Stability of Quantum Electrodynamics with Nonrelativistic Matter

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We prove stability for systems composed of arbitrarily many nonrelativistic Pauli electrons minimally coupled to the quantized, ultraviolet-cutoff electromagnetic field and of static nuclei interacting with each other through Coulomb forces. [S0031-9007(96)01414-7]

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In this Letter we prove that the quantum electrodynamics of nonrelativistic, quantum mechanical matter interacting with the quantized radiation field is stable, provided $\alpha^2(Z+1)$ is sufficiently small and an ultraviolet cutoff is imposed on the quantized electromagnetic vector potential. As usual, e denotes the elementary electric charge, $\hbar$ is Planck's constant, c is the velocity of light, and $\alpha = e^2/\hbar c \approx \frac{1}{137}$ is the dimensionless feinstructure constant; the charges of nuclei are assumed to be bounded above by Ze. A typical system described by this theory consists of an arbitrary number N of nonrelativistic electrons with electric charge $-e$, bare mass $m > 0$, spin $\frac{1}{2}$ and a bare gyromagnetic factor $g = 2$ (Pauli electrons), an arbitrary number K of static nuclei of nuclear charge $\leq Ze$, and arbitrarily many photons. In the Coulomb gauge, electrons and nuclei interact through Coulomb two body potentials, and the electrons are coupled to the transverse degrees of freedom of the radiation field by minimal substitution. Photons with energies large compared to typical atomic energies $[\propto mc^2(Z\alpha)^2]$ are not coupled to the electrons because of the ultraviolet cutoff imposed on the electromagnetic vector potential.

Stability is the statement that the energy per charged particle in such a system is bounded uniformly in N and K. Our result on stability also holds for systems of *dynamical* nuclei, provided the interactions between nuclear magnetic moments and the quantized electromagnetic field are neglected or suitably regularized. Much of atomic, molecular, and condensed matter physics is concerned with the study of detailed properties of the systems just described.

Our result extends earlier results on systems of electrons and nuclei coupled to *classical*, static magnetic fields proven in [1,2]; see also [3–6] for earlier partial results. An important part of our proof is based on methods developed in [2,7]. Our units are $\hbar^2(2me^2)^{-1}$ for length, $2me^4\hbar^{-2}$ for energy, and $2me^2\hbar^{-1}$ for the magnetic vector potential. In the Coulomb gauge, the Hamiltonian of a typical system is given by

$$H = H_m + H_f,$$

where

$$H_m = \sum_{i=1}^{N} \{[p_i + A_\Lambda(x_i)] \cdot \sigma_i\}^2 + V_C,$$

$$V_C = \sum_{\substack{i,j=1\\ i<j}}^{N} \frac{1}{|x_i - x_j|} - \sum_{i,k=1}^{N,K} \frac{Z}{|x_i - R_k|} + \sum_{\substack{k,l=1\\ k<l}}^{K} \frac{Z^2}{|R_k - R_l|},$$

$$H_f = \alpha^{-1} \int |k| \sum_{\lambda=\pm} a_\lambda(k)^* a_\lambda(k) d^3k. \tag{1}$$

The Hamiltonian H acts on $(\Lambda^N \mathcal{H}) \otimes \mathcal{F}$, where $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ and $\mathcal{F}$ is the bosonic Fock space over $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$. The factors $\mathbb{C}^2$ describe the spin of the electron and the helicity of the photon, respectively. The ultraviolet-cutoff electromagnetic vector potential in the Coulomb gauge is given by

$$A_\Lambda(x) \equiv A(x) = A_-(x) + A_-(x)^*,$$

$$A_-(x) = \frac{\alpha^{1/2}}{2\pi} \int \kappa(k)\, |k|^{-1/2} \sum_{\lambda=\pm} a_\lambda(k) e_\lambda(k) e^{ikx} d^3k.$$

The cutoff function $\kappa(k)$ satisfies $|\kappa(k)| \leq 1$ and $\mathrm{supp}\kappa \subset \{k \in \mathbb{R}^3 \mid |k| \leq \Lambda\}$, for some constant $\Lambda < \infty$. For each k, the direction of propagation $\hat{k} = k/|k|$ and the polarizations $e_\pm(k) \in \mathbb{C}^3$ are orthonormal. The operators $a_\lambda(k)^*$ and $a_\lambda(k)$ are creation and annihilation operators on $\mathcal{F}$ and satisfy canonical commutation relations

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

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

The main result of the Letter is the following theorem.

