Commun. Math. Phys. 104, 251–270 (1986)

Communications in Mathematical Physics

Stability of Coulomb Systems with Magnetic Fields

I. The One-Electron Atom

Jürg Fröhlich[1,★], Elliott H. Lieb[2,★★], and Michael Loss[2,★★★]

[1] Theoretical Physics, ETH-Hönggerberg, CH-8093 Zürich, Switzerland

[2] Departments of Mathematics and Physics, Princeton University, Jadwin Hall, P.O.B. 708, Princeton, NJ 08544 USA

Abstract. The ground state energy of an atom in the presence of an external magnetic field B (with the electron spin-field interaction included) can be arbitrarily negative when B is arbitrarily large. We inquire whether stability can be restored by adding the self energy of the field, $\int B^2$. For a hydrogenic like atom we prove that there is a critical nuclear charge, z_c, such that the atom is stable for $z<z_c$ and unstable for $z>z_c$.

1. Introduction

The problem of the stability of an atom (i.e. the finiteness of its ground state energy) was solved by the introduction of the Schrödinger equation in 1926. While it is true that Schrödinger mechanics nicely takes care of the $-ze^2/r$ Coulomb singularity at $r=0$ (here $z|e|$ is the nuclear charge), a more subtle problem that has to be considered is the interaction of the atom with an external magnetic field $B(x)$ with vector potential $A(x)$ and $B=\operatorname{curl} A$. In this paper the problem of the one-electron atom in a magnetic field is studied; in a subsequent paper [6] some aspects of the many-electron and many-nucleus problem will be addressed.

Units. Our unit of length will be half the Bohr radius, namely $l=\hbar^2/(2me^2)$. The unit of energy will be 4 Rydbergs, namely $2me^4/\hbar^2=2mc^2\alpha^2$, where α is the fine structure constant $e^2/(\hbar c)$. The magnetic field B is in units of $|e|/(l^2\alpha)$. The vector potential satisfies $B=\operatorname{curl} A$. The magnetic field energy ($\int B^2/8\pi$) is, in these units,

$$\varepsilon\int B^2\,,\qquad 1/\varepsilon=8\pi\alpha^2\,. \tag{1.1}$$

★ Work partially supported by U.S. National Science Foundation grant DMS-8405264 during the author's stay at the Institute for Advanced Study, Princeton, NJ, USA

★★ Work partially supported by U.S. National Science Foundation grant PHY-8116101-A03

★★★ Work partially supported by U.S. and Swiss National Science Foundation Cooperative Science Program INT-8503858. Current address: Institut f. Mathematik, FU Berlin, Arnimallee 3, D-1000 Berlin 33

The first problem to be considered is one in which the electron spin is neglected. The Hamiltonian in this case is

$$H' = (p - A)^2 - z/|x| \tag{1.2}$$

(with $p = i\nabla$). H' presents no interesting problem as far as stability is concerned because the effect of including A is *always* to raise the ground state energy. (Reason: For any ψ, $(\psi, (p-A)^2\psi) \geqq (|\psi|, p^2|\psi|)$. This is essentially Kato's inequality [4] (see e.g. [13]). On the other hand $(\psi, |x|^{-1}\psi) = (|\psi|, |x|^{-1}|\psi|)$, so we can lower the energy by replacing ψ by $|\psi|$ and setting $A = 0$.)

The problem becomes interesting when the electron spin is included, and this problem is the subject of this paper. The wave function ψ is a two-component (complex valued) spinor:

$$\psi(x) = (\psi_1(x), \psi_2(x)). \tag{1.3}$$

The Hamiltonian is

$$H = (p - A)^2 - \sigma \cdot B(x) - z/|x| \tag{1.4}$$

$$= [\sigma \cdot (p - A)]^2 - z/|x| \tag{1.5}$$

where $\sigma_1, \sigma_2, \sigma_3$ are the Pauli matrices. The first term in (1.5) is the Pauli kinetic energy and is the non-relativistic approximation to the Dirac operator.

The ground state energy $E_0(B, z)$ of H is always finite but depends on B in such a way that $E_0 \to -\infty$ as $B \to \infty$ (for a constant field), roughly as $-(\ln B)^2$, see [1]. What prevents B from spontaneously growing large and driving E_0 towards $-\infty$? (We do not inquire into the source of this B, but simply assume that nature will always contrive to lower the energy, if possible.) The answer, which we shall take as a hypothesis here, is that the price to be paid is the field energy $\int B^2/8\pi$. Thus, we are led to consider (in our units) $H + \varepsilon \int B(x)^2 dx$ and ask whether

$$E(B, z) = E_0(B, z) + \varepsilon \int B^2 \tag{1.6}$$

is bounded below *independent* of B. This problem is important in the analysis of stability in non-relativistic quantum electrodynamics [we have omitted the term $\int E^2$ which makes (1.6) a lower bound and which makes the magnetic field classical]. We define

$$E(z) = \inf_B E(B, z). \tag{1.7}$$

In the remainder of this introduction we shall first outline our results about $E(z)$, then discuss their physical interpretation and finally formulate some preliminary mathematical facts and notation.

We show that there is a critical value of z (called z_c) such that

$$\begin{aligned} E(z) &= -\infty \quad \text{for} \quad z > z_c, \\ E(z) &\text{ is finite} \quad \text{for} \quad z < z_c. \end{aligned} \tag{1.8}$$

The value of z_c is proportional to $1/\alpha^2$ (not $1/\alpha$ as in the case of the Dirac equation or the "relativistic" Schrödinger equation [3]). Section II (in conjunction with [8]) contains the proof that z_c is finite. The fact that $z_c \neq \infty$ is intimately connected with the fact that the equation

$$\sigma\cdot(p-A)\psi=0 \tag{1.9}$$

has a non-zero solution with $\psi\in H^1$ and $A\in L^6$. When we first worked on this problem we realized this connection and proved (Sect. II) that

$$z_c=\inf\varepsilon\int B^2/(\psi,|x|^{-1}\psi), \tag{1.10}$$

where the infimum is over all solutions to (1.9). (Clearly, any solution to (1.9) has zero kinetic energy so that if z exceeds the right side of (1.10) the total energy can be driven to $-\infty$ by the scaling $\psi(x)\to\lambda^{3/2}\psi(\lambda x)$, $A(x)\to\lambda A(\lambda x)$. The converse is the difficult part of Sect. II.) At first it was unknown whether or not (1.9) has a solution, but now several have been found [8].

Section III gives a lower bound to z_c (which we call z_c^L):

$$z_c>z_c^L=(24.0)/(8\pi\alpha^2)>17{,}900. \tag{1.11}$$

This is far better than that needed for physics. For all $z<z_c^L$ we also derive a lower bound for $E(z)$:

$$E(z)\geqq -\tfrac{1}{4}z^2-z^3(32z_c^L)^{-1}(1-\tfrac{3}{4}z/z_c^L)^{3/2}. \tag{1.12}$$

[Note that $E(z)$ is trivially less than $-\frac{1}{4}z^2$, which is the ground state energy for $B\equiv 0$.]

The B field that causes $E(z)$ to diverge when $z>z_c$ is highly inhomogeneous (both in magnitude and direction) near the nucleus. In astrophysical and other applications [9, 11] one is interested in studying atoms and ions in very strong, external magnetic fields with the property that the *direction of the magnetic field is constant* over distance scales many times the scales of atomic physics, to a very good approximation. Theoretical astrophysicists have carried out large-scale numerical calculations of the spectra of atoms and ions in very strong magnetic fields and have tried to correlate theoretical predictions with experimental data. As a modest contribution to the mathematical foundations of this kind of work, we establish stability of one-electron atoms in *arbitrarily strong* magnetic fields whose direction (but *not* magnitude) is *constant* in a neighborhood of the atom. This is done in Sect. IV, where we prove that $E(z)$ is always finite in this case. An open problem for further investigation is the analysis of $E_0(B,z)$ for magnetic fields that are curl free in a neighborhood of the atom.

Before proceeding to the physical interpretation, we note in passing that the electron g factor was taken to be 2 in (1.4). If we replace the $\sigma\cdot B$ term in (1.4) by $\frac{1}{2}g\sigma\cdot B$ then two cases arise:

$g<2$. Here we can write the kinetic energy as $\frac{1}{2}g[\sigma\cdot(p-A)]^2+(1-\frac{1}{2}g)(p-A)^2$. The first term is nonnegative and the second, when combined with $-z/|x|$ gives a Hamiltonian of type H' in (1.2). This is bounded below by $-\frac{1}{2}z^2/(2-g)$, and hence $E(z)$ is always finite.

$g>2$. Here, $E(z)=-\infty$ for all z, *including* $z=0$. To see this, let B be a field which is constant $=B(0,0,1)$ over a large cube of length L, with $A=\frac{1}{2}B(x_2,-x_1,0)$ inside this cube. Let B drop to zero outside the cube so that $I=\int B^2<\infty$. Take ψ to be a ground state Landau orbital (cut off in the x_3 direction so that $\psi\in L^2$), i.e.

$$\psi(x)=(\text{const})(1,0)\exp[-\tfrac{1}{4}B(x_1^2+x_2^2)]\cos(\pi x_3/L)$$

and $\psi(x)=0$ for $|x_3|>L/2$. With B fixed and with L big enough, we can have $(\psi,[\sigma\cdot(p-A)]^2\psi)\leqq\frac{1}{4}(g/2-1)B$ and $(\psi,\sigma\cdot B\psi)\geqq\frac{1}{2}B$. Also $I\leqq 2B^2L^3$. The total energy (with $z=0$) is less than $-\frac{1}{4}(g/2-1)B+2B^2L^3\varepsilon$. Now, let $\lambda>0$ and replace $\psi(x)$ by $\lambda^{3/2}\psi(\lambda x)$, $A(x)$ by $\lambda A(\lambda x)$ and $B(x)$ by $\lambda^2 B(\lambda x)$. The energy is then less than $-\frac{1}{4}\lambda^2(g/2-1)B+2\lambda B^2L^3\varepsilon$. (This scaling is exact and will be employed frequently in the sequel.) As $\lambda\to\infty$, the energy tends to $-\infty$, so stability never holds.

