STABILITY OF MATTER IN MAGNETIC FIELDS

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ABSTRACT: The proof of the stability of matter is three decades old, but the question of stability when arbitrarily large magnetic fields are taken into account was settled only recently. Even more recent is the solution to the question of the stability of relativistic matter when the electron motion is governed by the Dirac operator (together with Dirac's prescription of filling the "negative energy sea"). When magnetic fields are included the question arises whether it is better to fill the negative energy sea of the free Dirac operator or of the Dirac operator with magnetic field. The answer is found to be that the former prescription is unstable while the latter is stable.

I. Introduction

This will be a brief summary of recent work which solves the problem of the stability of matter in magnetic fields. The first part, which was the one reported in the Evora conference, concerns the usual Schrödinger equation with nonrelativistic kinetic energy, but with a Zeeman term $\sigma \cdot \mathbf{B}$. The second part is about some very recent work [1], not reported at the conference, on the relativistic problem with kinetic energy given by the Dirac operator. In both cases the electrons are treated quantum mechanically while the fields are regarded as classical fields.

It has been well understood for some time, starting with the work of Dyson and Lenard in 1967 [2], that matter consisting of N electrons and K static (but arbitrarily positioned) nuclei, and governed by nonrelativistic quantum mechanics, is stable. (See also [3] and see [4], [5] for reviews.) This means that the ground state energy (more generally, the bottom

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of the spectrum, in case there is no lowest eigenvalue) is finite and is bounded below by a universal constant times the number of particles, i.e., $E_0 \geq const.(N+K)$. The reason the nuclei are taken to be static is that they are so massive compared to the electron that if the nuclear mass (or the nuclear radius of 10^{-13}cm, for that matter) played any significant role then ordinary matter would have to look very different from what it does.

The Hamiltonian of our system in suitable units is

$$H_{\text{nonrelatvistic}} = \sum_{i=1}^{N} p_i^2 + \alpha V_{\text{c}} \ , \tag{1.1}$$

where $\alpha = e^2/\hbar c$ is the fine-structure constant and $\mathbf{p} = -i\nabla$, as usual. V_{c} is the Coulomb potential of K fixed nuclei with nuclear charge Ze (we take all the charges to be the same for simplicity only), with locations R_j in $\mathbf{R}^3$, and with N electrons.

$$V_{\text{c}} = -Z \sum_{i=1}^{N} \sum_{j=1}^{K} |x_i - R_j|^{-1} + \sum_{1 \leq i < j \leq N} |x_i - x_j|^{-1} + Z^2 \sum_{1 \leq i < j \leq K} |R_i - R_j|^{-1}. \tag{1.2}$$

We should like to generalize this stability question in two directions. One direction is to add magnetic fields and the other is to make the kinetic energy relativistic, which means replacing p^2 by $\sqrt{p^2 + m^2} - m$ or, equivalently and more simply by $|\mathbf{p}|$ (since the difference between these two expressions is bounded by m, and hence the change in energy is at most a term proportional to the number of electrons). It will turn out that these two problems (magnetic fields and relativity) are not as unrelated mathematically as one might think. Later on, we shall generalize still further by replacing the operator $|\mathbf{p}|$ by the Dirac operator; this is the content of the very recent work mentioned above.

II. Stability of non-relativistic matter with magnetic fields

Let us begin with the magnetic field problem, and with a simple example to illustrate its essence. We shall consider the nonrelativistic case first. We shall denote by $\mathbf{A}(x)$ the vector potential of a magnetic field and $\mathbf{B}(x) = \operatorname{curl} \mathbf{A}(x)$ is the magnetic field itself. Conceptually, we do not ask where this field comes from; it can be external or it can be generated by the current of the electrons themselves. The action of the field on the orbital motion of the electrons is given by the minimal substitution (recalling that the electron's charge is negative)

$$\mathbf{p} \longrightarrow \mathbf{p} + \mathbf{A}(x). \tag{2.1}$$

This has little effect on the ground state energy of our Hamiltonian in (1.1). Indeed, for one electron the field can only raise the energy. For several electrons it can lower the energy but by a controllable amount. In fact, all known proofs of the stability of matter hold with constants unchanged by the substitution (2.1).

