

Magnetic fields and spin

So far the spin of the electron did not have too much influence in our investigations of stability. This situation changes drastically when magnetic fields are included. The operator that describes the motion of an electron in a magnetic field is the **Pauli operator**

$$\left(\frac{1}{i}\nabla + A(x)\right)^2 \otimes I + \sigma \cdot B(x) . \quad (P)$$

Here σ denotes the vector of Pauli matrices $(\sigma_1, \sigma_2, \sigma_3)$ where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

and

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

The matrix I is the 2×2 identity. The wave function of a single electron is given by a ‘spinor’

$$\psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}$$

where

$$|\psi_1(x)|^2$$

is the probability density of finding the the electron at x with spin up and

$$|\psi_2(x)|^2$$

is the probability density of finding the the electron at x with spin down. These words, ‘spin up’ and ‘spin down’ mean the following. Take the spinor

$$\phi_1(x) = \begin{pmatrix} \psi_1(x) \\ 0 \end{pmatrix}$$

and calculate the vector with components

$$\langle \phi_1(x), \sigma \cdot i \phi_1(x) \rangle .$$

The vector is given by

$$(0, 0, 1)|\psi_1(x)|^2$$

likewise doing the same thing with

$$\psi_2(x) = \begin{pmatrix} 0 \\ \psi_2(x) \end{pmatrix}$$

one gets the vector

$$(0, 0, -1)|\psi_2(x)|^2 .$$

The Pauli matrices have useful commutation relations:

$$\sigma_i^2 = I$$

and

$$\sigma_1\sigma_2 = i\sigma_3 ,$$

and further relations follow by cyclically permuting the indices 1, 2, 3. Using these relations the Pauli equation can be written in the following compact form

$$\left(\frac{1}{i}\nabla + A(x)\right)^2 \otimes I + \sigma \cdot B(x) = \left[\sigma \cdot \left(\frac{1}{i}\nabla + A(x)\right)\right]^2$$

which shows that the Pauli operator is positive. We call

$$\sigma \cdot \left(\frac{1}{i}\nabla + A(x)\right)$$

the three dimensional Dirac operator.

The first system we analyze is hydrogen in a magnetic field. The Hamiltonian is given by

$$\left[\sigma \cdot \left(\frac{1}{i}\nabla + A(x)\right)\right]^2 - \frac{Z}{|x|} . \quad (1)$$

The example where the magnetic field is constant is already interesting. We shall assume that the field points in the z direction, i.e., is given by

$$(0, 0, B) ,$$

$B > 0$. Calculating the curl of

$$A(x, y, z) = \frac{B}{2}(-y, x, 0)$$

shows that A is a vector potential for this magnetic field. In this case it is better to write the Hamiltonian in the original form as

$$\left(\frac{1}{i}\nabla + A(x, y, z)\right)^2 + \sigma_3 B - \frac{Z}{|x|} .$$

We are interested in what happens when the magnetic field B gets large. It is not possible to solve for the ground state energy in terms of elementary functions, and hence one has to resort to trial functions. The trial function will be gleaned from solving the magnetic Hamiltonian first without the Coulomb potential.

The Hamiltonian in this case is given by

$$\left(\frac{1}{i}\frac{\partial}{\partial x} - \frac{B}{2}y\right)^2 + \left(\frac{1}{i}\frac{\partial}{\partial y} + \frac{B}{2}x\right)^2 - \frac{\partial^2}{\partial z^2} . \quad (2)$$

Note that the motion in the z direction is the free motion and completely decouples from the other degrees of freedom. Hence, it suffices to concentrate on the two dimensional problem which we write as

$$B(P^2 + Q^2) \tag{3}$$

where

$$Q = \frac{1}{\sqrt{2}} \left(\frac{1}{i} \frac{\partial}{\partial y} + x \right)$$

and

$$P = \frac{1}{\sqrt{2}} \left(\frac{1}{i} \frac{\partial}{\partial x} - y \right) .$$