Since physically $g>2$ because of Quantum Electrodynamics (QED) effects, it is clear that if we try to "improve" (1.4) by replacing $\sigma\cdot B$ by $\frac{1}{2}g\sigma\cdot B$ we shall get an inconsistent theory. The only truly consistent procedure is to include *all* QED effects, and this is outside the scope of this paper.

The foregoing aside about the g-factor leads us to the question of the physical content of the results of this paper, (1.8)–(1.12). There are two ways to view them. The first is to observe that (1.8) and (1.11) show that atomic physics with the Hamiltonian (1.4) contains no seeds of instability for small z (small meaning $z<17{,}900$) and that perturbation theory (in B) can be safely employed for very small B. (Of course one should also analyze the many-electron and many-nucleus problem to be certain about this conclusion. We are unable to do this fully, but in a subsequent paper [6] we do successfully analyze two problems: the one-electron, many-nucleus problem and the one-nucleus, many-electron problem, i.e. the full atom.) The fact that the theory is well behaved for small z is not entirely a trivial matter, especially when the situation is contrasted with that for spin-spin interactions (either electron-electron or electron-nucleus). Here, one adds a two-body term $\sigma^a\cdot\sigma^b|x|^{-3}-3(\sigma^a\cdot x)(\sigma^b\cdot x)|x|^{-5}$, where x is the vector between particles a and b. The $|x|^{-3}$ singularity is not integrable and, in particular it cannot be controlled by the kinetic energy. Thus, a system with this interaction is *always* unstable in our sense. The treatment of the interaction by perturbation theory, is not really a consistent procedure.

Of course, it is always possible to restore stability by cutting off the Coulomb or spin-spin interactions at the Compton wavelength of the electron, but then the theory would depend critically on this wavelength. Stability, in the sense we use it, implies that the Schrödinger equation for electrons and nuclei is independent of the electron's Compton wavelength-in conformity with what is always assumed to be the case.

The second viewpoint is to emphasize the breakdown of (1.4) when $z>z_c$ and to say that magnetic interactions impose an upper bound on $z\alpha^2$. Here we are treading on shaky ground. If we specify ψ and ask what B minimizes $(\psi,H\psi)+\varepsilon\int B^2$, we easily find that Maxwell's equation takes the form

$$2\varepsilon\,\mathrm{curl}\,B(x)=j(x)=2\,\mathrm{Re}\langle\psi,(p-A)\psi\rangle(x)+\mathrm{curl}\langle\psi,\sigma\psi\rangle(x)\,. \tag{1.13}$$

[Notation. $(\psi,H\psi)$ has been used to denote the usual expectation, including the x-integration. $\langle\psi,\sigma\psi\rangle(x)$ denotes the inner product with respect to the spinor indices *only*, and hence it is a function of x. $\langle\psi,\psi\rangle(x)\equiv|\psi(x)|^2=|\psi_1(x)|^2+|\psi_2(x)|^2$.]

The first term in j is the electron current ($p-A$ is the velocity). The second term is the "spin" current; it is conserved. The B field in (1.13) cannot be viewed as external; it is, in fact, generated by the electron as (1.13) shows. It is this B field that causes the breakdown when $z>z_c$. [Technical note. In Sect. II we choose a special pair ψ, A with $\sigma \cdot (p-A)\psi \equiv 0$, so that the right side of (1.13) is zero. For this ψ, the B field we use is not exactly optimal [because (1.13) is not satisfied], but the error becomes inconsequential when we employ the λ-scaling $\psi(x) \to \lambda^{3/2}\psi(\lambda x)$ and $A(x) \to \lambda A(\lambda x)$.]

The instability of (1.6) for $z > z_c$ might indicate a qualitative change in the behaviour of non-relativistic quantum electrodynamics (QED), e.g. some kind of phase transition or an intrinsic instability, as z becomes large. For a compelling argument in this direction we would, however, have to include the term $\int \mathbf{E}^2$ in the Hamiltonian, quantize the electromagnetic field and properly renormalize the theory. Our calculations can be viewed as a quasi-classical approximation to that theory. The fact that this approximation exhibits an instability, for large z, should, by experience, be seen as a warning that the full theory might also exhibit a drastic change in behaviour, for large z.

Physically, our instability result for $z > z_c$ is, of course, quite irrelevant, because $z_c > 17{,}000$. Nuclei with nuclear charge above ~ 100 are not known to exist in nature, and even if nuclei with $z \sim 10{,}000$ existed electrons moving in their field would be highly relativistic particles, so that our use of non-relativistic kinematics is not justified for values of z where the instability occurs. Nevertheless, we feel that it is an interesting mathematical problem to explore the consistency of this model even beyond the domain, where the approximation is justified.

As remarked after (1.12), the interaction given in (1.4) *lowers* the energy. In contrast to this, the Lamb shift, which is obtained from a proper QED calculation (but only in perturbation theory), is a *raising* of the energy. Furthermore the Lamb shift is of order $z^4\alpha^3$ (apart from logarithmic corrections) which contrasts with our lowering (1.12) which is of order $z^3\alpha^2$. Our result is not directly comparable with the Lamb shift since the latter requires a fully quantized theory with renormalization.

Now we turn to the mathematical preliminaries to the rest of this paper. Some notation will be introduced and, more importantly, a careful discussion of the class of functions (A, B, ψ) will be given.

First, consider the B field. In order that (1.1) make sense we obviously require $B \in L^2(\mathbb{R}^3)$. [Notation. For vector fields (A or B)

$$\|A\|_p \equiv \|(A \cdot A)^{1/2}\|_p, \tag{1.14}$$

where $A = (A_1, A_2, A_3)$ and $A \cdot A = \sum |A_i|^2$. For spinors ψ

$$\|\psi\|_p = \|\langle \psi, \psi \rangle^{1/2}\|_p, \tag{1.15}$$

where $\langle \psi, \psi \rangle(x) = |\psi_1(x)|^2 + |\psi_2(x)|^2 = \left\{\sum_i |\langle \psi, \sigma_i \psi \rangle(x)|^2\right\}^{1/2}$. For gradients

$$\|\nabla A\|_2 = \left\|\left(\sum_{i,j} |\partial_i A_j|^2\right)^{1/2}\right\|_2 = \left\{\sum_{i,j} \int |\partial_i A_j|^2\right\}^{1/2} \tag{1.16}$$

with $\partial_i = \partial/\partial x_i$, $i = 1, 2, 3$. A similar formula holds for $\|\nabla \psi\|_2$.] The vector potential, A, satisfies $\operatorname{curl} A = B$, but A is determined only up to a gauge (i.e. $A \to A + \nabla \Phi$). Gauge transformations on ψ (i.e. $\psi \to e^{i\Phi}\psi$) can be nasty ($e^{i\Phi}$ can have very bad differentiability properties). This problem is avoided by fixing a gauge, namely the Coulomb gauge, $\operatorname{div} A = 0$. Additionally, it will be convenient to have the formal identity (when $\operatorname{div} A = 0$)

$$\|B\|_2^2 = \int B^2 = \|\nabla A\|_2^2 . \tag{1.17}$$

The danger is that A might conceivably have bad decay properties at infinity which would prevent the necessary integrations by parts in (1.17). This problem is resolved in Appendix A. Notice that if $\nabla A \in L^2$ and if $A(x) \to 0$ as $|x| \to \infty$ in a weak sense, see [2], then, by the Sobolev inequality

$$\|\nabla A\|_2 \geqq S \|A\|_6 , \tag{1.18}$$

so A is automatically in L^6. Theorem A.1 in the appendix states that when $B \in L^2$ there is a *unique* A satisfying

$$\operatorname{curl} A = B, \quad \operatorname{div} A = 0 \text{ in } \mathscr{D}', \text{ and } \quad A \in L^6 , \tag{1.19}$$

and this A also satisfies (1.17), which implies $\nabla A \in L^2$. Here, $\mathscr{D}'$ denotes the usual space of distributions. This is the A we shall use (except in Theorems 2.1 and A.2 where only the assumption $A \in L^6$ is used).

Next we turn to the spinor field ψ which obviously must be in L^2. To avoid operator domain questions we shall interpret the first term in (1.5) as a quadratic form $Q = \|\sigma \cdot (p - A)\psi\|_2^2$. Theorem A.2 states that if $\sigma \cdot (p - A)\psi \in L^2$, $\psi \in L^2$, and $A \in L^6$, then automatically $\nabla \psi \in L^2$. This, in turn, implies that $(\psi, |x|^{-1}\psi) < \infty$ by (1.18), or by the well known uncertainty principle for the hydrogen atom,

$$\|\psi\|_2 \|\nabla \psi\|_2 \geqq (\psi, |x|^{-1}\psi) . \tag{1.20}$$

Therefore, we introduce the class of function pairs

$$\mathscr{C} = \{\psi, A \mid \psi \in H^1(\mathbb{R}^3), \|\psi\|_2 = 1, A \in L^6(\mathbb{R}^3), \operatorname{div} A = 0, \nabla A \in L^2(\mathbb{R}^3)\} . \tag{1.21}$$

[$\psi \in H^1$ means $\psi \in L^2$ and $\nabla \psi \in L^2$. The set of functions f satisfying $f \in L^6(\mathbb{R}^3)$, $\nabla f \in L^2(\mathbb{R}^3)$ is sometimes called $D^{1,2}(\mathbb{R}^3)$; it is the completion of $H^1(\mathbb{R}^3)$, not in the H^1-norm $(\|f\|_2^2 + \|\nabla f\|_2^2)^{1/2}$, but in the norm $\|\nabla f\|_2$.]

