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Stability of Coulomb Systems with Magnetic Fields

III. Zero Energy Bound States of the Pauli Operator

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Abstract. It is shown that there exist magnetic fields of finite self energy for which the operator $\sigma \cdot (p-A)$ has a zero energy bound state. This has the consequence that single electron atoms, as treated recently by Fröhlich, Lieb, and Loss [1], collapse when the nuclear charge number $z \geqq 9\pi^2/8\alpha^2$ (α is the fine structure constant).

I. Introduction

In an accompanying paper [1] the stability of the hydrogen atom in magnetic fields is studied. The authors considered the following Hamiltonian

$$H = [\sigma \cdot (p-A)]^2 - z/|x| \tag{1.1}$$

whose ground state energy was denoted by $E_0(B,z)$. Here the σ_i's are the Pauli matrices and A is the vector potential, $B = \operatorname{curl} A$. H acts on 2-component spinors ψ. In particular, it was shown that there is a critical number $z_c > 0$ such that $E(z) = \inf_B (E_0(B,z) + \varepsilon \int B^2)$ was finite whenever $z < z_c$ and $E(z) = -\infty$ for $z > z_c$. $\varepsilon = (8\pi\alpha^2)^{-1}$ and α is the fine structure constant $\simeq (137.04)^{-1}$. For the physical interpretation of these results see [1]. When they first did their work, the authors did not know whether z_c was finite or not. However they show, among other results, that a necessary and sufficient condition for the finiteness of z_c, is that the equation

$$\sigma \cdot (p-A)\psi = 0\,, \tag{1.2}$$

is valid for some A and some ψ, which satisfy

$$\psi \in H^1(\mathbb{R}^3)\,, \quad \text{i.e.} \quad \psi, \nabla\psi \in L^2(\mathbb{R}^3)\,, \tag{1.3a}$$

$$A \in L^6(\mathbb{R}^3)\,, \qquad \operatorname{div} A = 0 \quad \text{and} \quad B \equiv \operatorname{curl} A \in L^2(\mathbb{R}^3)\,. \tag{1.3b}$$

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Furthermore, they prove the following formula for z_c:

$$z_c = \min(\varepsilon \int B^2)(\psi, |x|^{-1}\psi)^{-1}, \tag{1.4}$$

where the minimum in (1.4) is taken over all normalized solutions of (1.2), (1.3).

The aim of this work is to show that (1.2), (1.3) has solutions. Some of the results were announced in [1]. We shall give a special class of solutions of (1.2), (1.3). One of these examples will be used to compute an upper bound on z_c via formula (1.4). This is carried out in Sect. II. The result is

$$z_c \leqq 9\pi^3\varepsilon = 9\pi^2/8\alpha^2,$$

which is ten times bigger than the lower bound for z_c given in [1].

Observe that while (1.2) is a gauge invariant equation, (1.3) imposes both gauge invariant and gauge dependent constraints. The gauge invariant conditions are

$$\psi \in L^2 \quad \text{and} \quad B \in L^2. \tag{1.5}$$

The constraints

$$\nabla\psi \in L^2 \quad \text{and} \quad A \in L^6, \quad \operatorname{div} A = 0, \tag{1.6}$$

are not gauge invariant.

Assuming (1.2) has a solution then, by (3.3), B can be expressed entirely in terms of the vector field

$$U = \langle \psi, \sigma\psi \rangle, \tag{1.7}$$

and its derivatives. (U = twice the spin density and $\langle\ ,\ \rangle$ denotes the usual inner product in $\mathbb{C}^2$.) U itself has to satisfy $\operatorname{div} U = 0$ if ψ satisfies (1.2). One is tempted to ask the following question: Suppose a vector field U is given satisfying $U \in L^1$, U smooth, $\operatorname{div} U = 0$ and the B associated with U by (3.3) is square integrable. Can one find ψ and A satisfying (1.2), (1.3), (1.7)? Under the assumption that U is nonvanishing the answer is yes. We prove this in Sect. III and thereby provide some examples of solutions that probably cannot be obtained by the method of Sect. II.

It is an interesting problem to ask how many solutions of (1.2) exist for a given A. We do not know a completely satisfactory answer to that question, however, by squaring (1.2) the problem is reduced to computing the number, N, of solutions of the equation

$$[(p-A)^2 - \sigma \cdot B]\psi = 0.$$

Since $|(\psi, \sigma \cdot B\psi)| \leqq (\psi, |B|\psi)$, by the minimax principle the number of bound-states of the Hamiltonian

$$(p-A)^2 - |B|$$

provides an upper bound on N given by

$$c \int |B|^{3/2},$$

c is some constant (see [2, 3]).

