

Stability of nonrelativistic quantum mechanical matter coupled to the (ultraviolet cutoff) radiation field

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ABSTRACT We announce a proof of *H*-stability for the quantized radiation field, with ultraviolet cutoff, coupled to arbitrarily many non-relativistic quantized electrons and static nuclei. Our result holds for arbitrary atomic numbers and fine structure constant. We also announce bounds for the energy of many electrons and nuclei in a classical vector potential and for the eigenvalue sum of a one-electron Pauli Hamiltonian with magnetic field.

In this note, we describe a variety of mathematical results concerning the quantum theory of systems of static nuclei and nonrelativistic electrons with spin coupled to a classical, static magnetic field and/or to the ultraviolet cutoff quantized radiation field. Our results and their proofs are based, in part, on earlier work in refs. 1 through 7. Details will appear in refs. 8–10.

A typical system we propose to study consists of an arbitrary number, N , of nonrelativistic electrons with electric charge $-e$, bare mass $m > 0$, spin $1/2$ and a bare gyromagnetic factor $g = 2$, an arbitrary number, M , of nuclei of atomic number $\leq Z$, for some arbitrary, but fixed integer $Z < \infty$, and an arbitrary number of photons which describe the transverse degrees of freedom of the quantized electromagnetic field. The dynamics of the system, generated by a self-adjoint Hamilton operator H , conserves the number of nuclei and electrons, but the number of photons is arbitrary and changes in time.

Our concern is to show that, in the ground state of the system corresponding to the infimum of the spectrum of H , the energy per charged particle (electron or nucleus) is bounded *uniformly* in N and M , for fixed $Z < \infty$. This property of nonrelativistic, quantum-mechanical matter is called *H-stability*. In ref. 11 the reader may find many important results and background material on stability of matter, as well as applications thereof.

When the coupling of nuclei to the transverse degrees of freedom of the electromagnetic field is turned off *H*-stability of the systems described above is a mathematical consequence of the *H*-stability of systems in which nuclei are treated as *static*. In this note we consider static nuclei, in accordance with the fact that their masses are much larger than the mass of an electron, but we emphasize that, because of their magnetic moments, this is not an entirely innocent approximation for most realistic nuclei; see the discussion in refs. 7 and 8. Furthermore, interactions between electrons and photons with energies large compared with a typical energy of an electron in an atom of atomic number $\leq Z$ are turned off with the help of an ultraviolet cutoff.

The Hilbert space of pure state vectors of a system of N electrons and an arbitrary number of photons is given by

$$\mathcal{H} = (L^2(\mathbb{E}^3, d^3x) \otimes \mathbb{C}^2)^{\wedge N} \otimes \mathcal{F}, \quad [1]$$

where $L^2(\mathbb{E}^3, d^3x) \otimes \mathbb{C}^2$ is the Hilbert space for one electron of spin $1/2$ in physical space \mathbb{E}^3 , \wedge denotes an antisymmetric tensor product, and \mathcal{F} is the photon Fock space—i.e., the symmetric tensor algebra—over the one-photon Hilbert space $L^2(\mathbb{R}^3, d^3k) \otimes \mathbb{C}^2$. The factors \mathbb{C}^2 account for the spin states of electrons and the helicities of photons, respectively. Electrons are fermions—i.e., they satisfy the Pauli principle, giving rise to antisymmetric tensor products—while photons are bosons corresponding to symmetric tensor products.

The Hamiltonian of the system, in the presence of M static nuclei, is given by

$$H = H_{\text{Pauli}} + H_{\text{field}}, \quad [2]$$

where

$$H_{\text{Pauli}} = \sum_{i=1}^N \mathcal{D}_i^2 + V_c, \quad [3]$$

$$\mathcal{D}_i = \sum_{\alpha=1}^3 \left(-i \frac{\partial}{\partial x_i^\alpha} - A_\alpha^{(\Lambda)}(\mathbf{x}_i) \right) \cdot \sigma_\alpha^{(i)}, \quad [4]$$

x_i^α is the α th component of the position, $\mathbf{x}_i \in \mathbb{E}^3$, of the i th electron; $A_\alpha^{(\Lambda)}(\mathbf{x})$ is the α th component of the quantized electromagnetic vector potential, $\mathbf{A}(\Lambda)(\mathbf{x})$, with an ultraviolet cutoff Λ , at the point $\mathbf{x} \in \mathbb{E}^3$ (see below); $\sigma_\alpha^{(i)}$ stands for the matrix