The problem comes in when we include the electron spin–field interaction. Thus, we replace $(\mathbf{p}+\mathbf{A})^2$ by the *Pauli operator* (in which σ denotes the triplet of Pauli matrices)

$$\mathcal{T}_{\mathbf{A}} \equiv [\sigma \cdot (\mathbf{p}+\mathbf{A})]^2 = (\mathbf{p}+\mathbf{A})^2 + \sigma \cdot \mathbf{B}. \tag{2.2}$$

It is a fact, which is not entirely easy to prove [6], that E_0 for a hydrogen-like atom $H = \mathcal{T}_{\mathbf{A}} - Z/r$, behaves as $-(\ln B)^2$ for a large, spatially uniform field $\mathbf{B}$. Thus, if we minimize E_0 over all possible fields (since nature will presumably find that value of the field that gives the lowest E_0) the minimum energy will be $-\infty$. However, we forgot to include the self energy of the magnetic field

$$H_{\text{field}} \equiv [8\pi\alpha]^{-1} \int B(x)^2 \, d^3x. \tag{2.3}$$

(The unconventional factor α^{-1} in (2.3) comes from the system of units we have been using.) Does the addition of H_{field} stabilize the system, i.e., is E_0 now bounded below, independent of $\mathbf{B}$?

The answer, perhaps not unsurprisingly in view of the appearance of α in (2.3), is yes *if and only if* α *is small enough.* More precisely it is the combination $Z\alpha^2$ that has to be small enough. This was proved in [7], where it was shown that the "hydrogenic" Hamiltonian

$$H_{hydrogenic} = \mathcal{T}_{\mathbf{A}} - Z\alpha/r + H_{\text{field}} \tag{2.4}$$

is bounded below if $Z\alpha^2 \le 9\pi^2/8$. Oddly, it was harder to prove that the atom is *unstable* if $Z\alpha^2$ is too large; this fact relied on a difficult calculation in [8] that the Pauli kinetic energy operator $\mathcal{T}_{\mathbf{A}}$ can have a zero mode for certain special choices of the $\mathbf{A}$ field. That is, the equation

$$\mathcal{T}_{\mathbf{A}}\Psi = 0 \tag{2.5}$$

has a solution for some magnetic field $\mathbf{B}$, whose energy H_{field} is finite, and some square integrable, electron wave function Ψ. The ordinary kinetic energy p^2 does not have this remarkable property, i.e., the property that in a suitable field the electron can "stand still". (This happens for the uniform magnetic field, to be sure, but that field has infinite energy.)

Obviously, the next question is whether the full many-electron, many-nucleus problem is stable when p^2 is replaced by $\mathcal{T}_{\mathbf{A}}$ and with the addition of H_{field}. Thus, we consider

$$H_{\text{Pauli}} \equiv \sum_{i=1}^{N} \mathcal{T}_{\mathbf{A}}(i) + \alpha V_{\text{c}} + H_{\text{field}} \ , \tag{2.6}$$

and ask whether it is bounded below (for all $\mathbf{A}$, N, K and all locations of the nuclei) by some universal constant times $N+K$. This problem was open for about 9 years and was first solved by Fefferman (unpublished) for sufficiently small α, Z (which does not include hydrogen in its range). A simple proof of stability with good constants was given shortly thereafter in [9]: A representative sufficient condition for stability in (2.6), obtained in [9], is

$$Z\alpha^2 \leq 0.041 \quad \text{and} \quad \alpha \leq 0.06. \tag{2.7}$$

Another sufficient condition is $Z \leq 1050$ when $\alpha = 1/137$. (A more recent result in [1] improves this to $Z \leq 2265$.) It is comforting to have this very large margin of stability in (2.6) because it means that the magnetic field-electron interaction can be treated perturbatively with confidence when $Z \leq 92$.