II. A First Example and an Upper Bound on z_c

A simple class of solutions of Eq. (1.2) is provided by the following remark. Instead of considering (1.2) we consider the problem

$$\sigma \cdot p\psi(x) = \lambda(x)\psi(x) \tag{2.1}$$

for some given real (scalar valued) $\lambda(x)$. Assuming that (2.1) has a solution and that $\langle\psi,\psi\rangle(x) \neq 0$, all x then, by setting

$$A(x) = \lambda(x)\langle\psi,\sigma\psi\rangle(x)/\langle\psi,\psi\rangle(x), \tag{2.2}$$

we find a solution of problem (1.2). For this, observe that the two by two matrix $Q = \sigma \cdot \langle\psi,\sigma\psi\rangle/\langle\psi,\psi\rangle$ has ψ as an eigenvector with eigenvalue $+1$ (a simple consequence of the relation $\langle\psi,\sigma\psi\rangle\langle\psi,\sigma\psi\rangle = \langle\psi,\psi\rangle^2$), and hence

$$\sigma \cdot A(x)\psi(x) = \lambda(x)\psi(x), \tag{2.3}$$

and we have at least a formal solution of (1.2). In general, the A of (2.2) will not satisfy (1.3b), so one has to add some $\nabla\chi$ to A and then check, in any particular case, that $A + \nabla\chi$ satisfies (1.3b).

Example. Choose

$$\psi = (1+x^2)^{-3/2}(1 + i\sigma \cdot x)\phi_0, \tag{2.4}$$

where ϕ_0 is an arbitrary, constant, normalized spinor. Call $w = \langle\phi_0, \sigma\phi_0\rangle$ and note that $|w| = 1$. A simple calculation shows that

$$\sigma \cdot p\psi = \frac{3}{1+x^2}\psi, \tag{2.5}$$

and hence, by using (2.2), (1.2) is satisfied with

$$A(x) = 3(1+x^2)\langle\psi,\sigma\psi\rangle, \tag{2.6}$$

where

$$\langle\psi,\sigma\psi\rangle = U = (1+x^2)^{-3}\{(1-x^2)w + 2(w \cdot x)x + 2w \times x\}. \tag{2.7}$$

It is easily seen that the B-field is

$$B = \operatorname{curl} A = 12U. \tag{2.8}$$

Observe that

$$\operatorname{div} A = 6\frac{(w \cdot x)}{(1+x^2)^2} \neq 0,$$

but, defining

$$A' = A + \nabla\chi, \qquad \psi' = e^{i\chi}\psi,$$

where $-\Delta\chi(x) = \operatorname{div} A(x)$ or

$$\chi(x) = \frac{6}{4\pi}\int |x-y|^{-1}\frac{(w \cdot y)}{(1+y^2)^2}dy = (w \cdot x)\frac{3}{r^3}(r - \arctan r),$$

it is easily seen that $A' \in L^6$ and $\operatorname{div} A' = 0$. Certainly, $\psi' \in H^1$ and $B \in L^2$. With this example we can compute the upper bound on z_c mentioned in the introduction. After normalizing (2.4) we obtain, upon inserting into (1.4), an upper bound in terms of Beta functions, and the result is

$$z_c \leqq \tfrac{9}{8}\pi^2\alpha^{-2}, \tag{2.9}$$

which is ten times larger than the lower bound given in [1].

The following might help the reader to visualize the field lines. The field lines of B can be found by solving the differential equation

$$\dot{x} = (1 - x^2)w + 2(w \cdot x)x + 2w \times x. \tag{2.10}$$

We assume w to point in the 3-direction. By passing to a rotating coordinate system

$$x = R(t)y, \qquad R(t) = \begin{pmatrix} \cos 2t & \sin 2t & 0 \\ -\sin 2t & \cos 2t & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

we find for y the equation

$$\dot{y} = (1 - y^2)w + 2(w \cdot y)y. \tag{2.11}$$

This system is rotation invariant around the 3-axis and it is easily seen that the flow lines of system (2.11) are 2 dimensional circles and the motion is periodic with the *same* period as that of $R(t)$. In other words, the y field is qualitatively the same as the field of a current loop with closed circular field lines that lie on torii. The effect of $R(t)$ is to twist the y lines in the (x_1, x_2) plane in such a way that they stay closed, because the period of the twist is the same as the period of the y motion.