$$\mathbf{I} \otimes \cdots \otimes \sigma_\alpha \otimes \cdots \otimes \mathbf{I}, \quad [5]$$

on spin space $(\mathbb{C}^2)^{\otimes N}$, where σ_α , $\alpha = 1, 2, 3$ are the three Pauli matrices, and the 2×2 matrix σ_α in Eq. 5 appears in the i th factor of the tensor product; V_c denotes the Coulomb potential—i.e.,

$$V_c = \sum_{1 \leq i < j \leq N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} - \sum_{\substack{i=1, \dots, N \\ l=1, \dots, M}} \frac{Z_l}{|\mathbf{x}_i - \mathbf{y}_l|} + \sum_{1 \leq l < k \leq M} \frac{Z_l Z_k}{|\mathbf{y}_l - \mathbf{y}_k|}, \quad [6]$$

where $\mathbf{y}_l \in \mathbb{E}^3$ denotes the position of the l th static nucleus and $Z_l \leq Z$ its atomic number, $l = 1, \dots, M$; finally,

$$H_{\text{field}} = \alpha^{-1} \sum_{\lambda=\pm} \int \alpha_\lambda^*(\mathbf{k}) |\mathbf{k}| a_\lambda(\mathbf{k}) d^3k \quad [7]$$

is the Hamiltonian of the transverse degrees of freedom of the quantized electromagnetic field. The constant $\alpha = e^2/\hbar c$ (\hbar is Planck's constant and c is the velocity of light) is the dimensionless fine-structure constant, with $\alpha \approx 1/137$ in nature. We have chosen units for energy where $2mc^2\alpha^2 = 1$, i.e., the ground state energy of a hydrogen atom is -4 . Furthermore,

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we impose the *Coulomb gauge* on our choice of electromagnetic potentials; in particular, V_C is purely electrostatic and $\nabla \cdot \mathbf{A}^{(\Lambda)}(\mathbf{x}) = 0$. The ultraviolet cutoff vector potential $\mathbf{A}^{(\Lambda)}(\mathbf{x})$ is given by

$$\mathbf{A}^{(\Lambda)}(\mathbf{x}) = \mathbf{A}^{(\Lambda)}_{-}(\mathbf{x}) + \mathbf{A}^{(\Lambda)}_{+}(\mathbf{x}),$$

where

$$\begin{aligned} \mathbf{A}^{(\Lambda)}_{-}(\mathbf{x}) &= \frac{\alpha^{1/2}}{2\pi} \sum_{\lambda=\pm} \int \Lambda(\mathbf{k}) |\mathbf{k}|^{-1/2} a_{\lambda}(\mathbf{k}) \varepsilon_{\lambda}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} d^3k, \\ \mathbf{A}^{(\Lambda)}_{+}(\mathbf{x}) &= (\mathbf{A}^{(\Lambda)}_{-}(\mathbf{x}))^{*}, \end{aligned} \quad [8]$$

\mathbf{k} denotes a wave vector, and the direction of propagation, $\mathbf{k}/|\mathbf{k}|$, and the two polarization vectors $\varepsilon_{\lambda}(\mathbf{k})$, $\lambda = \pm$, form an orthonormal basis of $\mathbb{R}^3 \otimes \mathbb{C}$, for each $\mathbf{k} \in \mathbb{R}^3$; moreover, the cutoff function $\Lambda(\mathbf{k})$ satisfies $0 \leq \Lambda(\mathbf{k}) \leq 1$, and

$$\text{supp } \Lambda(\cdot) \subseteq \{\mathbf{k} \mid |\mathbf{k}| \leq \Lambda\}, \quad [9]$$

where Λ is a finite constant. The operators $a_{\lambda}(\mathbf{k})^{*}$ and $a_{\lambda}(\mathbf{k})$ are creation and annihilation operators on \mathcal{F} satisfying the canonical commutation relations

$$[a_{\lambda}(\mathbf{k})^{\#}, a_{\lambda'}(\mathbf{k}')^{\#}] = 0, [a_{\lambda}(\mathbf{k}), a_{\lambda'}(\mathbf{k}')^{*}] = \delta_{\lambda\lambda'} \delta^{(3)}(\mathbf{k} - \mathbf{k}'), \quad [10]$$

where $a^{\#} = a$ or a^{*} .