For functions in $\mathscr{C}$ the following energy functional is a generalization of $(\psi, H\psi) + \varepsilon \int B^2$.

$$\mathscr{E}(\psi, A) = \|\sigma \cdot (p - A)\psi\|_2^2 + \varepsilon \|B\|_2^2 - z(\psi, |x|^{-1}\psi) , \tag{1.22}$$

and each term in (1.22) is well defined. The ground state energy is

$$E(z) = \inf\{\mathscr{E}(\psi, A) \mid (\psi, A) \in \mathscr{C}\} . \tag{1.23}$$

Theorem 2.4 states that when $E(z)$ is finite, the infimum in (1.23) is a minimum.

Another class we shall need is

$$\mathscr{F} = \{\psi, A \mid (\psi, A) \in \mathscr{C} \text{ and } \sigma \cdot (p - A)\psi = 0\} . \tag{1.24}$$

Notice that when $(\psi, A) \in \mathscr{C}$, then each term $p\psi$ and $A\psi$ makes sense as L^2 function. In Sect. II the formula

$$z_c = \varepsilon \inf\{\|B\|_2^2 / (\psi, |x|^{-1}\psi) \mid (\psi, A) \in \mathscr{F}\} \tag{1.25}$$

will be derived. Theorem 2.5 states that the infimum in (1.25) is actually a minimum.

II. A Basic Theorem and a Formula for z_c

Heuristically, if $\mathscr{E}(\psi, A)$ is unbounded for a certain z, we expect ψ and A to blow up in some sense. The following theorem is essential for understanding this blowup. It is stated in general terms, but its use for our problem will be clarified shortly; it will yield a formula for z_c.

Theorem 2.1. *Let ψ_n be a sequence of spinor valued functions on $\mathbb{R}^3$ and A_n a sequence of vector fields on $\mathbb{R}^3$ satisfying (for some fixed $3<p<\infty$)*

(i) $d_1 \leqq \|\psi_n\|_2 \leqq d_2$ *for some constants* $d_2 \geqq d_1 > 0$.

(ii) $\|\nabla\psi_n\|_2 \to \infty$ *as* $n \to \infty$.

(iii) $\|A_n\|_p \leqq D\|\nabla\psi_n\|_2^s$ *for some* $D>0$, *where* $s = 1 - \dfrac{3}{p}$.

(iv) $\|\sigma\cdot(p-A_n)\psi_n\|_2 \leqq C_n\|\nabla\psi_n\|_2$ *for some sequence* $\{C_n\}_{n=1}^{\infty}$ *with* $C_n \to 0$ *as* $n\to\infty$. *Define* $1/\lambda_n = \|\nabla\psi_n\|_2$ *(whence* $\lambda_n \to 0$ *as* $n\to\infty$*),* $\phi_n(x) = \lambda_n^{3/2}\psi_n(\lambda_n x)$ *and* $\alpha_n(x) = \lambda_n A_n(\lambda_n x)$. *Then*

(a) $\liminf\limits_{n\to\infty} \|\alpha_n\|_p \geqq c > 0$.

(b) *There exists a subsequence (which we continue to denote by n) and functions ϕ and α, and a sequence of points $x_n \in \mathbb{R}^3$ such that $\tilde{\phi}_n(x) \equiv \phi_n(x-x_n) \rightharpoonup \phi(x) \neq 0$ weakly in $H^1(\mathbb{R}^3)$, $\tilde{\alpha}_n(x) \equiv \alpha_n(x-x_n) \rightharpoonup \alpha(x) \neq 0$ weakly in $L^p(\mathbb{R}^3)$. Moreover,*

$$\sigma\cdot(p-\alpha)\phi = 0\,. \tag{2.1}$$

(c) *If the original sequence has the property that ϕ_n does not converge weakly to zero in $H^1(\mathbb{R}^3)$, then the statement in part* (b) *holds with* $x_n \equiv 0$.

Proof. Clearly by (i) and the definition of ϕ_n we have that ϕ_n is uniformly bounded in $H^1(\mathbb{R}^3)$. By (iii)

$$\|\alpha_n\|_p = \lambda_n^{\frac{p-3}{p}}\|A_n\|_p \leqq D\lambda_n^{1-s-3/p} = D\,, \tag{2.2}$$

so α_n is uniformly bounded in $L^p(\mathbb{R}^3)$. By (iv) $\|\sigma\cdot(p-\alpha_n)\phi_n\|_2 \leqq C_n \to 0$ as $n\to\infty$. By the triangle inequality and Hölder's inequality with $q = 2p/(p-2)$ we have

$$C_n \geqq \|\sigma\cdot(p-\alpha_n)\phi_n\|_2 \geqq \|\nabla\phi_n\|_2 - \|\alpha_n\phi_n\|_2 \geqq 1 - \|\alpha_n\|_p\|\phi_n\|_q\,. \tag{2.3}$$

Note that $\|(\sigma\cdot p)\phi\|_2 = \|\nabla\phi\|_2$ and that $\|(\sigma\cdot\alpha)\phi\|_2 = \|\alpha\phi\|_2$. The latter uses the trivial identity $(\sigma\cdot\alpha)^2 = \alpha^2$. The former uses the same identity in Fourier space $(\sigma\cdot p)^2 = p^2$, and this is justified since $\phi \in H^1$. Also note that $2<q<6$. Inequality (2.3) will be used in two ways. Since ϕ_n is uniformly bounded in H^1 we have, by Sobolev's inequality, that $\|\phi_n\|_q \leqq d_q$, and hence $\|\alpha_n\|_p \geqq (1-C_n)/d_q$, which proves (a). On the other hand using (2.2) together with (2.3) we find $\|\phi_n\|_q \geqq (1-C_n)/D$, and hence $\liminf\|\phi_n\|_q \geqq 1/D > 0$. Since $\|\phi_n\|_2 \leqq d_2$ and $\|\phi_n\|_6 \leqq d_6$, Lemma 2.1 and Lemma 2.2 below prove the existence of a sequence $x_n \in \mathbb{R}^3$ and a subsequence ϕ_n such that $\tilde{\phi}_n \rightharpoonup \phi \neq 0$ weakly in $H^1(\mathbb{R}^3)$. By passing, if necessary, to a further subsequence we can assume that $\tilde{\alpha}_n \rightharpoonup \alpha$ weakly in $L^p(\mathbb{R}^3)$. Next we show that $\tilde{\phi}_n\tilde{\alpha}_n \rightharpoonup \phi\alpha$ componentwise weakly in $L^2(\mathbb{R}^3)$. To show that $f_n \rightharpoonup f$ in $L^2(\mathbb{R}^3)$, it suffices to prove that $f_n \rightharpoonup f$ in $L^2(K)$ for every compact $K \subset \mathbb{R}^3$. By the Rellich-Kondrachov theorem, $\tilde{\phi}_n \to \phi$ strongly in $L^q(K)$ (since $2<q<6$), whence $\tilde{\phi}_n\tilde{\alpha} \rightharpoonup \phi\alpha$ in $L^2(K)$. Thus, we have proved that $g_n \equiv \sigma\cdot(p-\tilde{\alpha}_n)\tilde{\phi}_n \rightharpoonup \sigma\cdot(p-\alpha)\phi \equiv g$ weakly in $L^2(\mathbb{R}^3;\mathbb{C}^2)$. But we already noted that $\|g_n\|_2 \to 0$, which implies (by the weak lower semicontinuity of the norm) that $g=0$. Obviously, $\alpha \neq 0$ because otherwise we should have $(\sigma \cdot p)\phi=0$ with $\phi \neq 0$, which is impossible [recall that $\|(\sigma \cdot p)\phi\|_2 = \|\nabla\phi\|_2$]. This proves (b).

To prove (c) we note a trivial generalization of the Banach-Alaoglu theorem: Since $\phi_n \not\rightharpoonup 0$ we can find a subsequence such that $\phi_n \rightharpoonup \phi$ and $\phi \neq 0$. The rest of the proof is the same as in (b), except that Lemma 2.2 is not needed. □

Lemma 2.1. *Let g be a measurable function on a measure space such that for $p<q<r$ fixed and for some C_p, C_q, C_r all >0,*

(i) $\|g\|_p^p \leqq C_p$,
(ii) $\|g\|_r^r \leqq C_r$,
(iii) $\|g\|_q^q \geqq C_q > 0$.

Then $f(\varepsilon) \equiv \operatorname{meas}\{x \mid |g(x)| \geqq \varepsilon\} > C$ for some fixed $\varepsilon, C>0$ depending on p, q, r, C_p, C_q, C_r, but not on g.