Theorem 1.—There is a dimensionless, positive constant ε such that

$$H \geq -\mathrm{const} \times (Z+1)^2(N+K),$$

provided $\alpha^2(Z+1) \leq \varepsilon$ and $\alpha\Lambda^4 \leq \mathrm{const} \times (Z+1)^4$.

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Because of (1), the maximal cutoff allowed by the theorem corresponds to photon energies $\alpha^{-1}\Lambda = \text{const} \times \alpha^{-5/4}(Z+1)$. For $\alpha^5(Z+1)^4 \ll 1$, the maximal photon energy $\alpha^{-1}\Lambda$ is much larger than $(Z+1)^2$, which is the scale of typical atomic energies in our units (see Proposition 2).

Remark.—Our proof shows that

$$H \geq -\text{const}_\Lambda \times (Z+1)^2(N+K),$$

provided $\alpha^2(Z+1) \leq \varepsilon$, for arbitrary Λ; but the constant on the right hand side tends to ∞, as $\Lambda \to \infty$. (Note that H is the unrenormalized Hamiltonian.)

Stability of matter in a classical magnetic field.—Here we extend recent results in [2] concerning the stability of quantum mechanical matter in an arbitrary external magnetic field. In [2] the energy functional of the system contains the magnetic field energy. Here we show that the lower bound given in [2] for the combined energy of matter and magnetic field holds true, at least qualitatively, if the magnetic energy is retained only in a neighborhood of the nuclei of size at least that of a Bohr radius for nuclear charge Z. (A similar result is announced in [1].)

Proposition 2.—Let

$$\Omega = \{x \in \mathbb{R}^3 \,|\, |x - R_j| \leq (Z+1)^{-1} \text{ for some } j = 1, \ldots, K\}.$$

Then there is $\varepsilon > 0$ such that

$$H_m + \frac{1}{8\pi\alpha^2}\int_\Omega (\nabla \otimes A)^2(x)d^3x \geq -\text{const} \times (Z+1)^2(N+K), \quad (2)$$

for any classical vector potential $A(x)$, provided $\alpha^2(Z+1) \leq \varepsilon$.

The proof adds a localization argument to some results of [2]. Given $K \geq 1$ nuclei at positions $R_1, \ldots, R_K$, the physical space $\mathbb{R}^3$ is partitioned into Voronoi cells $\Gamma_j = \{x \,|\, |x - R_j| \leq |x - R_k| \text{ for } k = 1, \ldots, K\}$ $(j = 1, \ldots, K)$. Let $D_j = \min\{|R_j - R_k| \,|\, j \neq k\}/2$. A potential W is defined [2] cellwise as

$$W(x) = Z|x - R_j|^{-1} + F_j(x) \quad \text{for } x \in \Gamma_j, \quad (3)$$

where

$$F_j(x) = \begin{cases} (2D_j)^{-1}(1 - D_j^{-2}|x - R_j|^2)^{-1} & \text{for } |x - R_j| \leq \lambda D_j, \\ (\sqrt{2Z} + \frac{1}{2})|x - R_j|^{-1} & \text{for } |x - R_j| > \lambda D_j. \end{cases}$$

We set $\lambda = \frac{8}{9}$, as in [2]. In particular, for $x \in \Gamma_j$, one has $W(x) \leq [Z + \max(\lambda(1-\lambda^2)^{-1}/2, \sqrt{2Z} + \frac{1}{2})] \times |x - R_j|^{-1} \leq Q|x - R_j|^{-1}$, where $Q = Z + \sqrt{2Z} + 2.2$. If $K = 0$, we set $W = 0$.

Let h be the one-particle Pauli operator with potentials A and W, i.e.,

$$h = [(p + A) \cdot \sigma]^2 - W. \quad (4)$$

Then [2,7]

$$H_m \geq d\Gamma(h) + \frac{Z^2}{8}\sum_{j=1}^K D_j^{-1}, \quad (5)$$

where $d\Gamma$ is fermionic second quantization [8]. Note that $N = d\Gamma(1)$ is the number of electrons. It is proven in [2] [see Eqs. (3) and (18)] that

$$d\Gamma(h) \geq -4.13Q^2(N + 2K)/3 - b\int B(x)^2d^3x - c\sum_{j=1}^K D_j^{-1}, \quad (6)$$

where b, c are given following (18) in [2] and $B = \nabla \wedge A$.