Remark. Note that the solutions of $\sigma \cdot p\psi = \lambda(|x|)\psi$ can be classified according to the invariant subspaces of the total angular momentum operator $J = \frac{1}{2}\sigma + L$ (L = angular momentum) labeled by $j = \frac{1}{2}, \frac{3}{2}, \ldots$. The solutions constructed above belong to the subspace with $j = \frac{1}{2}$. In a similar fashion it is possible to find solutions of (1.2) and (1.3) where the ψ carries any j value.

Following [7, p. 62], define the spinor

$$u_{\ell,m} = (2\ell + 1)^{-1/2}((\ell + m + \tfrac{1}{2})^{1/2} Y_{\ell, m-\frac{1}{2}}, -(\ell - m + \tfrac{1}{2})^{1/2} Y_{\ell, m+\frac{1}{2}}),$$

where $Y_{\ell,m}$ are spherical harmonics and $-j \leqq m \leqq j$, with $j = \ell + \frac{1}{2}$ being the total angular momentum. The solution to (1.2) is then

$$\psi(x) = |x|^{\ell}(1 + x^2)^{-\ell - 3/2}[1 + i\sigma \cdot x]u_{\ell,m},$$

$$\begin{aligned} A(x) &= (2\ell + 3)(1 + x^2)^{-1}\langle\psi, \sigma\psi\rangle(x)/\langle\psi, \psi\rangle(x) \\ &= (2\ell + 3)(1 + x^2)^{-2}\{(1 - x^2)w(x) + 2(w(x) \cdot x)x + 2w(x) \times x\} \end{aligned}$$

with

$$w(x) = \langle u_{\ell,m}, \sigma u_{\ell,m}\rangle(x)/\langle u_{\ell,m}, u_{\ell,m}\rangle(x).$$

Unlike the $j = \frac{1}{2}$ case, w now depends on x. The A field given above does not satisfy $\operatorname{div} A = 0$ but, as before, one can add $\nabla\chi$ to A so that $\operatorname{div} A = 0$ and $B \in L^2$ and $A \in L^6$.

III. Another Class of Solutions of Eq. (1.2)

In this section (1.2) is viewed in a different way. We suppose that $\psi \in H^1$ is given and want to find A such that the pair ψ, A satisfies Eq. (1.2). Assuming $\langle\psi,\psi\rangle(x)$ is nonvanishing, this problem is easily solved, and we get

$$A=[\operatorname{curl}\tfrac{1}{2}\langle\psi,\sigma\psi\rangle+\operatorname{Im}\langle\psi,\nabla\psi\rangle]/\langle\psi,\psi\rangle, \tag{3.1}$$

provided ψ satisfies the additional constraint

$$\operatorname{div}\langle\psi,\sigma\psi\rangle=0. \tag{3.2}$$

A computation shows that for this A and ψ (1.2) is formally satisfied. A more tedious calculation shows that

$$B=\frac{1}{2|U|^3}\Big[\sum_j U_j(\operatorname{curl}U\times\nabla U_j)-|U|^2\Delta U+\tfrac{1}{2}\sum_{ijk}\varepsilon_{ijk}U_i\nabla U_j\times\nabla U_k\Big], \tag{3.3}$$

where $U=\langle\psi,\sigma\psi\rangle$. We emphasize that B depends only on U and its derivatives. This suggests that U essentially determines the whole problem. The following theorem shows that this is true in a certain sense. Let $C^{2,\alpha}$ be the space of functions which are C^2 and their second derivative is Hölder continuous of order α for some $0<\alpha<1$.

Theorem. *Let U be a $C^{2,\alpha}$ nonvanishing vector field which satisfies*
(a) $\operatorname{div}U=0$,
(b) $\int|U|dx<\infty$.
Further, suppose that the B-field given by formula (3.3) *is square integrable. Then there exists ψ and A which solve* (1.2), *i.e.* (1.2) *holds together with the conditions given by* (1.3). *Moreover, $\langle\psi,\sigma\psi\rangle=U$ and $\operatorname{curl}A=B$.*

Proof. Define

$$\eta_-=2^{-1/2}\begin{pmatrix}(|U|+U_3)^{1/2}\\(U_1+iU_2)/(|U|+U_3)^{1/2}\end{pmatrix}. \tag{3.4}$$