It is important to understand why there is a bound on α alone in (2.7), independent of the magnitude of Z (as long as $Z > 0$). The reason is that once one admits the possibility that a single atom can collapse if $Z\alpha^2$ is too large (or $Z\alpha$ is too large in the relativistic theories studied below) then one has to ask what prevents a large number of small nuclei from coming together to form a supercritical nucleus? The answer is the Coulomb repulsion among the nuclei, but this quantity is effectively governed by the parameter α^{-3} (or α^{-1} in the relativistic theory) because the nuclear repulsion is proportional to $Z^2\alpha = (Z\alpha^2)^2/\alpha^3$. In other words if $Z\alpha^2$ is truly the relevant atomic parameter then it should be regarded as fixed, which means that α^{-3} is the relevant parameter governing the nuclear repulsion. Anyway, whether or not the reader believes this heuristic discussion, the fact remains that the bound on α in (2.7) is essential.

Two proofs of stability are given in [9]. The simplest uses an ingredient that, at first sight appears to have nothing to do with the magnetic problem—*the stability of relativistic matter*. Let us turn to that next.

III. Relativistic matter without magnetic fields and its application to the nonrelativistic magnetic problem

The relativistic Hamiltonian looks like (1.1), with the substitution (2.1), but with p^2 replaced by $|\mathbf{p}|$. It contains no H_{field} term. Thus,

$$H_{\text{rel}} \equiv \sum_{i=1}^{N} |\mathbf{p} + \mathbf{A}|_i + \alpha V_{\text{c}} \ . \tag{3.1}$$

Admittedly, this Hamiltonian is not well motivated physically because the operator $|\mathbf{p}|$ is not local (unlike the Dirac operator). Minimal substitution does preserve gauge invariance, however. There is no spin-field interaction, as in the Pauli or Dirac Hamiltonians, but let us take one step at a time. It will turn out that the understanding of (3.1) is central to the whole story.

There are two important remarks to be made about (3.1). The first is that everything scales like 1/length (if we let the $\mathbf{A}$ field scale as 1/length as well). Because of this, there are exactly two possibilities for E_0 after we minimize over all possibilities for $\mathbf{A}$ and the nuclear locations:

$$E_0 = 0 \qquad \text{or} \qquad E_0 = -\infty \ . \tag{3.2}$$

(If we used $\sqrt{p^2+m^2} - m$ instead, then the first alternative, $E_0 = 0$ would be replaced by some negative number depending on m. The condition on α for the first alternative to hold does not depend on m.)

The second remark is that for the one-electron hydrogenic problem $E_0 = 0$ if and only if $Z\alpha \leq 2/\pi$ (due to Kato [10] and Herbst [11]). The reason for such a condition is that the kinetic and potential energies scale the same way. If the kinetic energy is larger, E_0 can be driven to zero by dilation; in the reverse case, E_0 can be driven to $-\infty$ by contraction. Closely related to this is a property of the Dirac hydrogenic atom that was known for a long time: Self adjointness of the Dirac operator requires $Z\alpha \leq 1$.

The stability of the many-body Hamiltonian (for all N and K) was first shown by Conlon [12] for $Z = 1$ and $\alpha < 10^{-200}$ and zero magnetic field. The situation was substantially improved in [13] to $Z\alpha \leq 2/\pi$ and $\alpha \leq 1/94$, but $\mathbf{A} = 0$. [13] also contains a simpler proof of stability which holds only up to a slightly smaller value of $Z\alpha$ but which has the advantage of holding with an arbitrary magnetic field. It is this slightly weaker, but more verstile version of the stability of relativistic matter that enters the proof of the stability of the Pauli Hamiltonian *with* the field energy H_{field}. (The ability to add a field was not explicitly stated in [13], but the extension is easy; it was first noted in [9].) The constants obtained in [13] have been improved recently in [14]. However, it remains true that the optimal value of $Z\alpha = 2/\pi$ has not been reached with a magnetic field present. The sufficient condition for stability in [14] (with a field) is

$$(\frac{\pi}{2})Z + 2.80\ Z^{2/3} + 1.30 \leq 1/\alpha\ , \tag{3.3}$$

which permits $Z \leq 59$ for $\alpha = 1/137$.