Proof of Proposition 2.—Let $l > 0$ be some length scale to be chosen later, and let $C(\beta)$, $C'(\beta)$, $C''(\beta)$ be open cubes of side l, $3l$, and $5l$, respectively, centered at $\beta \in l\mathbb{Z}^3$. The cubes $C(\beta)$ form a partition of $\mathbb{R}^3$ without their boundaries, whereas the $C'(\beta)$ form an open cover of $\mathbb{R}^3$. By scaling we can construct a partition of unity $\{j_\beta\}$ subordinate to $\{C'(\beta)\}$ satisfying

$$\sum_{\beta\in l\mathbb{Z}^3} j_\beta^2(x) = 1, \qquad \sum_{\beta\in l\mathbb{Z}^3}[\nabla j_\beta(x)]^2 \leq \text{const} \times l^{-2}.$$

We shall also need similarly constructed functions $\tilde{j}_\beta$ (not forming a partition of unity), with $\tilde{j}_\beta^2 \leq 1$ but $=1$ on $C'(\beta)$ and $=0$ outside $C''(\beta)$. We then set $A_\beta = \tilde{j}_\beta A + (1 - \tilde{j}_\beta)a_\beta$, where $a_\beta = |C''(\beta)|^{-1} \times \int_{C''(\beta)} A(x)d^3x$ is the average of A over the cube $C''(\beta)$. Clearly, $A_\beta = A$ on $C'(\beta)$.

Set $\mathcal{N}_\beta = \{j | R_j \in C''(\beta)\}$ and let $\Gamma_{\beta,j}$, $D_{\beta,j}$, $W_\beta(x)$ be the objects appearing in (3) if the set of nuclei is $\mathcal{N}_\beta$. We claim that

$$W(x) \leq W_\beta(x) + \text{const} \times Ql^{-1} \quad \text{for } x \in C'(\beta). \quad (7)$$

Indeed, let $x \in C'(\beta) \cap \Gamma_j$. If $j \notin \mathcal{N}_\beta$ then $W(x) \leq Q|x - R_j|^{-1} \leq Ql^{-1}$. If $j \in \mathcal{N}_\beta$, then $\Gamma_j \subset \Gamma_{\beta,j}$. Let k be such that $D_j = |R_j - R_k|/2$. We distinguish between $R_k \in C''(\beta)$ and $R_k \notin C''(\beta)$. In the first case, $D_j = D_{\beta,j}$ and $W(x) = W_\beta(x)$; in the second one, $l \leq |x - R_k| \leq |x - R_j| + 2D_j$, which gives (7) in view of $F_j(x) \leq \text{const} \times Q(|x - R_j| + 2D_j)^{-1}$.

All this yields

$$h = \sum_{\beta\in l\mathbb{Z}^3} j_\beta h j_\beta - \sum_{\beta\in l\mathbb{Z}^3}(\nabla j_\beta)^2 \geq \sum_\beta j_\beta h_\beta j_\beta - \text{const} \times (l^{-2} + Ql^{-1}),$$

where h_β is the Pauli Hamiltonian (4) with potentials A_β, W_β. A more convenient expression for the last sum is obtained by introducing a Hilbert space $\hat{\mathcal{H}} = \oplus_\beta \mathcal{H}$ and operators

$$\hat{h} : \hat{\mathcal{H}} \to \hat{\mathcal{H}}, \hat{h} = \oplus_\beta h_\beta, \quad j : \mathcal{H} \to \hat{\mathcal{H}}, j = \oplus_\beta j_\beta .$$

Then $\sum_\beta j_\beta h_\beta j_\beta = j^* \hat{h} j$ and $1 = j^* j$. Upon second quantization we have $d\Gamma(j^*\hat{h}j) = \Gamma(j)^* d\Gamma(\hat{h}) \times \Gamma(j) = \Gamma(j)^*[\sum_\beta d\Gamma(h_\beta)]\Gamma(j)$ and $N = d\Gamma(j^*j) = \Gamma(j)^*[\sum_\beta d\Gamma(1_\beta)]\Gamma(j)$. If $\mathcal{N}_\beta = \emptyset$ we simply note that $h_\beta \geq 0$. Otherwise, we apply (6) and obtain