One arrives at this form by scaling the wave function

$$\psi(x, y) \rightarrow \sqrt{\frac{B}{2}} \psi \left(\sqrt{\frac{B}{2}} (x, y) \right) .$$

The operators P and Q which are selfadjoint, have the commutation relation

$$PQ - QP = [P, Q] = \frac{1}{i}$$

and we see that the Hamiltonian in an algebraic sense is equivalent to the Harmonic oscillator and hence we get as the eigenvalues of the Hamiltonian (3) the numbers

$$B(2n + 1) , n = 0, 1, 2, 3 \dots .$$

The eigen-functions are trickier to find. for this we write

$$B(P^2 + Q^2) = 2BA^*A + B$$

where

$$A = \frac{1}{\sqrt{2}} (P - iQ)$$

and

$$A^* = \frac{1}{\sqrt{2}} (P + iQ) .$$

The eigen-functions belonging to the lowest eigenvalue are given by those functions ψ that satisfy

$$A\psi = 0$$

which means that

$$\frac{1}{\sqrt{2}i} \left(\frac{\partial}{\partial x} - i \frac{\partial}{\partial y} + x - iy \right) \psi = 0$$

which in complex notation $z = x + iy$ means that

$$\left(\frac{1}{2} \frac{\partial}{\partial z} + \bar{z} \right) \psi = 0 .$$

This is straightforward to solve and yields

$$\psi = e^{-|z|^2/2}\phi(z)$$

where $\phi(z)$ is an entire analytic function. Thus, we see that the ground state is in fact infinitely degenerate and we call this space of eigen - functions the **lowest Landau band**.

The eigen-functions of the next higher Landau band can be found by using commutation. If ψ is in the lowest Landau band then

$$A^*\psi$$

is not identically zero and

$$\begin{aligned} [2BA^*A + B]A^*\psi &= 2BA^*[A, A^*]\psi + A^*A^*A\psi + B\psi \\ &= 3BA^*\psi \end{aligned}$$

since $A\psi = 0$ and since $[A, A^*] = 1$. In this way one can ascend and get all the eigen - function of the Hamiltonian (3). In the usual units, the functions in the lowest Landau band of the Hamiltonian (2) are given by

$$e^{-\frac{B(x^2+y^2)}{4}}P(x + iy)$$

where P is any polynomial.

Returning to the Hamiltonian (2) we have to consider the kinetic energy in the z direction which commutes with the other term. This operator can be diagonalized using Fourier transform in the z variable only

$$\hat{f}(k) = \int e^{-2\pi ikz} f(z) dz ,$$

resulting in the Hamiltonian

$$\left(\frac{1}{i}\frac{\partial}{\partial x} + \frac{B}{2}y\right)^2 - \left(\frac{1}{i}\frac{\partial}{\partial y} + \frac{B}{2}x\right)^2 + (2\pi k)^2 . \quad (2F)$$

Hence we see that the spectrum of the Hamiltonian is given by

$$B(2n + 1) + (2\pi k)^2$$

where $n = 0, 1, \dots$ and $k \in R$. The spectrum is continuous because of the kinetic energy in the z direction hence there are no square integrable eigenfunctions.

Since the magnetic field is constant in the z direction, the dynamics of the spin is $\sigma_3 B$ which amounts to considering the matrix Hamiltonian

$$\begin{bmatrix} \left(\frac{1}{i}\nabla + A(x, y, z)\right)^2 + B & 0 \\ 0 & \frac{1}{i}\nabla + A(x, y, z))^2 - B \end{bmatrix} .$$