We are now ready to use (3.3) in the study of the stability of the nonrelativistic magnetic Hamiltonian (2.6). With Z fixed, let us define the number $\tilde{\alpha}$ by (3.3), i.e.,

$$1/\tilde{\alpha} \equiv (\frac{\pi}{2})Z + 2.80\ Z^{2/3} + 1.30\ . \tag{3.4}$$

Then from (3.1) we conclude the operator inequality

$$V_{\text{c}} \geq \frac{1}{\tilde{\alpha}} \sum_{i=1}^{N} |\mathbf{p} + \mathbf{A}|_i\ . \tag{3.5}$$

This inequality can be substituted in (2.6), and we see that it now suffices to study the spectrum of the one-body operator

$$h_{\mathbf{A}} \equiv \mathcal{T}_{\mathbf{A}} - \frac{\alpha}{\tilde{\alpha}} |\mathbf{p} + \mathbf{A}|\ . \tag{3.6}$$

In fact, what we require is a lower bound on the the sum of the lowest N eigenvalues of $h_{\mathbf{A}}$ (according to the Pauli principle). One can show [9] that this sum is bounded below by *const.* $\times N - H_{\text{field}}$, as required for stability, *provided that* the conditions given in (2.7), or the ones mentioned after (2.7), are satisfied.

An inequality that plays a key role in this proof is the CLR bound on the number of negative eigenvalues for a single particle in a potential (in $n \geq 3$-dimensions), i.e., for the Hamiltonian

$$\tilde{h} \equiv p^2 + U(x) \tag{3.7}$$

with $p^2 = -\nabla^2$ as usual and with U some arbitrary potential. We can always write U in terms of its positive and negative parts, $U(x) = U_+(x) - U_-(x)$, with $U_+(x) \equiv (1/2)\{|U(x)| + |U(x)\}$ and $U_-(x) \equiv (1/2)\{|U(x)| - U(x)\}$. Then there is the inequality for the number of negative eigenvalues of $\tilde{h}$, obtained independently by Cwikel, Lieb and Rosenblum,

$$\text{Number of negative eigenvalues} \leq L_{0,n} \int U_-(x)^{n/2} \; d^n x \tag{3.8}$$

with $L_{0,3} = 0.1156$. (The sharp value of $L_{0,3}$ is not known, but it is not much smaller than this value, obtained by Lieb.)

Closely related to this is a family of similar eigenvalue inequalities, derived earlier by Lieb and Thirring [3], about the power sums of the negative eigenvalues, e_j of $\tilde{h}$,

$$\sum_{e_j<0} |e_j|^\gamma \leq L_{\gamma,n} \int U_-(x)^{\gamma+n/2} \; d^n x \tag{3.9}$$

for $n \geq 1$, all $\gamma > 0$ for $n \geq 2$ and all $\gamma \geq 1/2$ for $n = 1$. This inequality, for $n = 3$ and $\gamma = 1$ is important in the proof [3] of the stability of nonrelativistic matter without magnetic fields. The case $n = 3$ and $\gamma = 1/2$ plays a role in the study of H_{Dirac} below. It is known that $L_{1,3} \leq 0.0404$ and $L_{\frac{1}{2},3} \leq 0.06003$.

IV. Putting it all together: Relativistic matter with magnetic fields

Up to now we have considered the nonrelativistic Schrödinger equation with a Zeeman term (i.e., with the Pauli operator) and showed that the magnetic field energy restores the otherwise lost stability provided $Z\alpha^2$ and α itself are small enough (but well within the range of physical parameters). We have also considered the "relativistic" Schrödinger operator, with no Zeeman term, and found that stability requires that $Z\alpha$ and α be small. The combination of the two might be expected to lead to insurmountable difficulties, and it was with some surprise that we found that these difficulties can be overcome if things are defined properly.