$$d\Gamma(h_\beta) \geq -\text{const} \times Q^2[d\Gamma(1_\beta) + |\mathcal{N}_\beta|] - b \int B_\beta^2 d^3x - c \sum_{j \in \mathcal{N}_\beta} D_{\beta,j}^{-1},$$

where $B_\beta = \nabla \wedge A_\beta = \tilde{j}_\beta B + \nabla \tilde{j}_\beta \wedge (A - a_\beta)$. Therefore

$$\int B_\beta^2 d^3x \leq 2 \int \tilde{j}_\beta^2 B^2 d^3x + 2 \int [\nabla \tilde{j}_\beta \wedge (A - a_\beta)]^2 d^3x$$
$$\leq 2 \int_{C''(\beta)} B^2 d^3x + \text{const} \times l^{-2} \int_{C''(\beta)} (A - a_\beta)^2 d^3x \leq \text{const} \times \int_{C''(\beta)} (\nabla \otimes A)^2 d^3x ,$$

since the second to last integral is bounded by $(5l)^2\pi^{-2} \int_{C''(\beta)} (\nabla \otimes A)^2 d^3x$ (Poincaré's inequality). Moreover, we note that $D_{\beta,j}^{-1} \leq D_j^{-1}$. Collecting estimates and using that the cubes $\{C''(\beta)\}$ have the uniform finite intersection property we find that

$$d\Gamma(h) \geq -\text{const} \times \Bigg[(Q^2 + l^{-2})(N + K) + b \int_{\cup_{\mathcal{N}_\beta \neq \emptyset} C''(\beta)} (\nabla \otimes A)^2 d^3x + c \sum_{j=1}^{K} D_j^{-1} \Bigg].$$

The domain of integration is contained in Ω for $5\sqrt{3}\, l = (Z + 1)^{-1}$, so that $Q^2 + l^{-2} \leq \text{const} \times (Z + 1)^2$. The conclusion, which we now sketch, is as in [2]. We use parameters $X = Z\alpha^2$, $Y = \alpha$ instead of Z, α. The conditions $\text{const} \times b = (8\pi\alpha^2)^{-1}$ and $\text{const} \times c \leq Z^2/8$ [see (5)] are seen to hold for $X = X_0$, $Y \leq Y_0$ for some $X_0, Y_0 > 0$, proving the bound (2) in that case. For $X \leq X_0$, $Y \leq Y_0$, a bound is obtained by using that the infimum of the left hand side of (2) is decreasing in α, if $Z \geq X_0 Y_0^{-2}$, and in Z otherwise. Thus $Z + 1$ in (2) gets replaced by $\max(Z, X_0 Y_0^{-2}) + 1 \leq \text{const} \times (Z + 1)$.

Stability of matter coupled to the quantized electromagnetic field.—The Hamiltonian of the modes allowed by the cutoff is

$$H_\kappa \equiv \alpha^{-1} \int |\kappa(k)|^2 |k| \sum_{\lambda = \pm} a_\lambda(k)^* a_\lambda(k) d^3k .$$

It follows from

$$(\nabla \otimes A_-)(x) = \frac{i\alpha^{1/2}}{2\pi} \int \kappa(k)\, |k|^{1/2} \sum_{\lambda=\pm} a_\lambda(k) \times [\hat{k} \otimes e_\lambda(k)] e^{ikx} d^3k$$

that

$$\int (\nabla \otimes A_-)(x)^* (\nabla \otimes A_-)(x) d^3x = 2\pi\alpha^2 H_\kappa , \qquad (8)$$

$$[(\nabla \otimes A_-)(x), (\nabla \otimes A_-)(x)^*] = 4\pi\alpha C_\kappa , \qquad (9)$$

with $C_\kappa = (2\pi)^{-3} \int |\kappa(k)|^2 |k| d^3k \leq (2\pi)^{-2}\Lambda^4/2$.