η_- is well defined and smooth outside the closed set

$$\Gamma_-=\{x\in\mathbb{R}^3|U_1^2+U_2^2=0,\ U_3<0\}.$$

Note that η_- is chosen such that $\langle\eta_-,\sigma\eta_-\rangle=U$. Now we invoke formula (3.1) and find (outside Γ_-) the vector potential associated with η_-:

$$A_-=(2|U|)^{-1}\operatorname{curl}U+\tfrac{1}{2}(1-U_3/|U|)\nabla\theta, \tag{3.5}$$

$$\theta=\operatorname{Arg}(U_1+iU_2), \tag{3.6}$$

$$\nabla\theta=(U_1\nabla U_2-U_2\nabla U_1)/(U_1^2+U_2^2). \tag{3.7}$$

Observe that θ is defined as a multiple valued function on the set $\mathbb{R}^3\backslash\Gamma$, where

$$\Gamma=\{x|U_1^2+U_2^2=0\}.$$

Because U is nonvanishing, $\Gamma=\Gamma_+\cup\Gamma_-$, where

$$\Gamma_+=\{x\in\mathbb{R}^3|U_1^2+U_2^2=0,\ U_3>0\}.$$

Also note that the second term in (3.5) is, in fact, well behaved on Γ_+ since η_-, and hence A_- is C^1 outside Γ_-. Formally, η_- and A_- solve (1.2). By Theorem A.1 in [1] we can find $A \in L^6$ such that $\operatorname{curl} A = B$ and $\operatorname{div} A = 0$. In [1] the A field is given by

$$A = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{x-y}{|x-y|^3} \times B(y) d^3 y .$$

Since $B \in C^\alpha$, it is easily seen by dividing the integration smoothly into $|x-y|>2$ and $|x-y| \leqq 1$ that the first part is C^∞ and the second part is C^1 by [6, p. 54] and hence A is C^1. By the lemma below there exists a function Φ_- such that $\langle \Phi_-, \sigma \Phi_- \rangle = U$ and the pair Φ_-, A satisfies (1.2) on $\mathbb{R}^3 \backslash \Gamma_-$. In addition, $\Phi_- \in L^2(\mathbb{R}^3 \backslash \Gamma_-$. Similarly using

$$\eta_+ = 2^{-1/2} \begin{pmatrix} (U_1 - iU_2)/(|U| - U_3)^{1/2} \\ (|U| - U_3)^{1/2} \end{pmatrix} .$$

We repeat the procedure and obtain Φ_+ with $\langle \Phi_+, \sigma \Phi_+ \rangle = U$ such that the pair Φ_+, A satisfy (1.2) on $\mathbb{R}^3 \backslash \Gamma_+$ and $\Phi_+ \in L^2(\mathbb{R}^3 \backslash \Gamma_+)$. Observe that Φ_+ and Φ_- give the same A on $\mathbb{R}^3 \backslash \Gamma$ and the same U. From the latter Φ_+ and Φ_- can only differ by a phase factor, say $e^{i\chi}$, and, by the former,

$$0 = \sigma(p-A)\Phi_+ = e^{i\chi}\sigma(p-A)\Phi_- + e^{i\chi}\sigma \nabla \chi \Phi_- .$$

Since Φ_- is nonvanishing and satisfies $\sigma(p-A)\Phi_- = 0$ we have that $\nabla \chi = 0$, and so χ is locally a constant, i.e. it is constant on all connected components of $\mathbb{R}^3 \backslash \Gamma$. Hence, in the case where $\mathbb{R}^3 \backslash \Gamma$ is connected, χ is a constant, c, and

$$\Phi = \begin{cases} \Phi_+ & \text{on} \quad \mathbb{R}^3 \backslash \Gamma_+ = \Omega_+ , \\ e^{ic}\Phi_- & \text{on} \quad \mathbb{R}^3 \backslash \Gamma_- = \Omega_- , \end{cases}$$

satisfies $\Phi \in L^2$, $A \in L^6$, and $\sigma \cdot (p-A)\Phi = 0$. Theorem A.2 in [1] proves that $\nabla \Phi \in L^2$. In the general case we know that Φ_+ and Φ_- differ by a locally constant phase factor on $\Omega = \Omega_+ \cap \Omega_-$. By the Mayer-Vietoris cohomology sequence (see [4, 5])

$$H^0(\Omega_+) \oplus H^0(\Omega_-) \to H^0(\Omega) \to H^1(\mathbb{R}^3) = \{0\} ,$$

one easily proves the existence of locally constant phase factors $e^{i\alpha_+}$ and $e^{i\alpha_-}$ such that $\Phi_+ e^{i\alpha_+} = \Phi_- e^{i\alpha_-}$ on Ω. □

Lemma. *Let η_- and A_- be given by* (3.4) *and* (3.5) *(with $U \in C^2$) and let A be any C^1 vector potential for B given by* (3.3). *Then there exists a gauge transformation $e^{i\chi(x)}$ such that the pair $\Phi_- = e^{i\chi}\eta_-$ and A satisfies* (1.2) *on* $\mathbb{R}^3 \backslash \Gamma_-$.