Proof. From the fact that $f(\varepsilon)$ is monotone non-increasing and that $\int g^p = p\int_0^\infty f(\varepsilon)\varepsilon^{p-1}d\varepsilon$, we have $C_p \geqq p\int_0^R \varepsilon^{p-1} f(\varepsilon)d\varepsilon \geqq R^p f(R)$ or

$$f(\varepsilon) \leqq \varepsilon^{-p} C_p, \quad \text{all } \varepsilon>0. \tag{2.4}$$

Similarly,

$$f(\varepsilon) \leqq \varepsilon^{-r} C_r, \quad \text{all } \varepsilon>0. \tag{2.5}$$

Define S and T by

$$qC_pS^{q-p} = \tfrac{1}{4}(q-p)C_q,$$
$$qC_rT^{q-r} = \tfrac{1}{4}(r-q)C_q.$$

From (2.4)

$$q\int_0^S f(\varepsilon)\varepsilon^{q-1}d\varepsilon \leqq qC_p\int_0^S \varepsilon^{q-p-1}d\varepsilon = \tfrac{1}{4}C_q. \tag{2.6}$$

Similarly, from (2.5)

$$q\int_T^\infty f(\varepsilon)\varepsilon^{q-1}d\varepsilon \leqq \tfrac{1}{4}C_q, \tag{2.7}$$

(2.6) and (2.7) imply that $S<T$ and that

$$I \equiv q\int_S^T f(\varepsilon)\varepsilon^{q-1}d\varepsilon \geqq \tfrac{1}{2}C_q.$$

But $I \leqq f(S)|T^q - S^q|$ since f is monotone nonincreasing. This proves the lemma (with $\varepsilon \equiv S$) since S and T are explicitly given independent of f. □

Lemma 2.2 [5]. *Let $1<p<\infty$ and let $\{f_n\}_{n=1}^\infty$, be a uniformly bounded sequence of functions in $W^{1,p}(\mathbb{R}^d)$ with the property that the Lebesgue measure of $\{x \mid |f_n(x)|>\varepsilon\} > C$ for some fixed constants C and $\varepsilon>0$. Then there exists a sequence of translations $\{\tau_n\}_{n=1}^\infty$ of $\mathbb{R}^d$, $\tau_n y = y + x_n$, $F_n(y) \equiv f_n(\tau_n y) = f_n(y+x_n)$, such that, for some subsequence, $F_n \rightharpoonup F$ weakly in $W^{1,p}$ and $F \neq 0$.*

Remark. The proof in [5] was given for real valued functions. It is easy to see that the lemma holds for complex valued functions by considering separately real and imaginary parts. The same argument then carries over to complex spinors. We recall that $W^{1,p}$ consists of all functions in L^p whose first derivatives are in L^p. Note that $W^{1,2}=H^1$.

Let us now apply Theorem 2.1 to the proof of formula (1.10) for z_c. Suppose that z is such that $E=-\infty$. This means there exists a sequence of pairs $(\psi_n, A_n)\in\mathscr{C}$ such that as $n\to\infty$,

$$E_n=\mathscr{E}(\psi_n, A_n)=\|\sigma\cdot(p-A_n)\psi_n\|_2^2-z(\psi_n,|x|^{-1}\psi_n)+\varepsilon\int B_n^2dx \tag{2.8}$$

tends to $-\infty$. We verify the assumptions of Theorem 2.1 for the sequence (ψ_n, A_n). (The usage of ϕ_n, α_n as in Theorem 2.1 will be continued.) (i) is trivial since $\|\psi_n\|_2=1$.

Observe that $-z(\psi_n,|x|^{-1}\psi_n)$ is the only negative term in (2.8) and hence $(\psi_n,|x|^{-1}\psi_n)\to\infty$ as $n\to\infty$. (ii) follows from the inequality $(\psi_n,|x|^{-1}\psi_n)\leqq\|\nabla\psi_n\|_2\|\psi_n\|_2$.

We can choose $E_n<0$ (all n) and we find

$$\|\sigma(p-A_n)\psi_n\|_2^2+\varepsilon\int B_n^2\leqq z(\psi_n,|x|^{-1}\psi_n)\leqq z\|\nabla\psi_n\|_2\,. \tag{2.9}$$

(iv) holds with $C_n=z^{1/2}\|\nabla\psi_n\|_2^{-1/2}$.

From (2.9) we also obtain $\|B_n\|_2^2\leqq(z/\varepsilon)\|\nabla\psi_n\|_2$. On the other hand, Sobolev's inequality gives

$$\|B_n\|_2^2=\sum_i\|\nabla A_{i,n}\|_2^2\geqq S^2\|A_n\|_6^2\,. \tag{2.10}$$

Thus, (iii) holds with $p=6$ and $s=\frac{1}{2}$.

The conclusions (a) and (b) of Theorem 2.1 thus hold for the sequence (ψ_n, A_n). It is easily seen that conclusion (c) also holds, for suppose $\phi_n\rightharpoonup 0$ weakly in $H^1(\mathbb{R}^3,\mathbb{C}^2)$. This would imply that $b_n\equiv(\phi_n,|x|^{-1}\phi_n)\to 0$ as $n\to\infty$. [To prove this, let B_R be the ball of radius R centered at 0 and χ_R its characteristic function. Note that, by Rellich-Kondrachov, $\phi_n\to 0$ strongly in $L^4(B_R)$. Then, writing $b_n=b_n^+ + b_n^-$, with $b_n^-=(\phi_n,|x|^{-1}\chi_R\phi_n)$, we have that $b_n^-\to 0$. However $b_n^+\leqq R^{-1}$ since $\|\phi_n\|_2=1$. Then let $R\to\infty$.] The energy can be written [using λ_n of Theorem 2.1, $\beta_n(x)\equiv\lambda_n^2B_n(\lambda_n x)$] as

$$E_n=\mathscr{E}(\psi_n, A_n)=\lambda_n^{-1}\{\lambda_n^{-1}\|\sigma\cdot(p-\alpha_n)\phi_n\|_2^2+\varepsilon\|\beta_n\|_2^2-zb_n\}\,. \tag{2.11}$$

If $b_n\to 0$ then, since $E_n<0$, $\beta_n\to 0$ strongly in L^2. By (2.10), $\alpha_n\to 0$ strongly in L^6, which contradicts conclusion (a) of Theorem 2.1.

In the foregoing we did not actually use the fact that $E_n\to-\infty$, but only the facts that $E_n<0$ and that the Coulomb energy diverges. The foregoing analysis was actually the proof of the following

Theorem 2.2. *Let* $(\psi_n, A_n)\in\mathscr{C}$ *be a sequence satisfying*

$$E_n<0 \quad \textit{and} \quad \limsup_{n\to\infty}(\psi_n,|x|^{-1}\psi_n)=\infty\,.$$

Then conclusions (a) *and* (c) *of Theorem 2.1 hold for this sequence. Moreover, for the subsequence given by Theorem 2.1* (c),

$$(\phi_n,|x|^{-1}\phi_n)\to(\phi,|x|^{-1}\phi)\neq 0\,.$$

Remark. For any minimizing sequence (for any z) we can always assume $E_n<0$, since one can always take the pair $\psi=$ ground state hydrogenic function and $A\equiv 0$.

Let us define

$$\hat{z}=\inf_{\mathscr{F}} \varepsilon\|B\|_2^2/(\psi,|x|^{-1}\psi). \tag{2.12}$$

Note that the set $\mathscr{F}$ (defined in Sect. I) is not empty (see [8]).

Theorem 2.3.

$$\hat{z}=z_c. \tag{2.13}$$

Proof. Assume that $E_n\to-\infty$. We shall show that $z\geqq\hat{z}$, which implies $z_c\geqq\hat{z}$. By the remark above (and passing to a subsequence), we can assume that

$$\phi_n\rightharpoonup\phi\neq 0 \text{ weakly in } H^1(\mathbb{R}^3),$$

$$(\phi_n,|x|^{-1}\phi_n)\to(\phi,|x|^{-1}\phi),$$

$$\beta_n\rightharpoonup\beta \text{ weakly in } L^2(\mathbb{R}^3).$$

From this, $\|\beta\|_2\leqq\liminf\|\beta_n\|_2$ and $\|\phi\|_2\leqq\liminf\|\phi_n\|_2=1$. By (2.11)

$$0\geqq\liminf\lambda_nE_n\geqq\varepsilon\|\beta\|_2^2-z(\phi,|x|^{-1}\phi).$$

Since ϕ might not be normalized, define $\hat{\phi}=\phi/\|\phi\|_2$. Then

$$z\geqq\varepsilon\|\beta\|_2^2/(\phi,|x|^{-1}\phi)\geqq\varepsilon\|\beta\|_2^2/(\hat{\phi},|x|^{-1}\hat{\phi})\geqq\hat{z},$$

since $(\hat{\phi},\alpha)\in\mathscr{F}$.

On the other hand, if $z_c>\hat{z}$, then there exists $(\psi,A)\in\mathscr{F}$ such that the ratio on the right side of (2.12) is less than $\bar{z}\equiv\hat{z}+\frac{1}{2}(z_c-\hat{z})$. Define $\psi_n(x)=n^{3/2}\psi(nx)$, $A_n(x)=nA(nx)$. Then for the $\bar{z}$ just defined

$$\mathscr{E}(\psi_n,A_n)=n\{-\bar{z}(\psi,|x|^{-1}\psi)+\varepsilon\|B\|_2^2\},$$

which tends to $-\infty$ as $n\to\infty$. This is a contradiction since $\bar{z}<z_c$. □

Remark. We have repeatedly used the facts that $z<z_c \Rightarrow E>-\infty$ and $z>z_c \Rightarrow E=-\infty$. For the case $z=z_c$ we do not know whether E is finite or $E=-\infty$. This is an open question.

Two natural questions arise. Is there a minimizing $(A,\psi)\in\mathscr{C}$ for $\mathscr{E}$ when $z<z_c$? Is there a minimizing $(A,\psi)\in\mathscr{F}$ for the ratio in (2.12) defining $z_c=\hat{z}$? The answer to both questions is yes.