Lemma 3.—Let $f \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ be real valued. Then

$$\frac{1}{8\pi} \int f(x) [\nabla \otimes A(x)]^2 d^3x \leq \alpha^2 \|f\|_\infty H_\kappa + \alpha C_\kappa \|f\|_1 . \qquad (10)$$

Proof.—We set $A' = \nabla \otimes A$ for brevity and estimate

$$f(x)A'(x)^2 = f(x)[A'_-(x)^* A'_-(x) + A'_-(x)A'_-(x)^* + A'_-(x)^* A'_-(x)^* + A'_-(x)A'_-(x)]$$
$$\leq [f(x) + |f(x)|][A'_-(x)^* A'_-(x) + A'_-(x)A'_-(x)^*] = 4f_+(x)[A'_-(x)^* A'_-(x) + 2\pi\alpha C_\kappa]$$

by making use of $B^*B \geq 0$ for $B = |f(x)|^{-1/2} \times (|f(x)|A'_-(x) - f(x)A'_-(x)^*)$ as well as of (9). Integration and (8) then yield (10).

We are now able to reduce the stability problem to the case of a classical field.

Proof of Theorem 1.—Let $\alpha^2(Z + 1) \leq \varepsilon$, where ε is the bound in Proposition 2. By using $H_f \geq H_\kappa$ and (10) with f the characteristic function of Ω we find

$$H \geq H_m + \alpha^2(Z + 1)\varepsilon^{-1} H_\kappa \geq H_m + \frac{Z + 1}{8\pi\varepsilon} \times \int_\Omega [\nabla \otimes A(x)]^2 d^3x - \varepsilon^{-1}(Z + 1)\alpha C_\kappa |\Omega| .$$

All fields on the right hand side are multiplication operators in the same Schrödinger representation of $\mathcal{F}$ [3,8]. Hence (2) applies to $\varepsilon(Z+1)^{-1}$ instead of α^2 and yields

$$H \geq -\text{const} \times [(Z+1)^2 + \varepsilon^{-1}\alpha\Lambda^4(Z+1)^{-2}] \times (N+K).$$

Remarks.—(1) Carefully rearranging the calculations presented above and keeping track of the explicit values of various constants, one finds that the stability result of Theorem 1 holds for $Z \leq 6$ and $\alpha \leq \frac{1}{132}$, for example. These bounds are certainly far from optimal but cover a physically relevant range. For $Z \leq 6$, $\alpha \leq \frac{1}{137}$ and for $\Lambda = 1$ (which, in physical units corresponds to an ultraviolet cutoff at $4\alpha^{-1}$ Ryd) we have $H \geq -1920(N+K)$. (2) It is easy to prove (see, e.g., [9]) that, for *arbitrary* values of $\alpha^2(Z+1)$ and arbitrary $N < \infty$, $K < \infty$, the Hamiltonian H is bounded below, more precisely $H \geq -\text{const} \times (N^2 + K)$, provided the ultraviolet cutoff $\Lambda < \infty$. Of course, the constant in this estimate depends on Z and Λ and diverges, as Z or Λ tend to ∞. We conjecture that, for *arbitrary* $\alpha^2(Z+1)$, $H \geq -\text{const}' \times (N+K)$, for a finite constant depending on Z and Λ that diverges, as Λ or Z tend to ∞. (3) Ultimately, the dependence of our stability bounds on the ultraviolet cutoff Λ is due to the fact that we are studying the *unrenormalized* Hamiltonian of quantum electrodynamics with nonrelativistic matter. The renormalization of this theory can be understood by considering a single Pauli electron ($N = 1, K = 0$) interacting with the quantized radiation field. One can show that, in this theory, charge renormalization is *finite* and that, for a fixed bare electron mass $m > 0$, the radiative corrections to the energy of an electron are $O(\Lambda^2)$. Furthermore, a perturbative renormalization group calculation suggests that, for a fixed value of the physical electron mass, the bare electron mass $m = m_\Lambda$ must be chosen to depend on the ultraviolet cutoff Λ:

$$m_\Lambda = m_0 M_\Lambda, \quad \text{with } M_\Lambda \sim \Lambda^{-8\pi\alpha + O(\alpha^2)},$$

for some positive m_0. Thus the renormalized Hamiltonian of the theory is given by

$$H_\Lambda = \sum_{i=1}^{N} M_\Lambda^{-1}\{[p_i + A_\Lambda(x_i)] \cdot \sigma_i\}^2 - \mu_\Lambda N + V_C + H_f,$$

with $M_\Lambda \to 0$ and $\mu_\Lambda \to \infty$, as $\Lambda \to \infty$. The problems of finding the correct *(nonperturbative)* expressions for M_Λ and μ_Λ and of proving stability for H_Λ, *uniformly* in Λ, remain open.

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