q) + PE(\psi,Q) \ \ge\ -C'B_0^{1/2}\delta^{-1}\langle \mathcal{N}_Q\psi,\psi\rangle. \tag{5.23}$$

Also, the KE Lower Bound (5.15) shows, roughly speaking, that

$$C\,B_0^{1/2}\delta \cdot T_{\mathrm{Pauli}}(\psi,\boldsymbol{\mathcal{A}},Q) \ \ge\ c\,K\,B_0^{1/2}\delta^{-1}\langle \mathcal{N}_Q\psi,\psi\rangle - C\,K^{5/2}B_0^{3/2}\delta^{-1}. \tag{5.24}$$

(Here, we have rescaled (5.15) from the unit cube to the cube Q.) Adding (5.23) and (5.24), we obtain

$$\begin{aligned} &C\,B_0^{1/2}\delta \cdot T_{\mathrm{Pauli}}(\psi,\boldsymbol{\mathcal{A}},Q) \ +\ PE(\psi,Q) \ \ge \\ &\qquad (c\,K - C')\,B_0^{1/2}\delta^{-1}\langle \mathcal{N}_Q\psi,\psi\rangle \ -\ C\,K^{5/2}B_0^{3/2}\delta^{-1}. \end{aligned} \tag{5.25}$$

If we take K to exceed a large enough universal constant, then (5.25) implies (5.20). The proof of local Pauli Stability is complete, modulo polite fictions.

So far, we have worked with a constant magnetic field B. If we suppose instead that B varies only slightly on Q, then we can write the vector potential $\boldsymbol{\mathcal{A}}$ in the form $\boldsymbol{\mathcal{A}} = \boldsymbol{\mathcal{A}}_c + \boldsymbol{\mathcal{A}}^\#$ on Q, where $\boldsymbol{\mathcal{A}}_c$ has constant magnetic field, and $\boldsymbol{\mathcal{A}}^\#$ is small. We may then apply local Pauli stability (5.20) to the vector potential $\boldsymbol{\mathcal{A}}_c$, and regard $\boldsymbol{\mathcal{A}}^\#$ as a small perturbation. In this spirit, we can extend (5.20) as follows.

Local Pauli Stability (Varying Magnetic Fields): Let K, B_0 be large constants to be picked later, and let Q be a cube with side δ. Suppose the magnetic field $\boldsymbol{\mathcal{B}} = \text{curl}\ \boldsymbol{\mathcal{A}}$, satisfies

$$\int_Q |\boldsymbol{\mathcal{B}}(\mathbf{x})|^2\, d^3x \ \le\ B_0^2\, \delta^{-1} \quad \text{and} \tag{5.26}$$

$$\int_Q |\boldsymbol{\mathcal{B}}(\mathbf{x}) \ - \ \text{mean}_Q\, \boldsymbol{\mathcal{B}}|^2\, d^3x \ \le\ B_0^{-1}\, \delta^{-1}\ . \tag{5.27}$$

Then we have that

$$C\, B_0^{1/2}\delta \cdot T_{\text{Pauli}}\,(\psi, \boldsymbol{\mathcal{A}}, Q)\ +\ PE(\psi, Q)\ \ge\ -C\, K^{5/2} B_0^{3/2}\delta^{-1} + c\,\frac{K\, B_0^{1/2}}{\delta}\langle \mathcal{N}_Q\psi, \psi\rangle. \tag{5.28}$$

We omit all discussion of the proof, but just point out that (5.26) and (5.27) suggest that

$$\int_Q |\boldsymbol{\mathcal{B}}(\mathbf{x}) \ - \ \text{mean}_Q\, \boldsymbol{\mathcal{B}}|^2\, d^3x \ \ll\ \int_Q |\boldsymbol{\mathcal{B}}(\mathbf{x})|^2\, d^3x,$$

so that $\boldsymbol{\mathcal{B}}$ varies only slightly on Q.