Theorem 2.4. *When $z<z_c$ there exists a pair $(\psi,A)\in\mathscr{C}$ such that*

$$\mathscr{E}(\psi,A)=E\equiv\inf\{\mathscr{E}(\psi',A')|(\psi',A')\in\mathscr{C}\}.$$

Theorem 2.5. *There exists $(\psi,A)\in\mathscr{F}\equiv\{(\psi',A')\in\mathscr{C}|\sigma\cdot(p-A')\psi'=0\}$ such that $\varepsilon\|B\|_2^2/(\psi,|x|^{-1}\psi)=z_c=\hat{z}$ (given by (2.12)).*

Proof of Theorem 2.4. Let $(\psi_n,A_n)\in\mathscr{C}$ be a minimizing sequence. By Theorem 2.2, $b_n\equiv(\psi_n,|x|^{-1}\psi_n)$ is a bounded sequence (since $z<z_c$). From (2.8) we see that $\|B_n\|_2$ and $\|\sigma\cdot(p-A_n)\psi_n\|_2$ are also bounded sequences (since $E_n<0$). Now,

$$\|\nabla\psi_n\|_2=\|\sigma\cdot p\psi_n\|_2\leqq\|\sigma\cdot(p-A_n)\psi_n\|_2+\|(\sigma\cdot A_n)\psi_n\|_2.$$

However $\|(\sigma\cdot A_n)\psi_n\|_2 = \|A_n\psi_n\|_2 \leqq \|A_n\|_6 \|\psi_n\|_6^{1/2}\|\psi_n\|_2^{1/2}$. By the Sobolev inequality (2.10) applied to A_n and ψ_n, (and with $\|\psi_n\|_2 = 1$),

$$\|\nabla\psi_n\|_2 \leqq \|\sigma\cdot(p-A_n)\psi_n\|_2 + S^{-3/2}\|B_n\|_2\|\nabla\psi_n\|_2^{1/2}. \tag{2.14}$$

This implies that $\|\nabla\psi_n\|_2$ is also bounded and hence that ψ_n is bounded in H^1.

By passing to a subsequence we have

$$\begin{aligned} &\psi_n \rightharpoonup \psi \quad \text{weakly in } H^1, \\ &A_n \rightharpoonup A \quad \text{weakly in } L^6, \\ &B_n \rightharpoonup B \quad \text{weakly in } L^2, \\ &\operatorname{div} A = 0 \quad \text{and} \quad \operatorname{curl} A = B, \\ &(\psi_n, |x|^{-1}\psi_n) \to (\psi, |x|^{-1}\psi). \end{aligned} \tag{2.15}$$

The proof of the last statement is as in Theorem 2.2. Furthermore, $\psi_n A_n \rightharpoonup \psi A$ in L^2 (as in the proof of Theorem 2.1). By lower semicontinuity of the norms we obtain $E \geqq \mathscr{E}(\psi, A)$. If we knew that $\|\psi\|_2 = 1$ [and hence that $(\psi, A) \in \mathscr{C}$] we would be done. However, $\|\psi\|_2 \leqq 1$ by lower semicontinuity. Suppose that $\gamma = \|\psi\|_2^{-1} > 1$. Define $\hat{\psi} = \gamma\psi$. Then

$$\mathscr{E}(\hat{\psi}, A) = \gamma^2\{\|\sigma\cdot(p-A)\psi\|_2^2 - z(\psi, |x|^{-1}\psi)\} + \varepsilon\|B\|_2^2.$$

The term in { } must be negative [since $\mathscr{E}(\psi, A) \leqq E < 0$]. Therefore, $E \leqq \mathscr{E}(\hat{\psi}, A) < \mathscr{E}(\psi, A) \leqq E$. Hence $\gamma = 1$ and the proof is complete. □

Proof of Theorem 2.5. Let $(\psi_n, A_n) \in \mathscr{F}$ be a minimizing sequence. By scaling

$$\psi_n(x) \to \lambda^{3/2}\psi_n(\lambda x),\ A_n(x) \to \lambda A_n(\lambda x),$$

we can assume that $\|B_n\|_2 = 1$. Also $\|\psi_n\|_2 = 1$ and $\|\nabla\psi_n\|_2 \leqq S^{-3}$ [by (2.14) and $\sigma\cdot(p-A_n)\psi_n = 0$]. Thus ψ_n is bounded in H^1. Again, (2.15) holds for some subsequence. By lower semicontinuity, $\|B\|_2 \leqq \|B_n\|_2$ and $\gamma = \|\psi\|_2^{-1} \geqq 1$. Note that $\psi \neq 0$ by the last line of (2.15). Replacing ψ by $\hat{\psi} = \gamma\psi$ we have that

$$\hat{z}/\varepsilon = \lim\{\|B_n\|_2^2/(\psi_n, |x|^{-1}\psi_n)\} \geqq \|B\|_2^2/(\psi, |x|^{-1}\psi) \geqq \|B\|_2^2/(\hat{\psi}, |x|^{-1}\hat{\psi}).$$

If we can show that $\sigma\cdot(p-A)\psi = 0$, we can conclude from this that $\gamma = 1$ and that (ψ, A) is a minimizing pair. However, $\nabla\psi_n \rightharpoonup \nabla\psi$ and $A_n\psi_n \rightharpoonup A\psi$ weakly in L^2, so $0 = \sigma\cdot(p-A_n)\psi_n \rightharpoonup \sigma\cdot(p-A)\psi$ weakly in L^2. But the weak limit of 0 can only be 0. □

III. A Lower Bound for z_c

In the previous section z_c was shown to be finite (since $\mathscr{F}$ is not empty) and a formula for z_c was given. While we are unable to evaluate that formula, we shall show here that z_c is not too small. The methods of this section are completely different from those of the previous section.

Let $(\psi, A) \in \mathscr{C}$ be given and let

$$T(\psi, A) \equiv \|(p-A)\psi\|_2^2\,, \tag{3.1}$$

$$Q(\psi) \equiv \frac{1}{4\varepsilon} \int \{\langle \psi, \psi \rangle (x)\}^2 dx\,, \tag{3.2}$$

$$\mathcal{T}(\psi, A) \equiv \|\sigma \cdot (p-A)\psi\|_2^2 + \varepsilon \|B\|_2^2\,. \tag{3.3}$$

$$X(\psi, A) \equiv \tfrac{1}{2} T(\psi, A)/Q(\psi)\,. \tag{3.4}$$

Lemma 3.1.

$$\mathcal{T}(\psi, A) \geqq T(\psi, A) \cdot \begin{cases} \tfrac{1}{2} X(\psi, A) & \text{if} \quad X(\psi, A) \leqq 1 \\ 1 - \{2X(\psi, A)\}^{-1} & \text{if} \quad X(\psi, A) \geqq 1\,. \end{cases} \tag{3.5}$$

Proof. Let $0 \leqq t \leqq 1$ and observe that

$$\mathcal{T}(\psi, A) \geqq t \|\sigma \cdot (p-A)\psi\|_2^2 + \varepsilon \|B\|_2^2\,.$$

Expanding the first term on the right we get

$$\mathcal{T}(\psi, A) \geqq t T(\psi, A) - t \int B(x) \cdot \langle \psi, \sigma\psi \rangle (x) dx + \varepsilon \|B\|_2^2\,. \tag{3.6}$$

Note that in obtaining this result we performed a partial integration in the second term which is easily justified. Minimizing the second and the third term with respect to $B(B(x) = (t/2\varepsilon) \langle \psi, \sigma\psi \rangle (x))$ we find for these two terms the lower bound

$$-t^2 Q(\psi)\,. \tag{3.7}$$

We have used the identity

$$\langle \psi, \sigma\psi \rangle \cdot \langle \psi, \sigma\psi \rangle = \langle \psi, \psi \rangle^2\,, \qquad \text{all } x\,. \tag{3.8}$$

The sum of the first term in (3.6) together with (3.7) has its maximum as a function of t at $t_0 = X(\psi, A)$. If $t_0 \leqq 1$ we find

$$\mathcal{T}(\psi, A) \geqq \tfrac{1}{2} T(\psi, A) X(\psi, A)\,,$$

and if $t_0 > 1$ we set $t = 1$ and get

$$\mathcal{T}(\psi, A) \geqq T(\psi, A) - Q(\psi)\,. \quad \square$$

Lemma 3.1 provides us with two alternatives.

Alternative 1. $X(\psi, A) \geqq 1$. In this case $\mathcal{T}(\psi, A) \geqq \frac{1}{2} T(\psi, A)$, and thus

$$\mathscr{E}(\psi, A) \geqq \tfrac{1}{2} T(\psi, A) - z(\psi, |x|^{-1}\psi) \geqq -\tfrac{1}{2} z^2\,. \tag{3.9}$$

Here we have used the diamagnetic inequality [4]

$$T(\psi, A) \geqq T(|\psi|, 0) = \|\nabla \phi\|_2^2\,, \quad \text{with} \quad \phi(x)^2 = \langle \psi, \psi \rangle (x)\,, \tag{3.10}$$

together with the well-known hydrogenic ground state energy. We shall return to this alternative later.

Alternative 2. $X(\psi, A) < 1$. Then

$$\mathscr{E}(\psi, A) \geqq \mathscr{D}(\psi, A) \equiv \tfrac{1}{4} T(\psi, A)^2 / Q(\psi) - z(\psi, |x|^{-1}\psi)\,. \tag{3.11}$$

The two terms in $\mathscr{D}(\psi, A)$ scale (with x) in the same way, and hence the infimum of $\mathscr{D}$ is either 0 or $-\infty$. Let us define

$$\tilde{z}_c = \sup\{z | \inf \mathscr{D}(\psi, A) = 0\}. \tag{3.12}$$

Clearly

$$\tilde{z}_c \leqq z_c. \tag{3.13}$$

Another expression for $\tilde{z}_c$ [which uses the common x-scaling of the terms in $\mathscr{D}$ and (3.10)] is

$$\tilde{z}_c = \varepsilon \inf_{\phi} \|\phi\|_2^2 \|\nabla\phi\|_2^4 \|\phi\|_4^{-4} (\phi, |x|^{-1}\phi)^{-1}. \tag{3.14}$$

Here ϕ is an ordinary real valued function in $H^1(\mathbb{R}^3)$.

