Stability of Matter in Classical and Quantized Fields

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Abstract. In recent years considerable activity was directed to the issue of stability in the case of matter interacting with an *electromagnetic field*. We shall review the results which have been established by various groups, in different settings: relativistic or non-relativistic matter, classical or quantized electromagnetic fields. Common to all of them is the fact that electrons interact with the field both through their charges *and* the magnetic moments associated to their spin. Stability of non-relativistic matter in presence of magnetic fields requires that $Z\alpha^2$ (where Z is the largest nuclear charge in the system) as well as the fine structure constant α itself, do not exceed some critical value. If one imposes an ultraviolet cutoff to the field, as it occurs in unrenormalized quantum electrodynamics, then stability no longer implies a bound on α, $Z\alpha^2$. An important tool is given by Lieb–Thirring type inequalities for the sum of the eigenvalues of a one–particle Pauli operator with an arbitrary inhomogeneous magnetic field.

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Introduction

Ordinary matter consists of molecules and atoms which are largely empty inside. Yet matter does not shrink. A related — and more fundamental — aspect of stability is the fact that the energy per particle is bounded below, independently of the number of particles. This is what is usually referred to as stability of matter. It should be stressed that it goes well beyond the stability of individual atoms. Basic thermodynamic properties such as extensivity (e.g., two moles of water occupy with good approximation twice the volume occupied by a single mole) also depend on this property. These topics are reviewed in [19, 20].

Stability of matter could not hold without quantum mechanics and, in particular, without the uncertainty principle, but the Pauli principle and screening properties of the interaction (Coulomb) potential are equally important (see [34] for the consequences of tampering with these tenets). The first instance where stability was established, by Dyson and Lenard [9], is non-relativistic matter consisting of N electrons which move in the field of M nuclei having fixed but arbitrary positions. We denote by $q_i = -1$, resp. $q_i = Z$, the charge of an electron

($i = 1, \dots, N$), resp. of a nucleus ($i = N+1, \dots, N+M$). According to the Pauli principle a (pure) state of the N electrons is given by a normalized wave function

$$\Psi \in \bigwedge_{i=1}^{N} \mathrm{L}^2(\mathbb{R}^3, \mathbb{C}^2) \tag{1}$$

in the N-fold antisymmetric tensor product of the single particle Hilbert space $\mathrm{L}^2(\mathbb{R}^3, \mathbb{C}^2)$. Here, $\mathbb{C}^2$ accounts for the spin of the electron, whose role is however unessential so far. The Hamiltonian is, in appropriate units,

$$H = \sum_{i=1}^{N} t_i + V_{\mathrm{c}} \ , \tag{2}$$

where the kinetic energy of a single electron is $t = p^2$, $p = -\mathrm{i}\nabla$ and the index i refers to the variables of the i-th electron. The Coulomb potential V_{c} is

$$V_{\mathrm{c}} = \sum_{i<j} \frac{q_i q_j}{|x_i - x_j|} \ .$$

Theorem 1. *There is a constant $C(Z)$ independent of the position of the nuclei, such that*

$$H \geq -C(Z)(N+M) \ . \tag{3}$$

Subsequently, Lieb and Thirring [27] obtained a much better constant $C(Z)$ which is of order unity for $Z \approx 1$. They also provided a simpler proof, thereby linking (3) to stability of Thomas-Fermi theory. (See however [17] for a short proof closer in spirit to [9]).

In recent years considerable activity was directed to the issue of stability in the case of matter interacting with an electromagnetic field, which brings the model closer to physical reality. Results have been established by various groups, in different settings: relativistic or non-relativistic matter, classical or quantized electromagnetic fields.