The proof of our theorem proceeds by making a Calderón-Zygmund decomposition of $\mathbb{E}^3$ into cubes $\{Q_\nu\}$ that satisfy (5.26) and (5.27). We apply Local Pauli Stability (5.28) to each Q_ν, and sum the result over ν. To construct the Q_ν, we begin by partitioning $\mathbb{E}^3$ into cubes $\{Q_\alpha^0\}$ of side L, where L is as in the statement of our theorem. We retain all the Q_α^0 that satisfy (5.26), (5.27), and we cut all the other Q_α^0 into subcubes of side $L/2$. Thus, we obtain a collection $\{Q_\alpha^1\}$ of cubes of side $L/2$. We retain all the Q_α^1 that satisfy (5.26), (5.27), and we cut all the other Q_α^1 into subcubes of side $L/4$. Thus, we obtain a collection $\{Q_\alpha^2\}$ of cubes of side $L/4$. We continue in this way, and let $\{Q_\nu\}$ denote the collection of all the cubes Q_α^j (j, α arbitrary) retained during the above construction.

Thus $\mathbb{E}^3$ is partitioned into cubes $\{Q_\nu\}$ that satisfy (5.26) and (5.27). Let $\delta_\nu = \text{side}\,(Q_\nu)$, and note that $\delta_\nu \le L$.

Let Q_ν be one of the Calderón-Zygmund cubes with side δ_ν strictly less than L. Then Q_ν arose by cutting a cube Q_ν^+ with side $2\delta_\nu$. We know that Q_ν^+ cannot satisfy (5.26) and (5.27), since we cut Q_ν^+ to arrive at Q_ν. If (5.26) fails for Q_ν^+, then, roughly speaking, we have

$$\int_{Q_\nu} |\boldsymbol{\mathcal{B}}(\mathbf{x})|^2 \, d^3x \; > \; c\, B_0^2 \, \delta_\nu^{-1} \; . \tag{5.29}$$

If (5.27) fails for Q_ν^+, then, roughly speaking, we have that

$$\int_{Q_\nu} |\boldsymbol{\mathcal{B}}(\mathbf{x}) \; - \; \mathrm{mean}_{Q_\nu} \, \boldsymbol{\mathcal{B}}|^2 \, d^3x \; > \; c\, B_0^{-1} \, \delta_\nu^{-1} \; ,$$

so that

$$\int_{Q_\nu} \delta_\nu^2 \; \Big| \, (\boldsymbol{\nabla} \otimes \boldsymbol{\mathcal{B}})(\mathbf{x}) \, \Big|^2 \; d^3x \; > \; c\, B_0^{-1} \, \delta_\nu^{-1} \; , \tag{5.30}$$

by the Poincaré inequality. Hence, for every Q_ν, we have $\nu \in \mathcal{S}_1 \cup \mathcal{S}_2 \cup \mathcal{S}_3$, where

$$\mathcal{S}_1 \; = \; \{\nu \, : \, (5.29) \text{ holds}\}, \quad \mathcal{S}_2 \; = \; \{\nu \, : \, (5.30) \text{ holds}\}, \quad \mathcal{S}_3 \; = \; \{\nu \, : \, \delta_\nu \; = \; L\} \; . \tag{5.31}$$

Next, we bring in the function $D(\mathbf{x}) = \min \{|\mathbf{x} - \mathbf{y}_k| \; \big| \; 1 \, \leq \, \mathbf{k} \, \leq \, M\}$ from the statement of our theorem. We set

$$\theta_\nu \; = \; \max\nolimits_{\mathbf{x} \, \in \, Q_\nu} \, e^{- \, D(\mathbf{x})/L} \; . \tag{5.32}$$

Since Q_ν has side $\delta_\nu \, \leq \, L$, definition (5.32) shows at once that (for a constant c)

$$c\, \theta_\nu \; \leq \; e^{- \, D(\mathbf{x})/L} \; \leq \; \theta_\nu \text{ for all } \mathbf{x} \, \in \, Q_\nu \; . \tag{5.33}$$

The basic estimate for our Calderón-Zygmund cubes, apart from (5.26) and (5.27), is the following bound.