As an aside, it is worth mentioning that the fact that $z_c \geqq \tilde{z}_c$ [given by (3.14)] – but not Lemma 3.1 – can be derived directly from the formula (2.12). If $\sigma \cdot (p - A)\psi = 0$, then $0 = \int |\sigma \cdot (p-A)\psi|^2 = \int |(p-A)\psi|^2 - \int B \cdot \langle \psi, \sigma\psi \rangle$. (A justified integration by parts was used in the last term.) Using the Schwarz inequality on the last term, and (3.8), we have

$$T(\psi, A) \leqq \|B\|_2 Q(\psi)^{1/2} (4\varepsilon)^{1/2}. \tag{3.15}$$

Equation (3.14) then follows from (3.15), (3.10) and formula (2.12).

Our next goal is to find a lower bound to the right side of (3.14), which we shall call z_c^L:

$$z_c^L \leqq \tilde{z}_c \leqq z_c. \tag{3.16}$$

(Of course one can try to compute the infimum in (3.14) directly – which leads to an interesting differential equation.) First note that

$$\|\nabla\phi\|_2 \|\phi\|_2 \geqq (\phi, |x|^{-1}\phi), \tag{3.17}$$

which is the uncertainty principle and follows from the hydrogen ground state by scaling in x. Hence

$$\tilde{z}_c \geqq z_c^L \equiv \varepsilon \inf_{\phi} \|\nabla\phi\|_2^3 \|\phi\|_4^{-4} \|\phi\|_2. \tag{3.18}$$

The minimization problem in (3.18) is equivalent to the following. Let $e < 0$ be the ground state energy of $-\Delta - V(x)$. In [7] it is proved that

$$|e|^{1/2} \leqq L^1_{\frac{1}{2},3} \|V\|_2^2. \tag{3.19}$$

$L^1_{\frac{1}{2},3}$ is obtained by solving an ordinary differential equation [7] and is found numerically (to 3 significant figures) to be

$$L^1_{\frac{1}{2},3} = 0.0135. \tag{3.20}$$

By choosing $V(x) = C\phi(x)^2$ one deduces from (3.19), that $\|\nabla\phi\|_2^2 \geqq C\|\phi\|_4^4 - C^4 (L^1_{\frac{1}{2},3})^2 \|\phi\|_4^8$ when $\|\phi\|_2 = 1$. Optimizing with respect to C and inserting the result in (3.18) gives

$$z_c^L = \varepsilon (3/4)^{3/2} \{2L^1_{\frac{1}{2},3}\}^{-1} \geqq (24.0)\varepsilon. \tag{3.21}$$

This lower bound to $\tilde{z}_c$ is surprisingly accurate. Inserting the function $\phi(x) = \exp(-|x|)$ in (3.14) yields

$$z_c^L \leqq \tilde{z}_c \leqq 8\pi\varepsilon = (25.1)\varepsilon . \tag{3.22}$$

Recalling that $\varepsilon = \{8\pi\alpha^2\}^{-1} = 747.2$, we have that

$$z_c \geqq z_c^L \geqq 17{,}900 . \tag{3.23}$$

In [8] a solution to $\sigma \cdot (p - A)\psi = 0$ is found which, when inserted into (2.12), yields

$$z_c \leqq 9\pi^3\varepsilon = (279)\varepsilon = 208{,}000 . \tag{3.24}$$

So far we have shown that if $z \leqq \tilde{z}_c$ then alternative 2 above is irrelevant, for otherwise we should conclude that $E \geqq 0$, which is false. Our next goal is to find a lower bound for E, and we shall do so under the slightly stronger condition that $z \leqq z_c^L$. To this end, we need only consider $(\psi, A) \in \mathscr{C}$ such that $X(\psi, A) \geqq 1$. By Lemma 3.1, a lower bound, $\tilde{E}$, for E is given by

$$E \geqq \tilde{E} = \inf\{T(\psi, A) - Q(\psi) - z(\psi, |x|^{-1}\psi)\} \tag{3.25}$$

under the conditions $(\psi, A) \in \mathscr{C}$ and $T(\psi, A) \geqq 2Q(\psi)$.

The problem posed by (3.25) is too difficult (in particular it is not clear that $A = 0$ is an optimal choice). Therefore we seek a lower bound to the right side of (3.25) as follows. Recall that $T(\psi, A)$ satisfies (for $\|\psi\|_2 = 1$)

$$T(\psi, A) \geqq [4z_c^L Q(\psi)]^{2/3} , \tag{3.26}$$

which follows from (3.18) and (3.10),

$$T(\psi, A) \geqq (\psi, |x|^{-1}\psi)^2 , \tag{3.27}$$

$$T(\psi, A) \geqq 2Q(\psi) . \tag{3.28}$$

Define $\tau(\psi)$ by

$$\tau(\psi) = \max\{\text{right sides of (3.26), (3.27), (3.28)}\} .$$

Then, if we define E^L by

$$E^L = \inf_{\psi} \{\tau(\psi) - Q(\psi) - z(\psi, |x|^{-1}\psi)\} \tag{3.29}$$

(with $\|\psi\|_2 = 1$), we have that

$$E^L \leqq \tilde{E} \leqq E . \tag{3.30}$$

The problem posed by (3.29) is, in fact, algebraic. It is solved in Appendix B with the result that for all $z \leqq z_c^L$

$$E^L = -\tfrac{1}{4}(\tfrac{4}{3})^3 (z_c^L)^2 [3\gamma - 2 + 2(1-\gamma)^{3/2}] , \tag{3.31}$$

where $\gamma = \frac{3}{4} z / z_c^L$.

When the right side of (3.31) is Taylor expanded for small z, the leading two terms are

$$\approx -\tfrac{1}{4}z^2 - \frac{1}{32 z_c^L} z^3 . \tag{3.32}$$

On the other hand using Taylor's theorem with remainder and taking the maximum of d^3E^L/dz^3 in the interval $[0,z]$, we can derive a lower bound to (3.31) for all $z \leqq z_c^L$, which agrees with (3.32) to the first two orders:

$$E \geqq -\tfrac{1}{4}z^2 - (32z_c^L)^{-1}z^3(1-\gamma)^{-3/2}. \tag{3.33}$$

A crude upper bound for E can be obtained with the trial function

$$\begin{gathered} \psi(r) = \begin{pmatrix} \phi(r) \\ 0 \end{pmatrix}, \qquad \phi(r) = (z/2)^{3/2}\pi^{-1/2}e^{-zr/2}, \\ A = \tfrac{1}{2}\alpha^2 z^3 (2/3)^4 e^{-zr/2}(-y, x, 0). \end{gathered} \tag{3.34}$$

(This choice does not satisfy $\operatorname{div} A = 0$, but that does not matter.) A computation with this (ψ, A) gives

$$E \leqq -\tfrac{1}{4}z^2 - \tfrac{1}{2}(\tfrac{2}{3})^8 z^3\alpha^2 + 2^4 3^{-8} z^4 \alpha^4. \tag{3.35}$$

Remark. We do not know whether E diverges as $z \to z_c$. Of course, E is an upper semicontinuous, monotone decreasing function of z, so $E(z_c) = \lim_{z \to z_c} E(z)$.

IV. A Single Electron Atom in a Magnetic Field of Constant Direction

In the previous two sections we considered a single electron atom in an arbitrary magnetic field and showed that z_c is finite (but huge) and estimated the shift in the ground state energy for $z < z_c^L$. The magnetic field that causes the energy to diverge when $z > z_c$ has to be highly contorted (which is consistent with the example given in [8]). If, on the other hand, certain constraints are placed on B near the nucleus, the divergence will not occur and z_c will be infinite.

In this section we display one such condition-namely that B has a constant direction (but not necessarily constant magnitude) near the nucleus. This is one possible version of the external field problem and is relevant for astrophysics. We shall content ourselves with showing merely that z_c is infinite and will not bother to try to find a good estimate on the energy; in fact we shall obtain $E \geqq -(\text{const})(1+z^4)$ for all z. The crucial point, of course, is that the bound is independent of B (but it does depend on the size of the region in which the direction of B is constant).

It should be noted that something a bit stronger is actually proved in the following. Namely for *any* B the energy will be bounded below if we replace the troublesome term $\sigma \cdot B$ by $\sigma_3 B_3$. Such a replacement is physically meaningful only when $B_1 = B_2 = 0$.

Let R be a fixed radius and assume that inside the ball K_R of radius R centered at the origin (which is also the location of the nucleus)

$$B(x) = (0, 0, b(x)). \tag{4.1}$$

(The choice of the 3 direction is arbitrary.) $b(x)$ can be anything inside K_R and $B(x)$ can also be anything outside of K_R.

Let $\psi(x)$ be given on $\mathbb{R}^3$, and we want to localize it inside and outside K_R. Define η_1, η_2 both C^∞ such that $\eta_1(x) = 1$ for $x \in K_{R/2}$ and $\eta_1(x) = 0$ for $x \notin K_R$ and

$\eta_1(x)^2+\eta_2(x)^2=1$. Also define $\psi_i(x)=\eta_i(x)\psi(x)$, $i=1,2$. Thus $\psi^2=\psi_1^2+\psi_2^2$. It is easy to see that

$$\|\sigma\cdot(p-A)\psi_1\|_2^2+\|\sigma\cdot(p-A)\psi_2\|_2^2=(\psi,f\psi)+\|\sigma\cdot(p-A)\psi\|_2^2, \tag{4.2}$$

where $f=(\nabla\eta_1)^2+(\nabla\eta_2)^2$. (The cross terms cancel.) We can easily choose η_i such that $f(x)\leqq dR^{-2}$ for some constant, d. Hence we get for $(\psi,A)\in\mathscr{C}$,

$$\mathscr{E}'(\psi,A)\geqq\|\sigma\cdot(p-A)\psi_1\|_2^2-z(\psi_1,|x|^{-1}\psi_1)+\varepsilon\|B\|_2^2-d/R^2-2z/R. \tag{4.3}$$

Here we used the fact that $(\psi_2,|x|^{-1}\psi_2)\leqq 2/R$, since $\psi_2(x)=0$ for $|x|<R/2$ and $\|\psi_2\|_2\leqq 1$.