Stability and instability in classical magnetic fields

To begin with, consider the addition of a classical, external magnetic field $B = \nabla \wedge A$. There, stability — uniformly in the magnetic vector potential A — persists [1, 7] if the field is included through minimal substitution, i.e., for $t = D^2$, $D = p + A$. This follows by means of the diamagnetic inequality. To actually describe matter in magnetic fields one must however also add the interaction of the electrons with the field through their spins or, more precisely, through the associated magnetic moments. The corresponding kinetic energy is

$$t = D^2 + \frac{g}{2} B \cdot \sigma \ ,$$

where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices and g is known as the gyromagnetic factor. Its physical value is $g = 2$, as long as radiative corrections from quantum electrodynamics are neglected. Stability (3) extends straightforwardly to any $g < 2$, while for $g > 2$ the Hamiltonian is not even bounded below. In the critical case $g = 2$, to which we shall henceforth restrict, the kinetic energy may be written as

$$t = D^2 + B \cdot \sigma = \not{D}^2 , \qquad \not{D} = D \cdot \sigma .$$

Dynamical spins confer new aspects to the issue of stability. A first indication of this is the following: Whereas the equation $D\psi = 0$ admits (by the uncertainty principle) only $\psi = 0$ as a solution in $\mathrm{L}^2(\mathbb{R}^3, \mathbb{C}^2)$, there exist [30] field configurations A such that $\not{D}\psi = 0$ has non-trivial solutions called zero-modes. This effectively invalidates the uncertainty principle and, as a result, stability as defined above. To see this, just consider the case $N = M = 1$ with Hamiltonian

$$H_A = \not{D}_A^2 - Z|x|^{-1} .$$

By scaling both the field and its zero-mode,

$$A_\lambda(x) = \lambda^{-1} A(x/\lambda) , \qquad \psi_\lambda(x) = \lambda^{-3/2} \psi(x/\lambda) , \tag{4}$$

we obtain $\not{D}_{A_\lambda}\psi_\lambda = 0$ and

$$(\psi_\lambda, H_{A_\lambda}\psi_\lambda) = -Z\lambda^{-1}(\psi, |x|^{-1}\psi) , \tag{5}$$

which can be made arbitrarily large and negative by letting $\lambda \to 0$.

However, a proper formulation of stability should incorporate the field energy

$$H_{\mathrm{cf}} = \frac{1}{8\pi\alpha^2} \int B(x)^2 d^3x \tag{6}$$

into the Hamiltonian:

$$H = \sum_{i=1}^{N} t_i + V_{\mathrm{c}} + H_{\mathrm{cf}} . \tag{7}$$

Here $\alpha > 0$ is the fine structure constant. The physical value of this dimensionless parameter is $\alpha = e^2/\hbar c \approx 1/137$. Note that under (4) the magnetic field scales as $B_\lambda(x) = \lambda^{-2} B(x/\lambda)$, so that H_{cf} scales as λ^{-1}, just as the Coulomb energy (5). Thus already from the case $N = M = 1$ one sees that stability for (7) may hold only if $Z\alpha^2$ is sufficiently small. Another necessary condition is that α itself be small enough. To see the latter, consider $N = 1$ and M large. As above, let the electron be in a zero-mode of a fixed field A. Distribute the many nuclei according to some limiting density, e.g., uniformly over a ball. The repulsion energy between the nuclei is $\leq C_1(ZM)^2$, and the attraction of the electron $\leq -C_2(ZM)$, with C_1, $C_2 > 0$ independent of Z, M. By minimizing the sum of the two bounds we obtain $(\psi, V_{\mathrm{c}}\psi) \leq -C_2^2/4C_1$ for $ZM = C_2/2C_1$. Thus,

$$(\psi, H\psi) \leq -\frac{C_2^2}{4C_1} + \frac{1}{8\pi\alpha^2} \int B(x)^2 d^3x < 0$$

for α large enough. Since both the Coulomb and the field energy scale the same way, the expectation value of the Hamiltonian can in fact be made arbitrarily large and negative. The above two conditions are in fact sufficient for stability:

Theorem 2. *The Hamiltonian (7) is stable, i.e.,*

$$H \geq -C(N+M) ,$$

provided α and $Z\alpha^2$ are small enough.