Remark. Note that since $\mathbb{R}^3 \backslash \Gamma_-$ is not necessarily connected χ is determined only up to a locally constant function.

Proof. Denote $\mathbb{R}^3 \backslash \Gamma_\pm$ by $\Omega_\pm$, and let $\{\Omega^i_\pm\}$ be the connected components (indexed by i) of $\Omega_\pm$, respectively. Let $p^i \in \Omega^i_-$, $i = 1, 2, \ldots$. Define

$$\chi(x) = \int_{p^i}^{x} (A - A_-) \cdot dx \quad \text{if} \quad x \in \Omega^i_- . \tag{3.8}$$

Equation (3.8) is a line integral. Although χ is not single valued, we want to prove that the branches differ by 2π times an integer, which makes $e^{i\chi}$ and $\nabla\chi$ well defined. (Observe that χ is C^2.) This, however, follows once we have shown that

$$\frac{1}{2\pi}\int_{\gamma}(A-A_-)\cdot dx\in\mathbb{Z}, \tag{3.9}$$

for every closed curve $\gamma\in\Omega_-$. Observe that the integration depends only on the homology class of γ in Ω_- denoted by $[\gamma]\in H_1(\Omega_-)$. By the Mayer-Vietoris homology sequence (see [4])

$$\{0\}=H_2(\mathbb{R}^3)\longrightarrow H_1(\Omega_-\cap\Omega_+)\xrightarrow{j} H_1(\Omega_-)\oplus H_1(\Omega_+)\longrightarrow H_1(\mathbb{R}^3)=\{0\},$$

the map j, defined by

$$j([\beta])=[\beta]\oplus-[\beta],$$

is hence an isomorphism. $[\beta]$ on the left side is considered as a homology class in $H_1(\Omega_+\cap\Omega_-)$ and β on the right side as a homology class in $H_1(\Omega_-)$ and $H_1(\Omega_+)$, respectively. Hence for any $[\gamma]\in H_1(\Omega_-)$ there exists $[\beta]\in H_1(\Omega_-\cap\Omega_+)$ such that $j([\beta])=[\gamma]\oplus 0$, and hence

$$\begin{aligned}\frac{1}{2\pi}\int_{[\gamma]}(A-A_-)\cdot dx&=\frac{1}{2\pi}\int_{[\beta]}(A-A_-)\cdot dx\\&=\frac{1}{2\pi}\int_{[\beta]}(A-A_-+\nabla\theta)\cdot dx-\frac{1}{2\pi}\int_{[\beta]}\nabla\theta\cdot dx,\end{aligned} \tag{3.10}$$

where θ and $\nabla\theta$ are given by (3.6) and (3.7), respectively. Since $A-A_-+\nabla\theta$ is C^1 and has vanishing curl on Ω_+, the first term in (3.10) is zero and the second, by the definition of θ, is an integer. That Φ_- together with A satisfy (1.2) is obvious. □

In the following the above theorem is used to give examples of solutions different from the ones given in Sect. II. Let

$$U_1=\left[\frac{1}{\beta}(x_1^2+x_3^2)-(2n-1)x_2^2+1/\beta\right]/D^{n+1},$$

$$U_2=[x_1^2+\beta x_2^2+2nx_1x_2/\beta-(2n-1)x_3^2+1]/D^{n+1},$$

$$U_3=2n\beta x_2x_3/D^{n+1},$$

where $D=x_1^2+\beta x_2^2+x_3^2+1$, n is a positive integer and $\beta^3>n^2$ a positive constant. It is easy to check that U is a non-vanishing divergenceless vector field and has the following asymptotic properties:

(a) By considering the leading order of the numerator (it is homogeneous and vanishes only at the origin), we have $U\sim r^{-2n}$, where $r=(x_1^2+x_2^2+x_3^2)^{1/2}$, i.e. $\exists R>0$, $C_1,C_2>0$, such that

$$C_1r^{-2n}\leqq U(x)\leqq C_2r^{-2n}\quad\text{for}\quad r>R.$$

(b) $|\partial_iU_j|\lesssim C\cdot r^{-2n-1}$, $|\Delta U_j|\lesssim C\cdot r^{-2n-2}$ for some constant C.

It is easy to check that the assumptions on U and B of the previous theorem are satisfied.

Remark. The example above provides solutions which are stable in the sense that if f is any C^2 vector field with compact support satisfying $\operatorname{div} f = 0$, then εf can be added to U and, for ε sufficiently small, all the assumptions of the theorem continue to be satisfied.

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