From now on we drop the subscript 1 and denote ψ_1 by ψ (with $\|\psi\|_2\leqq 1$). Define

$$T_3(\psi,A)=\|(p_3-A_3)\psi\|_2^2\geqq\|p_3|\psi|\,\|_2^2\equiv T_3(\psi), \tag{4.4}$$

$$T_\perp(\psi,A)=\|(p_\perp-A_\perp)\psi\|_2^2\geqq\|p_\perp|\psi|\,\|_2^2\equiv T_\perp(\psi), \tag{4.5}$$

where $p_\perp=(p_1,p_2)$, etc. [The inequality (3.10) holds in any dimensions.] Since $B(x)$ is given by (4.1) on the set where $\psi(x)\neq 0$, we have

$$\|\sigma\cdot(p-A)\psi\|_2^2=T_3(\psi,A)+T_\perp(\psi,A)-\int b\langle\psi,\sigma_3\psi\rangle, \tag{4.6}$$

which can be rewritten as

$$T_3(\psi,A)+U_\perp(\psi,A), \tag{4.7}$$

where

$$U_\perp(\psi,A)\equiv\|\sigma_\perp\cdot(p_\perp-A_\perp)\psi\|_2^2. \tag{4.8}$$

Consider E', which is defined to be the infimum over $(\psi,A)\in\mathscr{C}$ of

$$\mathscr{E}'(\psi,A)=T_3(\psi)+U_\perp(\psi,A)+\varepsilon\|b\|_2^2-z(\psi,|x|_R^{-1}\psi), \tag{4.9}$$

where $|x|_R^{-1}=|x|^{-1}$ if $|x|\leqq R$ and zero otherwise. Here b is defined to be the 3-component of $B=\operatorname{curl}A$, even if B does not point in the 3-direction (note that $\|B\|_2\geqq\|b\|_2$, and that (4.6)–(4.8) is still true, namely $U_\perp=T_\perp-\int b\langle\psi,\sigma_3\psi\rangle$). It is obvious that

$$E\geqq E'-d/R^2-2z/R. \tag{4.10}$$

To analyze E' we observe that each of the four terms in (4.9) involves a 3-dimensional integral, and $\int d^3x=\int dx_3\int dx_\perp$. Think of $\psi, A, B, |x|_R^{-1}$ as functions of $x_\perp$ parameterized by x_3. Then

$$\mathscr{E}'(\psi,A)=T_3(\psi)+\int dx_3\mathscr{E}''(\psi,A), \tag{4.11}$$

$$\mathscr{E}''(\psi,A)=\int dx_\perp|\sigma_\perp\cdot(p_\perp-A_\perp)\psi|^2+\varepsilon\int dx_\perp b^2-z\int_{D(x_3)}dx_\perp\langle\psi,\psi\rangle\,(x_\perp^2+x_3^2)^{-1/2}, \tag{4.12}$$

where $D(x_3)$ is the domain in $x_\perp$ given by

$$x_\perp^2\leqq R^2-x_3^2. \tag{4.13}$$

To analyze (4.12) we utilize the t trick of Sect. III. For each value of x_3, let $t(x_3)$ be chosen to satisfy $0\leqq t(x_3)\leqq 1$. Replace $|\sigma\cdot(p_\perp-A_\perp)\psi|^2$ in (4.12) by $t(x_3)$ times this quantity and use (3.10) to obtain the lower bound on this first term:

$$t(x_3)T_\perp(\psi)-t(x_3)\int |b|\,\langle\psi,\psi\rangle dx_\perp\,.$$

[Here $T_\perp$ means $\int dx_\perp(\nabla_\perp|\psi|)^2$.] We used $|\langle\psi,\sigma\psi\rangle|=\langle\psi,\psi\rangle$.

Now minimize with respect to b and then maximize with respect to $t(x_3)$, as in Sect. III. For the first two terms on the right side of (4.12) we obtain the bound

$$\min\{(J_\perp)^2/4\varepsilon,\,\varepsilon(T_\perp/J_\perp)^2\} \tag{4.14}$$

with $(J_\perp)^2=\int dx_\perp\langle\psi,\psi\rangle^2$.

The last term in (4.12) can be bounded below as $-zJ_\perp W(x_3)$, and

$$W(x_3)^2=\int_{D(x_3)}(x_\perp^2+x_3^2)^{-1}dx_\perp=\begin{cases}2\pi\ln(R/|x_3|) & \text{for}\quad |x_3|<R\\ 0 & \text{for}\quad |x_3|\geqq R\,.\end{cases} \tag{4.15}$$

To bound (4.14) below, the Sobolev inequality in $\mathbb{R}^2$ is used:

$$T_\perp\geqq S(J_\perp)^2/g(x_3)^2\,, \tag{4.16}$$

where

$$g(x_3)^2=\int dx_\perp\langle\psi,\psi\rangle\,. \tag{4.17}$$

(The constant S can be found in [7].)

Substituting (4.14)–(4.17) in (4.12),

$$\mathscr{E}''(\psi,A)\geqq J_\perp^2\min\{(4\varepsilon)^{-1},S^2\varepsilon g(x_3)^{-4}\}-zJ_\perp W(x_3)\,. \tag{4.18}$$

Since $J_\perp=J_\perp(x_3)$ is unknown, we simply minimize (4.18) with respect to $J_\perp$ and obtain

$$\mathscr{E}''(\psi,A)\geqq -\tfrac{1}{4}z^2W(x_3)^2\cdot\max\{4\varepsilon,g(x_3)^4/S^2\varepsilon\}\,. \tag{4.19}$$

According to (4.11), (4.19) must be integrated over x_3. Since we do not know which term in the max{ , } in (4.19) holds for any given x_3, we shall simply take the sum of the two. The first yields

$$-\varepsilon z^2\int_{-R}^{R}dx_3W(x_3)^2=-4\pi\varepsilon z^2R\,. \tag{4.20}$$

To control the second possibility we invoke the $T_3(\psi)$ term in (4.11). An application of the Schwarz inequality [12] gives

$$T_3(\psi)\geqq\int dx_3(dg(x_3)/dx_3)^2=\|g'\|_2^2\,. \tag{4.21}$$

It is also a fact that for all x_3 and $g\in L^2(\mathbb{R}^1)$

$$g(x_3)^4\leqq\|g\|_2^2\|g'\|_2^2\leqq T_3(\psi)\,. \tag{4.22}$$

[This follows from $g(x)^2=2\int_{-\infty}^{x}gg'$ and $g(x)^2=-2\int_{x}^{\infty}gg'$. Hence $g(x)^2\leqq\int_{-\infty}^{\infty}|gg'|$. We recall also that $\|g\|_2^2=\int\langle\psi,\psi\rangle d^3x=1.$] Inserting (4.20)–(4.22) in (4.11), we obtain the following lower bound for the second possibility in (4.19).

$$T_3(\psi)\{1-\tfrac{1}{4}z^2S^{-2}\varepsilon^{-1}\int W^2\}=T_3(\psi)\{1-\pi Rz^2/S^2\varepsilon\}\,. \tag{4.23}$$

While the value of $T_3(\psi)$ is unknown, the term (4.23) can be eliminated by the following trick. Call R_0 the original radius inside of which (4.1) holds. A fortiori, (4.1) holds for any $R<R_0$. If $\{\ \bar{}\ \}$ in (4.23) is nonnegative, use R_0. Otherwise, use

$$R=S^2\varepsilon/\pi z^2\,.$$

Then (4.23)$\geqq 0$ and can be ignored.

Combining all the terms we obtain

$$E\geqq -d/R^2-2z/R-4\pi\varepsilon z^2 R \tag{4.24}$$

with

$$R=\min\{R_0, S^2\varepsilon/\pi z^2\}\,. \tag{4.25}$$

Appendix A

In the following, $\mathscr{D}'$ is the space of distributions.

Theorem A.1. *Let* $B\in L^2(\mathbb{R}^3)$ *be a given vector field and let* $\operatorname{div}B=0$ *in* $\mathscr{D}'$. *Define the vector field*

$$A(x)=\frac{1}{4\pi}\int |x-y|^{-3}(x-y)\times B(y)dy\,. \tag{A.1}$$

Then:

(a) $A\in L^6(\mathbb{R}^3)$ *and* $\operatorname{curl}A=B$, $\operatorname{div}A=0$ *in* $\mathscr{D}'$.

(b) *The distribution* $\partial_i A_j$ *is an* L^2*-function and we have the formula*

$$\sum_i \int |\nabla A_i|^2 d^3x=\int B^2 dx\,.$$

(c) *The* $A(x)$ *given by* (A.1) *is the only vector field having the three properties in* (a) *above.*

Proof. Let us write $A=T(B)$. The kernel in (A.1) is bounded by $|x-y|^{-2}$ and $|x|^{-2}\in L^{3/2}_w$. Let V be a vector field in $L^p(\mathbb{R}^3)$ with $1<p<3$. By the weak Young inequality, $T(V)\in L^r$ where $1/3+1/r=1/p$, and $\|T(V)\|_r\leqq C_p\|V\|_p$ for a suitable constant C_p. By Fubini's theorem

$$(W, T(V))=(T(W), V) \tag{A.2}$$

when $W\in L^q$ and $V\in L^p$, with $q=r'$, $1/q=4/3-1/p$. In (A.2), (W,U) means $\sum_{i=1}^{3}\int \overline{W_i(x)}U_i(x)dx$.