We are now prepared to describe our main results concerning H -stability of the systems described above.

THEOREM 1. (i) For an arbitrary number, N , of electrons, an arbitrary number, M , of static nuclei of atomic numbers $\leq Z$, for arbitrary values of $Z < \infty$ and of the fine-structure constant α , and for an arbitrary ultraviolet cutoff Λ (see expression 9), there exists a finite constant $E(\alpha, Z)$ (depending only on α and Z) such that

$$H \geq -E(\alpha, Z)\Lambda \cdot M. \quad [11]$$

(ii) For arbitrary N , M , and Z , as above, for an ultraviolet cutoff $\alpha^{-1}\Lambda \leq Z^2\alpha^{-3/4}$, and for sufficiently small values of αZ and $\alpha^{5/2}Z^3$, there exists a finite constant $\varepsilon(Z) \leq \text{const. } Z^{3/2}$ independent of α , N , and M such that

$$H \geq -\varepsilon(Z)Z^2 \cdot M. \quad [12]$$

Remarks: (i) The linear dependence on M (and independence of N) in bounds 11 and 12 implies H -stability of the systems considered here. The linear dependence on Λ of our bound 11 is related to the fact that the Hamiltonian H is the *unrenormalized* Hamiltonian of quantum electrodynamics with nonrelativistic matter (see the discussion in ref. 8 and, especially, in ref. 7).

(ii) In our units, a typical energy of an inner electron bound in an atom of atomic number Z is $-Z^2$. Thus the ultraviolet cutoff energy $\alpha^{-1}\Lambda \sim Z^2\alpha^{-3/4}$ for photons is *much larger* than a typical energy of such an electron, because, in nature, $\alpha \approx 1/137$. A nucleus of atomic number Z can bind of the order of Z electrons (12). The ground state energy of the resulting bound state (an atom or ion) is therefore bounded from below by $-\text{const. } Z^3$, in our units. We therefore conjecture that our estimates on $\varepsilon(Z)$ in inequality 12 can be improved to $\varepsilon(Z) \leq \text{const. } Z$ (see also *Theorem 2* below).

(iii) A proof of *Theorem 1* can be found in ref. 8. It combines arguments in ref. 7 with a new result on H -stability of nonrelativistic quantum-mechanical matter in an arbitrary static, external magnetic field established in ref. 9, which is stated below.

Let $\mathbf{A}(\mathbf{x})$ be an arbitrary, classical electromagnetic vector potential with square-integrable second derivatives in \mathbf{x} and with $\nabla \cdot \mathbf{A}(\mathbf{x}) = 0$ (Coulomb gauge). Let $\mathbf{B}(\mathbf{x}) = \text{curl } \mathbf{A}(\mathbf{x})$

denote the corresponding magnetic field. We set

$$D(\mathbf{x}) = \min_{1 \leq k \leq M} |\mathbf{x} - \mathbf{y}_k|. \quad [13]$$

Let $\psi \in (L^2(\mathbb{E}^3, d^3x) \otimes \mathbb{C}^2)^{\wedge N}$. We consider the energy functional

$$\begin{aligned} \varepsilon(\psi, \mathbf{A}) &= \langle \psi, H_{\text{Pauli}} \psi \rangle \\ &+ \int_{\mathbb{E}^3} \{ \Gamma |\mathbf{B}(\mathbf{x})|^2 + C(\Gamma, Z) L^2 |(\nabla \otimes \mathbf{B})(\mathbf{x})|^2 \} \\ &\times e^{-L^{-1}D(\mathbf{x})} d^3x, \end{aligned} \quad [14]$$

where H_{Pauli} is the N -electron Hamiltonian defined in eqs. 3 and 4, but with $\mathbf{A}^{(\Lambda)}$ replaced by the *classical* vector potential \mathbf{A} , and Γ , $C(\Gamma, Z)$, and L are constants yet to be chosen.

The proof of *Theorem 1* is based on a lower bound for the energy functional ε which we describe next.