The theorem was first established by Fefferman [12], for $Z = 1$. Soon thereafter, Lieb, Loss, and Solovej [23] found a simpler proof which furthermore ensures stability at physical values of the parameters Z, α and produces a realistic lower bound $-C$ on the energy per particle. An additional improvement of Lieb, Siedentop and Solovej [24, 25] and Loss [29] yields the following sufficient condition for stability:

$$\frac{\pi}{2}Z + 2.7919Z^{2/3} + 1.2987 \leq 0.2153\alpha^{-2} . \tag{8}$$

In particular, for $\alpha = 1/137$ stability holds if $Z \leq 2264$. Precursors of Theorem 2 are found in [16, 21], where the cases $N = 1$ and $M = 1$, resp. $N = 1$ or $M = 1$, were proved.

Let us present the proof of Theorem 2 given in [25], but for brevity we shall not keep track of best constants. The stability of (7) is brought into relation with stability of an apparently unrelated Hamiltonian H_{rel}, namely that of relativistic matter without dynamical spins. It is defined by (2), but with $t = \alpha^{-1}|D|$. The corresponding stability result was proven in [8, 15, 28, 22].

Theorem 3.

$$H_{\mathrm{rel}} \geq 0 , \tag{9}$$

if α and $Z\alpha$ are sufficiently small.

Note that H_{rel} can be uniformly bounded below only if it is non-negative, since both its terms scale as λ^{-1}. Explicitly, stability is assured [22] if the l.h.s. of (8) does not exceed α^{-1}. On the other hand, H_{rel} is unbounded below [18] if $Z\alpha > 2/\pi$.

The other ingredients of the proof of Theorem 2 are:

- The Birman-Koplienko-Solomyak inequality [3]: For any operators A, $B \geq 0$,

$$\mathrm{tr}(A-B)_+ \leq \mathrm{tr}(A^2 - B^2)_+^{1/2} , \tag{10}$$

  where $s_+ = \max(s, 0)$, provided the operator on the r.h.s. is trace class.
- The Lieb-Thirring estimate [27]:

$$\mathrm{tr}(-h)_+^{\gamma} \leq L_\gamma \int v(x)^{\gamma+\frac{3}{2}} d^3x \tag{11}$$

  for $\gamma \geq 0$ and any Schrödinger operator $h = D^2 - v$ on $\mathrm{L}^2(\mathbb{R}^3)$ with $v = v(x) \geq 0$. The l.h.s. can be written as $\sum_k |e_k|^\gamma$, where $e_k < 0$ are the negative eigenvalues of h.

Let us denote by $\tilde{\alpha}$ the fine structure constant in $H_{\rm rel}$, to avoid confusion. Using (9), the first two terms in (7), $H_{\rm m} = \sum_{i=1}^{N} \not{p}_i^2 + V_{\rm c}$, can be estimated as

$$H_{\rm m} \geq \sum_{i=1} (\not{p}^2 - \tilde{\alpha}^{-1}|D|)_i \geq -\operatorname{tr}(\tilde{\alpha}^{-1}|D| - 2\beta|\not{p}|)_+ - \beta^2 N \ ,$$

for any $\beta > 0$. Here we used $\not{p}^2 \geq 2\beta|\not{p}| - \beta^2$ and the Pauli principle. Now (10) can be used to bound the trace (setting $4\beta^2 = 2\tilde{\alpha}^{-2}$) as

$$\tilde{\alpha}^{-1} \operatorname{tr}(D^2 - 2\not{p}^2)_+^{1/2} = \tilde{\alpha}^{-1} \operatorname{tr}(-D^2 - 2B\cdot\sigma)_+^{1/2} \leq 2\tilde{\alpha}^{-1} L_{1/2} \int 4B(x)^2 d^3x \ ,$$

where, in the last step, we used $-B\cdot\sigma \leq |B|$ and (11). Summing up, one obtains

$$H = H_{\rm cf} + H_{\rm m} \geq \Big(\frac{1}{8\pi\alpha^2} - \frac{8L_{1/2}}{\tilde{\alpha}}\Big) \int B(x)^2 d^3x - \frac{1}{2}\tilde{\alpha}^{-2}N \ ,$$

showing that stability holds for $\alpha^2 \leq \tilde{\alpha}/(64\pi L_{1/2})$.