$$\begin{aligned} \sum_\nu \theta_\nu \, \delta_\nu^{-1} \; \leq \; & C\, B_0^{-2} \int_{\mathbb{E}^3} |\boldsymbol{\mathcal{B}}(\mathbf{x})|^2 \, e^{-D(\mathbf{x})/L} d^3x \; + \\ & C\, B_0 \int_{\mathbb{E}^3} L^2 \; \Big| \, (\boldsymbol{\nabla} \otimes \boldsymbol{\mathcal{B}}) \, (\mathbf{x}) \, \Big|^2 \; e^{-D(\mathbf{x})/L} d^3x \; + \; \frac{C}{L} \, M. \end{aligned} \tag{5.34}$$

To prove (5.34), we argue as follows. If $\nu \, \in \, \mathcal{S}_1$, then (5.29) and (5.33) imply that

$$\theta_\nu \, \delta_\nu^{-1} \; \leq \; C\, B_0^{-2} \int_{Q_\nu} \Big| \, \boldsymbol{\mathcal{B}}(\mathbf{x}) \, \Big|^2 \; e^{-D(\mathbf{x})/L} \, d^3x \; .$$

Summing over $\nu \, \in \, \mathcal{S}_1$, we obtain the bound

$$\sum_{\nu \, \in \, \mathcal{S}_1} \theta_\nu \, \delta_\nu^{-1} \; \leq \; C\, B_0^{-2} \int_{\mathbb{E}^3} \Big| \, \boldsymbol{\mathcal{B}}(\mathbf{x}) \, \Big|^2 \; e^{-D(\mathbf{x})/L} \, d^3x \; . \tag{5.35}$$

Similarly, if $\nu \in \mathcal{S}_2$, then (5.30) and (5.33) imply that

$$\theta_\nu\, \delta_\nu^{-1} \;\leq\; C\, B_0 \int\limits_{Q_\nu} L^2 \,\big|\, (\boldsymbol{\nabla} \otimes \boldsymbol{\mathcal{B}})\,(\mathbf{x})\,\big|^2 \;\; e^{-D(\mathbf{x})/L}\; d^3x, \qquad \text{since } \delta_\nu \;\leq\; L\;.$$

Summing over $\nu \in \mathcal{S}_2$, we get

$$\sum_{\nu \in \mathcal{S}_2} \theta_\nu\, \delta_\nu^{-1} \;\leq\; C\, B_0 \int\limits_{\mathbb{E}^3} L^2 \,\big|\, (\boldsymbol{\nabla} \otimes \boldsymbol{\mathcal{B}})\,(\mathbf{x})\,\big|^2 \;\; e^{-D(\mathbf{x})/L}\; d^3x\;. \tag{5.36}$$

For $\nu \in \mathcal{S}_3$, we have that

$$\theta_\nu\, \delta_\nu^{-1} \;=\; \theta_\nu\, L^{-1} \;\leq\; C\, L^{-4} \int\limits_{Q_\nu} e^{-D(\mathbf{x})/L}\; d^3x \;\leq\; C\, L^{-4} \sum_{k=1}^{M} \int\limits_{Q_\nu} e^{-|\mathbf{x}-\mathbf{y}_k|/L}\; d^3x,$$

by (5.33) and the definition of $D(\mathbf{x})$. Summing over $\nu \in \mathcal{S}_3$, we find that

$$\sum_{\nu \in \mathcal{S}_3} \theta_\nu\, \delta_\nu^{-1} \;\leq\; C\, L^{-4} \sum_{k=1}^{M} \int\limits_{\mathbb{E}^3} e^{-|\mathbf{x}-\mathbf{y}_k|/L}\; d^3x \;=\; \frac{C'}{L}\, M\;. \tag{5.37}$$

Combining estimates (5.35), (5.36) and (5.37), we obtain the desired result (5.34).

At last we are ready to prove our theorem. For each ν, we have

$$\begin{aligned} C\, B_0^{1/2} \delta_\nu \,\cdot\, T_{\text{Pauli}}\;(\psi, \boldsymbol{\mathcal{A}}, Q_\nu) \;+\; PE(\psi, Q_\nu) \;\geq\; -C\, B_0^{3/2} \delta_\nu^{-1} \theta_\nu K^{5/2} \;+ \\ c\, B_0^{1/2}\, \theta_\nu\, \delta_\nu^{-1} K \langle \mathcal{N}_{Q_\nu} \psi, \psi\rangle\;. \end{aligned} \tag{5.38}$$