THEOREM 2. Given $\Gamma > 0$ and $Z < \infty$, and for a suitable choice of the constant $C(\Gamma, Z) < \infty$ in Eq. 14, there are finite, positive constants $c(\Gamma, Z)$ and $C'(\Gamma, Z)$ depending only on Γ and Z such that, for arbitrary $L \leq c(\Gamma, Z)$,

$$\inf_{\|\psi\|=1, \mathbf{A}} \varepsilon(\psi, \mathbf{A}) \geq -C'(\Gamma, Z)L^{-1}M, \quad [15]$$

where M is the number of nuclei. If $\Gamma \geq Z^2$ there are finite, positive constants c and C such that, for the choices $c(\Gamma, Z) = cZ^{-1}$ [i.e., $c(\Gamma, Z)$ is proportional to the Bohr radius of an electron bound to a nucleus of atomic number Z] and $C(\Gamma, Z) = CZ^2$, one has that

$$C'(\Gamma, Z) \leq CZ^2. \quad [16]$$

Remarks: (i) The proof of *Theorem 2* is outlined in ref. 8 and carried out in full detail in ref. 9. In ref. 9, bounds on the constants $c(\Gamma, Z)$, $C(\Gamma, Z)$, and $C'(\Gamma, Z)$ are given in the three regimes $\Gamma \geq Z^2$, $Z^2 \geq \Gamma \geq 1$, and $\Gamma \leq 1$. In using *Theorem 2* to prove *Theorem 1*, one sets $\Gamma = \text{const. } \alpha^{-2}$. Since, in nature, $\alpha \approx 1/137$ and $Z < 100$, the regime $\Gamma \geq Z^2$ is the most important one for physics.

(ii) If $\Gamma \geq Z^2$ the bounds in *Theorem 2* imply that

$$\inf_{\|\psi\|=1, \mathbf{A}} \varepsilon(\psi, \mathbf{A}) \geq -C'Z^3M, \quad [17]$$

for some finite constant C' independent of the number N of electrons. In our units of energy, the ground state energy of an atom or ion consisting of a nucleus of atomic number Z and an arbitrary number of electrons is $\geq -\text{const. } Z^{7/3}$ (see refs. 12 and 13). The fact that, in part *ii* of *Theorem 1*, we only have that $H \geq -\text{const. } Z^{7/2}M$ is a consequence of the *ultraviolet divergence* of the zero-point energy of the quantized electromagnetic field (see ref. 8).

(iii) The strategy developed in ref. 9 (see also ref. 6) to prove *Theorem 2* is to reduce the stability bound 15 to local stability of matter in small cubes of physical space \mathbb{E}^3 whose sizes are chosen to depend on the configuration of nuclei and on the local behavior of the magnetic field \mathbf{B} . These cubes form a Caldéron-Zygmund decomposition of \mathbb{E}^3 .

To show that *Theorem 2* implies *Theorem 1*, we write the Hamiltonian H introduced in Eqs. 2-7 as the sum of two terms,

$$H = H_I + \mathbb{1} \otimes H_{II},$$

where

$$H_I = H_{\text{Pauli}} + \varepsilon_{\text{field}}(\mathbf{A}^{(\Lambda)}),$$

with

$$\varepsilon_{\text{field}}(\mathbf{A}) = \int_{\mathbb{E}^3} \{ \Gamma |\mathbf{B}(\mathbf{x})|^2 + C(\Gamma, Z)L^2 \times |(\nabla \otimes \mathbf{B})(\mathbf{x})|^2 \} e^{-L^{-1}D(\mathbf{x})} d^3\mathbf{x},$$

and

$$H_{II} = H_{\text{field}} - \varepsilon_{\text{field}}(\mathbf{A}^{(\Lambda)}).$$

It is clear that *Theorem 2* proves an appropriate lower bound on H_I [because, in the ‘‘Schrödinger representation’’ of Fock space \mathcal{F} , $\mathbf{A}^{(\Lambda)}$ can be treated as a classical vector potential (8)], while a lower bound on H_{II} follows from surprisingly simple Fock space estimates (7, 8).

In refs. 7 and 10 the following result related to *Theorem 2* is proven: Let

$$\Omega = \{ \mathbf{x} \in \mathbb{E}^3 \mid |\mathbf{x} - \mathbf{y}_l| \leq (Z + 1)^{-1}, l = 1, \dots, M \}$$

and define the classical field energy in the region Ω by

$$\varepsilon_{\text{field}}(\mathbf{A}; \Omega) = \Gamma \int_{\Omega} |(\nabla \otimes \mathbf{A})(\mathbf{x})|^2 d^3\mathbf{x},$$

with $\Gamma = (8\pi\alpha^2)^{-1}$.