Finally, Lieb, Siedentop and Solovej [24, 25] considered relativistic matter with dynamical spins. The appropriate kinetic energy is given by the Dirac operator

$$t = D\cdot\alpha + \beta m$$

acting on $\mathrm{L}^2(\mathbb{R}^3, \mathbb{C}^4)$, where $m \geq 0$ is the mass and $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, β are the Dirac matrices. Except for this modification, the many-body Hamiltonian $H_{\rm Dirac}$ is still given by (7). Clearly $H_{\rm Dirac}$, just as t, is unbounded below, but the proper interpretation, going in essence back to Dirac, is 'to fill the Fermi sea' for t. In other words, one should only consider expectation values for $H_{\rm Dirac}$ in states

$$\Psi \in \bigwedge_{i=1}^{N} \mathfrak{h}_+ \ ,$$

where $\mathfrak{h}_+ \subset \mathrm{L}^2(\mathbb{R}^3, \mathbb{C}^4)$ is the positive spectral subspace for t.

Theorem 4.

$$(\Psi, H_{\rm Dirac}\Psi) \geq 0$$

(uniformly also in $m \geq 0$), provided α and $Z\alpha$ are small enough.

For $\alpha = 1/137$ stability holds up to $Z \leq 56$. The proof is related to the one sketched above.

Stability and instability in quantized electromagnetic fields

We shall consider only the case of non-relativistic matter. The model is formally still defined by the Hamiltonian (7), but with the following changes. First, the Hilbert space now is $\mathcal{H} = \mathcal{H}_{\rm m} \otimes \mathcal{F}$, where $\mathcal{H}_{\rm m}$ is the Hilbert space (1) for matter and $\mathcal{F}$, the Hilbert space for the field, is the bosonic Fock space over $\mathrm{L}^2(\mathbb{R}^3, \mathbb{C}^2)$.

Here, $\mathbb{C}^2$ accounts for the helicity of the photon. Second, the ultraviolet-cutoff electromagnetic vector potential in the Coulomb gauge is given by

$$A_\Lambda(x) = A_-(x) + A_-(x)^* \ , \quad A_-(x) = \frac{\alpha^{1/2}}{2\pi} \int_{|k|\le\Lambda} |k|^{-1/2} \sum_{\lambda=\pm} a_\lambda(k) e_\lambda(k) \mathrm{e}^{\mathrm{i}kx} d^3k \ ,$$

where $\Lambda < \infty$ is the cutoff. 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

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

The vacuum state $\Omega \in \mathcal{F}$, $(\Omega, \Omega) = 1$, is distinguished by $a_\lambda(k)\Omega = 0$, for all $k \in \mathbb{R}^3$. The kinetic energy in (7), $t = \not{D}^2$, is now defined with $D = p + A_\Lambda(x)$. Finally, the quantum field energy is

$$H_{\mathrm{qf}} = \alpha^{-1} \int |k| \sum_{\lambda=\pm} a_\lambda(k)^* a_\lambda(k) d^3k \ . \tag{12}$$

This completes the definition of the Hamiltonian, which we denote by H_Λ. To see how (12) relates to the previous definition (6), we introduce the (tranverse) electric field $E(x) = -\mathrm{i}[H_{\mathrm{qf}}, A_\Lambda(x)]$ and the magnetic field $B(x) = (\nabla \wedge A_\Lambda)(x)$. Then,

$$H_{\mathrm{qf}} = \frac{1}{8\pi\alpha^2} \int :E(x)^2 + B(x)^2: d^3x \ , \tag{13}$$

where $: \ldots :$ denotes Wick ordering; explicitly, $:B(x)^2: = B(x)^2 - (\Omega, B(x)^2\Omega)$, and analogously for $E(x)^2$. In contrast to (6), the integrand of (13) may also take negative (expectation) values.