We shall try to combine the two by using a Dirac operator for the electron kinetic energy. Thus, we define the Dirac operator for a particle of mass m in a magnetic field by

$$\mathcal{D}_{\mathbf{A}} \equiv \not{\mathbf{p}} + \not{\mathbf{A}} + \beta m. \tag{4.1}$$

As usual, $\not{O} \equiv \alpha \cdot O$, where α_i and β are Dirac matrices. Our many-body Hamiltonian is formally similar to the one in (2.6), namely,

$$H_{\mathrm{Dirac}} \equiv \sum_{i=1}^{N} \mathcal{D}_{\mathbf{A}}(i) + \alpha V_{\mathrm{c}} + H_{\mathrm{field}} \ ,. \tag{4.2}$$

There is, however, one very important difference from (2.6): H_{Dirac} is unbounded below because the Dirac operator itself is unbounded below (recall that the Pauli operator, $\mathcal{T}_{\mathbf{A}}$ is not only bounded below, it is positive). According to Dirac the remedy is to fill all the negative energy states of the Dirac operator which (because of the Pauli principle) is the same thing as saying that the electron wave function must lie in the positive spectral subspace of the Dirac operator.

There's the rub! Which Dirac operator are we talking about? There are at least two significant ones in our problem. One is the free Dirac operator $\mathcal{D}_0 = \not{\mathbf{p}} + \beta m$. The other is the Dirac operator with the magnetic field $\mathcal{D}_{\mathbf{A}}$. It would seem that the latter is the more important one since an electron can never get rid of its own magnetic field. Moreover, the choice $\mathcal{D}_0$, is *not gauge invariant*, i.e., the multiplication of an electron wave function by a spatially varying phase usually takes a positive energy function into a mixture of positive and negative energy functions. The second choice is manifestly gauge invariant. (To avoid possible confusion it is to be noted that the Hamiltonian is always given by (4.2); the only question is what condition to impose on the electron wave function.)

This issue is usually not clearly stated in field theory textbooks, but whatever one might think about the appropriateness of either definition the interesting fact is that "stability" of matter can settle the argument. The following two things are proved in [1]. They show that one choice is valid and the other is not. (Recall that $\tilde{\alpha}$ was defined in (3.4).)

THEOREM:

(i). *If the electron wave functions are restricted to lie in the positive spectral subspace of the free Dirac operator then the Hamiltonian H_{Dirac} is unstable. More precisely, for any given values of $\alpha > 0$ and $Z > 0$, there are (sufficiently large) particle numbers N and K for which the bottom of the spectrum of H_{Dirac} is $-\infty$.*

(ii). *If the electron wave functions are restricted to lie in the positive spectral subspace of the Dirac operator $D_{\mathbf{A}}$ then H_{Dirac} is stable (i.e., $H_{\mathrm{Dirac}} > 0$) provided α and Z are small enough. In particular, if we define α_c to be the unique solution to the equation*

$$1 - (\alpha_c/\tilde{\alpha})^2 = (8\pi L_{\frac{1}{2},3}\alpha_c)^{2/3} \tag{4.3}$$

then $\alpha \le \alpha_c$ suffices for stability.

As a final remark, we draw attention to a recent result [15]. If we consider the Dirac hydrogenic atom *without* magnetic field, with Hamiltonian $\mathcal{D}_0 - Z\alpha/r$, and if the electron's wave function is required to lie in the positive spectral subspace of $\mathcal{D}_0$, the critical value of $Z\alpha$, below which this Hamiltonian is bounded below, is *raised* from the value $2/\pi$ (which is the corresponding value for the "relativistic" Hamiltonian in Sect. 3) to the value $(Z\alpha)_{\text{crit}} = 2/(\pi/2 + 2/\pi)$. As yet it is unknown to what extent a magnetic field will change this value further.

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