THEOREM 3. *There is a constant $\varepsilon > 0$ such that if $\Gamma^{-1}(Z + 1) < \varepsilon$, then*

$$H_{\text{Pauli}} + \varepsilon_{\text{field}}(\mathbf{A}; \Omega) \geq -K(Z + 1)^2(N + M),$$

for some finite constant K (depending only on Γ).

Theorem 3 can be used to prove a variant of part *ii* of *Theorem 1* (see ref. 7) in the (physically relevant) range $\alpha \leq 1/132$, $Z \leq 6$, and $\alpha^{-1}\Lambda \leq \alpha^{-5/4}(Z + 1)$.

The proof of *Theorem 3* is based on methods developed in ref. 5. Estimates extending the key estimates underlying the results in refs. 5 and 7 are proven in ref. 10. They have the following flavor: As in Eq. 4, define

$$\mathcal{D} = \sum_{\alpha=1}^3 \left(-i \frac{\partial}{\partial x^\alpha} - A_\alpha(\mathbf{x}) \right) \cdot \sigma_\alpha,$$

where $\mathbf{A}(\mathbf{x}) = (A_1(\mathbf{x}), A_2(\mathbf{x}), A_3(\mathbf{x}))$ is an arbitrary vector potential, and let $\mathbf{B} = \text{curl } \mathbf{A}$ be the magnetic field corresponding to \mathbf{A} . Let $v(\mathbf{x})$ be a positive (bounded, measurable) function on \mathbb{E}^3 . We consider the one-electron Pauli Hamiltonian

$$H^{(1)} = \mathcal{D}^2 - v. \tag{18}$$

Let $\{e_i\}_{i=0,1,2,\dots}$ be the negative eigenvalues of $H^{(1)}$ (ordered such that $e_0 \leq e_1 \leq e_2 \leq \dots$). We define a basic, \mathbf{B} -dependent length scale $r(\mathbf{x})$ as the solution of the equation

$$r(\mathbf{x})^{-1} = \int \varphi(r(\mathbf{x})^{-1}(\mathbf{y} - \mathbf{x})) |\mathbf{B}(\mathbf{y})|^2 d^3\mathbf{y}, \tag{19}$$

with $\varphi(\mathbf{x}) = (1 + 1/2|\mathbf{x}|^2)^{-2}$. For a homogeneous magnetic field \mathbf{B} , $r(\mathbf{x})$ is proportional to $|\mathbf{B}|^{-1/2}$, which is the cyclotron radius

of an electron, in our units. We also define $b(\mathbf{x}) = r(\mathbf{x})^{-2}$ as the strength of an effective magnetic field.

Our main result on $H^{(1)}$, proven in ref. 10, is the following theorem.

THEOREM 4. *There are finite, positive constants C, C', C'' such that, for an arbitrary vector potential $\mathbf{A}(\mathbf{x})$,*

$$-\sum_i e_i \leq C' \int_{\mathbb{E}^3} v(\mathbf{x})^{5/2} d^3\mathbf{x} + C'' \int_{\mathbb{E}^3} b(\mathbf{x})^{3/2} v(\mathbf{x}) d^3\mathbf{x}, \tag{20}$$

and

$$\int_{\mathbb{E}^3} b(\mathbf{x})^2 d^3\mathbf{x} \leq C \int_{\mathbb{E}^3} |\mathbf{B}(\mathbf{x})|^2 d^3\mathbf{x}. \tag{21}$$

As a corollary one obtains a result of ref. 5: There is a finite, positive constant K such that

$$-\sum_i e_i \leq K \left\{ \int_{\mathbb{E}^3} v(\mathbf{x})^{5/2} d^3\mathbf{x} + \left(\int_{\mathbb{E}^3} |\mathbf{B}(\mathbf{x})| b^2 d^3\mathbf{x} \right)^{3/4} \times \left(\int_{\mathbb{E}^3} v(\mathbf{x})^4 d^3\mathbf{x} \right)^{1/4} \right\}. \tag{22}$$

The relevance of inequalities 20, 21, or 22 for proofs of stability of matter in magnetic fields is explained in ref. 10, respectively ref. 5. See also ref. 14.

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