Let us remark that the model represents, apart from the cutoff needed to make it well-defined, a physically correct description of the coupled system consisting of matter and field, since the Hamiltonian yields the correct equations of motion. The spectral theory of a similar model is discussed in [2].

The stability of Theorem 2 carries over to this situation [6, 5], but not with the same explicit bounds.

Theorem 5. *For any* $\Lambda > 0$,

$$H_\Lambda \ge -C(\alpha, Z, \Lambda)(N + M) \ , \tag{14}$$

for small enough α, $Z\alpha^2$, *with* $C(\alpha, Z, \Lambda) = \mathrm{const} \cdot \tilde{Z} \max(\tilde{Z}, \alpha^{1/4}\Lambda)$ *and* $\tilde{Z} = Z+1$.

Actually, the ultraviolet cutoff prevents the instability explained before Theorem 2. As a result, the restriction to small values of α, $Z\alpha^2$ may be dropped, as shown by Fefferman [13] and Fefferman, Fröhlich and Graf [14]:

Theorem 5'. *For any* α, Z, Λ, *the estimate (14) holds with* $C(\alpha, Z, \Lambda) = \mathrm{const} \cdot \tilde{Z}(1 + \beta^5 \log\beta)(\beta^{-2}\tilde{Z} + \Lambda)$ *with* $\beta = \tilde{Z}\alpha^2 + 1$.

This fact is not of direct physical significance, however. Rather, one should consider a renormalized Hamiltonian

$$H_{\Lambda,\mathrm{ren}} = \sum_{i=1}^{N} m_\Lambda^{-1} \not{p}_i^2 + V_\mathrm{c} + H_\mathrm{qf} - \mu_\Lambda N \ , \tag{15}$$

where the mass m_Λ and the chemical potential μ_Λ are to be chosen so that the energy of a one electron state with small total momentum p is p^2. It appears conceivable that stability for (15) holds uniformly in Λ, for small enough α, $Z\alpha^2$.

The proof of Theorem 5 can be reduced to stability statements for matter in classical, external fields [12, 4], but with a different expression for the field energy H_cf than before. For reasons related to the vacuum energy subtraction mentioned above, the classical field energy (6) should be replaced by

$$H_\mathrm{cf} = \frac{1}{8\pi\alpha^2} \int_U B(x)^2 d^3x \ , \tag{16}$$

where the integration is now restricted to a small neighborhood U of the nuclei. A similar expression [13, 5], involving also the field gradient, occurs in the proof of Theorem 5'.

Magnetic Lieb-Thirring type inequalities

An issue of related, but also independent interest is found in Lieb-Thirring inequalities corresponding to (11) for Pauli, rather than Schrödinger, Hamiltonians, i.e., for $h = \not{p}^2 - v$ on $\mathrm{L}^2(\mathbb{R}^3, \mathbb{C}^2)$. (We shall focus on $\gamma = 1$, corresponding to the sum of the negative eigenvalues of h). The first such estimate, by Lieb, Solovej and Yngvason [26] applies to constant magnetic fields $B(x) = B$.

Theorem 6. *For constant fields,*

$$\sum_k |e_k| \le a_\delta \int v(x)^{5/2} d^3x + b_\delta |B| \int v(x)^{3/2} d^3x \ , \tag{17}$$

for any $0 < \delta < 1$, *with* $a_\delta = 0.3119\,\delta^{-2}$ *and* $b_\delta = 0.2123(1-\delta)^{-1}$.