Now we apply (A.2) to $V=B$ and $W=\nabla f$ with $f\in C_0^\infty(\mathbb{R}^3)$,

$$T(W)=-\frac{1}{4\pi}\operatorname{curl}\{|x|^{-1}*\nabla f\}=-\frac{1}{4\pi}\operatorname{curl}\operatorname{grad}\{|x|^{-1}*f\}=0\,.$$

(The first equality, namely exchanging integration and differentiation, follows by dominated convergence.) Then $(\nabla f, A)=0$ for all $f\in C_0^\infty$, and hence $\operatorname{div}A=0$ in $\mathscr{D}'$. A second application of (A.2) is to $V=B$ and $W=\operatorname{curl}G$, with $G\in C_0^\infty$.

$$T(W)=-\frac{1}{4\pi}\operatorname{curl}\operatorname{curl}\{|x|^{-1}*G\}=-G-\nabla\operatorname{div}\frac{1}{4\pi}\{|x|^{-1}*G\}\equiv -G-\nabla g\,.$$

Then $(W,A)=(-G-\nabla g, B)=(-G,B)-(\nabla g,B)$. We claim that $(\nabla g,B)=0$, which will imply that $\operatorname{curl}A=B$ in $\mathscr{D}'$. While $g\in C^\infty$ it does not generally have compact support; otherwise we would have $(\nabla g,B)=0$ since $\operatorname{div}B=0$ in $\mathscr{D}'$.

However $B \in L^2$, and therefore $(\nabla g, B) = \lim_{R \to 0} (\nabla(g f_R), B)$, where $f_R(x) = f(Rx)$ and $f(x)$ is a C_0^∞ function satisfying $f(x) = 1$ for $|x| < 1$, $f(x) = 0$ for $|x| > 2$. Since $(\nabla(g f_R), B) = 0$, we have the desired result, and (a) is proved.

To prove (b) we define $T_j(B) = i\partial_j T(B) = iT(\partial_j B)$ for B smooth and of compact support. It is a standard result about the Riesz transform that $T_j(B)$ has a bounded extension to $L^2(\mathbb{R}^3)$, see [10], so we can assume merely that $B \in L^2$. Furthermore T_j is selfadjoint. Now for any vector field V in $L^2(\mathbb{R}^3)$ we have

$$\sum_j (T_j(B), T_j(V)) = \sum_j (B, T_j^2(V)) = (B, V). \tag{A.3}$$

Indeed, when V is smooth and of compact support $\sum_j T_j^2(V)(x) = V(x) + \frac{1}{4\pi} \nabla \operatorname{div}\{|x|^{-1} * V\}(x)$. Using the previous approximation argument (namely $g \to g f_R$) and the fact that $\operatorname{div} B = 0$ in $\mathscr{D}'$ gives (A.3). Since T_j is bounded, (A.3) is true for all $V \in L^2(\mathbb{R}^3)$. Hence, by setting $V = B$, (b) is also proven.

To prove (c), suppose there were another $\tilde{A}$ with the properties in (a) and let $\alpha = \tilde{A} - A$. Then $\alpha \in L^6$, $\operatorname{curl}\alpha = 0$, $\operatorname{div}\alpha = 0$ in $\mathscr{D}'$. Let $j_\varepsilon(x)$ be a C_0^∞ approximation to the identity and $\alpha_\varepsilon = j_\varepsilon * \alpha$. It is easy to see that $\alpha_\varepsilon \in C^\infty$, $\operatorname{div}\alpha_\varepsilon = 0$, $\operatorname{curl}\alpha_\varepsilon = 0$ and $\alpha_\varepsilon(x) \to 0$ as $|x| \to \infty$. From this, $\Delta\alpha_\varepsilon = -\operatorname{curl}\operatorname{curl}\alpha_\varepsilon + \operatorname{grad}\operatorname{div}\alpha_\varepsilon = 0$. So each component of α_ε is harmonic, but since $\alpha_\varepsilon \to 0$ at ∞, α_ε must be zero for all $\varepsilon > 0$. But as $\varepsilon \to 0$, $\alpha_\varepsilon \to \alpha$ (in L^6 and in $\mathscr{D}'$), so $\alpha = 0$. □

Theorem A.2. *For any* $A \in L^6(\mathbb{R}^3)$ *and* $\psi \in L^2(\mathbb{R}^3)$, $\|\sigma \cdot (p - A)\psi\|_2 < \infty$ *implies* $\psi \in H^1(\mathbb{R}^3)$.

Proof. Observe that by assumption

$$\sigma \cdot p\psi = \sigma \cdot A\psi + u, \quad u \in L^2, \quad \text{and} \quad A\psi \in L^{3/2}$$

by Hölder's inequality ($A \in L^6, \psi \in L^2$). Since $(\sigma \cdot p)^{-1} = \sigma \cdot p|p|^{-2}$, we find

$$\psi = \frac{i}{4\pi} \int |x - y|^{-3} \sigma \cdot (x - y)\, [(\sigma \cdot A\psi)(y) + u(y)]\, dy.$$

Again, by the weak Young inequality, $\psi = v_1 + v_2$, $v_1 \in L^3$, $v_2 \in L^6$ which implies (since $\psi \in L^2$) $\psi \in L^2 \cap L^3$. Hence $A\psi \in L^2$ (again by Hölder's inequality) and thus $\sigma \cdot p\psi \in L^2$.

Appendix B: Proof of Eq. (3.31)

Given ψ, define

$$S(\psi) = (\psi, |x|^{-1}\psi).$$

As ψ ranges over all functions satisfying $\|\psi\|_2 = 1$, $Q(\psi)$ and $S(\psi)$ independently take on all values between 0 and ∞. Therefore we are entitled to think of S and Q simply as an unknown pair of positive numbers.

According to (3.29), then, we have to minimize $e = \tau - Q - zS$ under the conditions $\tau \geqq 2Q$, $\tau \geqq S^2$, $\tau \geqq KQ^{2/3}$ with $K^{3/2} = 4z_c^L$. There are two cases:

case (a): $2Q^{1/3} \geqq K$ or $Q \geqq 2(z_c^L)^2$,

case (b): $2Q^{1/3} < K$.

If case (a) holds, we set $\tau = 2Q$, $S^2 = 2Q$, and then $\tau - Q - zS \geqq 0$, since $z \leqq z_c^L$ and $Q \geqq 2(z_c^L)^2$. If case (b) holds then, similarly,

$$E^L = \min\{KQ^{2/3} - Q - zK^{1/2}Q^{1/3} | Q \leqq 2(z_c^L)^2\}\,.$$

Change the variable to $Q \equiv 2(z_c^L)^2 x^3$. Then E^L is the minimum of

$$-2(z_c^L)^2[x^3 - 2x^2 + \tfrac{4}{3}\gamma x]$$

subject to $0 \leqq x \leqq 1$ and $\gamma = \frac{3}{4}z/z_c^L \leqq \frac{3}{4}$. The minimum occurs at

$$x = \tfrac{2}{3}[1 - (1-\gamma)^{1/2}]$$

and yields (3.31) for the lower bound.

Acknowledgement. It is a pleasure to acknowledge valuable discussions at the Aspen Center for Physics with David Boulware and Lowell Brown.

References

1. Avron, J., Herbst, I., Simon, B.: Schrödinger operators with magnetic fields: III. Atoms in homogeneous magnetic field. Commun. Math. Phys. **79**, 529–572 (1981)
2. Remark 3 in Brezis, H., Lieb, E.H.: Minimum action solution of some vector field equations. Commun. Math. Phys. **96**, 97–113 (1984)
3. Daubechies, I., Lieb, E.H.: One-electron relativistic molecules with Coulomb interaction. Commun. Math. Phys. **90**, 497–510 (1983)
4. Kato, T.: Schrödinger operators with singular potentials. Israel J. Math. **13**, 135–148 (1972)
5. Lieb, E.H.: On the lowest eigenvalue of the Laplacian for the intersection of two domains. Invent. Math. **74**, 441–448 (1983)
6. Lieb, E.H., Loss, M.: Stability of Coulomb systems with magnetic fields: II. The many-electron atom and the one-electron molecule. Commun. Math. Phys. **104**, 271–282 (1986)
7. Lieb, E.H., Thirring, W.: Inequalities for the moments of the eigenvalues of the Schrödinger Hamiltonian and their relation to Sobolev inequalities. In: Studies in mathematical physics, essays in honor of Valentine Bargmann. Lieb, E.H., Simon, B., Wightman, A.S. (eds.). Princeton, NJ: Princeton University Press 1976
8. Loss, M., Yau, H.T.: Stability of Coulomb systems with magnetic fields: III. Zero energy bound states of the Pauli operator. Commun. Math. Phys. **104**, 283–290 (1986)
9. Michel, F.C.: Theory of pulsar magnetospheres. Rev. Mod. Phys. **54**, 1–66 (1982)
10. Stein, E.M.: Singular integrals and differentiability properties of functions. Princeton, NJ: Princeton University Press 1970
11. Straumann, N.: General relativity and relativistic astrophysics. Berlin, Heidelberg, New York, Tokyo: Springer 1984
12. Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T.: Schrödinger inequalities and asymptotic behavior of the electron density of atoms and molecules. Phys. Rev. A **16**, 1782–1785 (1977)
13. Avron, J., Herbst, I., Simon, B.: Schrödinger operators with magnetic fields: I. General Interactions. Duke Math. J. **45**, 847–883 (1978)

Communicated by A. Jaffe

Received October 2, 1985; in revised form January 2, 1986