On one hand, (5.38) reduces to local Pauli stability (inequality (5.28)) if Q_ν contains at least one nucleus, since then we have $\theta_\nu = 1$ by (5.32). On the other hand, if Q_ν contains no nuclei, then a glance at definition (5.7) gives $PE(\psi, Q_\nu) = 0$, so that (5.38) is an immediate consequence of the KE Lower Bound (5.15). (Recall, we are ignoring the last term on the right side in (5.15).) Thus, (5.38) holds in all cases. Summing (5.38) over all ν, and invoking (5.8) and (5.9), we obtain the estimate

$$\begin{aligned} C\, B_0^{1/2} L \left\langle \sum_{k=1}^{N} \Big[\boldsymbol{\sigma}^{(\mathbf{k})} \cdot (i \boldsymbol{\nabla}_{\mathbf{x}_k} - \boldsymbol{\mathcal{A}}(\mathbf{x}_k))\Big]^2 \psi, \psi \right\rangle \;+\; \langle V_C\; \psi, \psi\rangle \;\geq\; -\,C\, K^{5/2} B_0^{3/2} \sum_{\nu} \theta_\nu\, \delta_\nu^{-1} \\ +\left\{ c\, K\, B_0^{1/2} \left\langle \sum_{\nu} \theta_\nu \delta_\nu^{-1}\, \mathcal{N}_{Q_\nu} \psi, \psi \right\rangle \;-\; C \sum_{\nu} \theta_\nu \delta_\nu^{-1}\, \mathcal{M}_{Q_\nu} \right\}\;, \end{aligned} \tag{5.39}$$

since $\delta_\nu \;\leq\; L$ and $\theta_\nu = 1$ when $\mathcal{M}_{Q_\nu} \neq 0$.

We have agreed to suppose that $\mathcal{N}_{Q_\nu}$ and $\mathcal{M}_{Q_\nu}$ are comparable. Therefore, the term in curly brackets in (5.39) is positive, since K and B_0 are large constants. Let us restrict the parameter L, by demanding that

$$C\, B_0^{1/2}\, L \;\leq\; 1\;. \tag{5.40}$$

Then (5.34), (5.39) and (5.40) imply

$$\langle H_{\text{Pauli}}\ \psi,\psi\rangle \ +\ C_K B_0^{-1/2}\int\limits_{\mathbb{E}^3} \mid \boldsymbol{\mathcal{B}}(\mathbf{x}) \mid^2 \ e^{-D(\mathbf{x})/L}\, d^3x \ +$$

$$C_K B_0^{5/2}\int\limits_{\mathbb{E}^3} L^2 \mid (\boldsymbol{\nabla}\otimes\boldsymbol{\mathcal{B}})(\mathbf{x}) \mid^2 \ e^{-D(\mathbf{x})/L} d^3x \ \geq\ -\frac{C_K\, B_0^{3/2}}{L}\, M\ , \qquad (5.41)$$

where C_K depends on K.

Our theorem follows easily from (5.41). We first take K to be a large enough universal constant. Then, with Γ as in our theorem, we pick B_0 so large that $C_K B_0^{-1/2} \leq \Gamma$. Finally we take $c\,(\Gamma, Z) = \left(C\, B_0^{1/2}\right)^{-1}$, with C as in (5.40). Thus, for $L < c\,(\Gamma, Z)$, (5.40) holds; hence, (5.41) holds and tells us that

$$\langle H_{\text{Pauli}}\ \psi,\psi\rangle \ +\ \Gamma\int\limits_{\mathbb{E}^3} \mid \boldsymbol{\mathcal{B}}(\mathbf{x}) \mid^2 \ e^{-D(\mathbf{x})/L} d^3x$$

$$+\, C\,(\Gamma, Z)\int\limits_{\mathbb{E}^3} L^2 \mid (\boldsymbol{\nabla}\otimes\boldsymbol{\mathcal{B}})(\mathbf{x}) \mid^2 \ e^{-D(\mathbf{x})/L}\, d^3x \ \geq\ -\,C\,(\Gamma, Z)\,\frac{M}{L}\,. \qquad (5.42)$$

This is the conclusion of our theorem.

Of course we have repeatedly oversimplified the argument. For full details, see [12].

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