The second term represents the contribution of the lowest Landau level, i.e., of the lowest (degenerate) eigenvalue of $\not{p}^2$, whereas the higher levels are accounted for by the familiar first term. Note that a generalization to arbitrary non-constant fields cannot be obtained by just pulling $|B(x)|$ in (17) under the integral sign. Such a bound would be too small (for small v), since, due to the possible existence of zero-modes $\not{p}\psi = 0$, the bound has to be at least $(\psi, v\psi)$.

Estimates for non-constant fields are due to Erdős [10], followed by [23, 32, 33, 4, 5, 31]. Some of them are useful in proofs of stability of matter. In this context we mention the bound of Lieb, Loss and Solovej [23]:

Theorem 7.

$$\sum_k |e_k| \le a_\delta \int v(x)^{5/2} d^3x + b_\delta \Big(\int B(x)^2 d^3x\Big)^{3/4} \Big(\int v(x)^4 d^3x\Big)^{1/4} \ , \tag{18}$$

for any $0 < \delta < 1$*, with* $a_\delta = 0.0654\,\delta^{-1}$ *and* $b_\delta = 0.1005\,\delta^{-5/8}(1-\delta)^{-3/8}$.

One may be tempted to believe that the second term could be replaced by $\int |B(x)|^{3/2} v(x)\, d^3x$, which would imply (18) by Hölder's inequality. It turns out — essentially by arguments of Erdős [10] — that this is not true: The interplay between the field $B(x)$ and the potential $v(x)$ is not strictly local. It is however possible to define an effective scalar field $b(x) \geq 0$ which allows for a semi–local version of (18). This is of interest in connection with the definition (16) and is the content of the following result of Bugliaro et al. [4]:

Theorem 8.

$$\sum_k |e_k| \leq C' \int v(x)^{5/2} d^3x + C'' \int b(x)^{3/2} v(x) d^3x \ , \tag{19}$$

$$\int b(x)^2 d^3x \leq C \int B(x)^2 d^3x \ . \tag{20}$$

In particular, the two estimates together imply (18), except for the constants. The construction of $b(x)$ can be explained as follows. The interplay between the field B and V takes place on a length scale $r(x)$ which depends on B itself (see below), and $b(x)^2$ is the average of $B(y)^2$ over that length scale:

$$b(x)^2 = \int r(x)^{-3} \varphi\Big(\frac{y-x}{r(x)}\Big) B(y)^2 d^3y \ ,$$

with appropriate decay of $\varphi(z) \geq 0$ as $|z| \to \infty$. To determine $r(x)$, note that in the constant field case it is proportional to $|B|^{-1/2}$, the radius of a Landau orbit in the lowest Landau level. In the general case, it is determined self-consistently as $r(x) = b(x)^{-1/2}$. A different definition of $b(x)$ due to Sobolev [32, 33], which motivated the one just presented, also implies (19), but not (20).

Yet another generalization of (17) aims at estimating the contributions of the field gradient $\nabla \otimes B = (\partial_i B_j)_{i,j=1,2,3}$. This was done by Erdős and Solovej [11] and, under somewhat different conditions, by Bugliaro, Fefferman and Graf [5]. To this end a length scale $l(x)$ is introduced which is related to $\nabla \otimes B$ in a similar way as $r(x)$ is related to B.

Theorem 9.

$$\sum e_i \leq C' \int V(x)^{3/2} (V(x) + \widehat{B}(x)) d^3x + C'' \int V(x) P(x)^{1/2} (P(x) + \widehat{B}(x)) d^3x \ ,$$

where $\widehat{B}(x)$ *is the average of* $|B(y)|$ *over a ball of radius* $l(x)$ *centered at* x*, and* $P(x) = l(x)^{-1}(r(x)^{-1} + l(x)^{-1})$.

By the variational principle, this estimate implies a bound on the density $n(x) = \sum_j |\psi_j(x)|^2$ of orthonormal zero-modes ψ_j of $\not{D}$. The bound is

$$n(x) \leq C'' P(x)^{1/2} (P(x) + \widehat{B}(x)) \ ,$$

and, as it should, it vanishes in the case of a homogeneous magnetic field.

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