Although there is not really a ground state we see that the infimum of the spectrum of the Hamiltonian (P) for a constant magnetic field is 0. Note that the spin terms subtracts the kinetic energy. This infimum can be found by considering spinors of the type

$$\sqrt{\frac{B}{2\pi}} e^{-(x^2+y^2)B/4} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \phi(x+iy) f(z) \quad (4)$$

where f is any normalized function of one real variable and ϕ is an analytic function obeying the normalization

$$\frac{B}{2\pi} \int e^{-(x^2+y^2)B/2} |\phi(x+iy)|^2 dx dy = 1 .$$

Returning to the hydrogenic Hamiltonian (1) we would like to obtain some estimates on the ground state energy. Using trial functions of the form (4) we get the expectation value for the energy

$$\int_{-\infty}^{\infty} |f'(z)|^2 dz - Z \frac{B}{2\pi} \int e^{-(x^2+y^2)B/2} \frac{1}{\sqrt{x^2+y^2+z^2}} |f(z)|^2 dx dy dz$$

where we assume that

$$\int_{-\infty}^{\infty} |f(z)|^2 dz = 1 .$$

Since

$$r \rightarrow \frac{1}{\sqrt{r^2+z^2}}$$

is a convex function we have that

$$Z \frac{B}{2\pi} \int e^{-(x^2+y^2)B/2} \frac{1}{\sqrt{x^2+y^2+z^2}} |f(z)|^2 dx dy dz \geq Z \frac{1}{\sqrt{\frac{2}{B}+z^2}} |f(z)|^2 dz$$

and hence we have the upper bound

$$\begin{aligned} & \int_{-\infty}^{\infty} |f'(z)|^2 dz - Z \int_{-\infty}^{\infty} \frac{1}{\sqrt{\frac{2}{B}+z^2}} |f(z)|^2 dz \\ & \leq \int_{-\infty}^{\infty} |f'(z)|^2 dz - Z \int_{-\infty}^{\infty} \frac{1}{\frac{2}{B}+|z|} |f(z)|^2 dz . \end{aligned}$$

Finally, if we choose the function

$$f(z) = \left(\frac{1}{2\pi}\right)^{1/4} e^{-z^2/2}$$

we see that the expectation of the energy is a fixed number while the expectation of the potential energy behaves as

$$-\text{const.} \log B$$

as $B \rightarrow \infty$.

Thus, there is no diamagnetic inequality and large magnetic fields squeeze the electron into the nucleus because of the interaction of the spin with the magnetic field. It is, however, impossible to produce large magnetic fields without expenditure of energy. Hence we define the stability of matter problem as follows.

Let $E(N, B, Z)$ be the ground state energy of matter interacting with a magnetic field $B(x)$. Consider (in our units) the total energy

$$E(N, K, B, Z) + \frac{1}{8\pi\alpha^2} \int |B(x)|^2 dx .$$

We say that the system is stable of the second kind if there exists a constant $C(Z)$ independent of the number of particles N and K and **independent** of the magnetic field such that

$$E(N, K, B, Z) + \frac{1}{8\pi\alpha^2} \int |B(x)|^2 dx \geq -C(Z)(N + K) .$$

Let us return to the hydrogen atom and report the bad news.

Theorem *The hydrogenic atom interacting with a magnetic field is unstable in the sense that if $Z\alpha^2$ is large enough then*

$$\inf \left\{ E(Z, B) + \frac{1}{8\pi\alpha^2} \int |B(x)|^2 dx \right\} = -\infty .$$

PROOF: The proof depends critically on the existence of **zero modes of the three dimensional Dirac operator**. Consider a vector potential $A(x)$ which

$$\int |\text{curl} A(x)|^2 dx < \infty .$$

A spinor $\psi(x)$ is called a zero mode if it is square integrable and if

$$\sigma \cdot \left(\frac{1}{i} \nabla + A(x) \right) \psi(x) = 0$$

everywhere. Once such a zero mode is given we can scale it

$$\psi \rightarrow \psi_\lambda(x) = \lambda^{3/2} \psi(\lambda x)$$

and

$$A(x) \rightarrow A_\lambda(x) = \lambda A(\lambda x) .$$

Clearly

$$\sigma \cdot \left(\frac{1}{i} \nabla + A_\lambda(x) \right) \psi_\lambda(x) = 0$$

and hence the expectation value of the hydrogenic Hamiltonian is given by

$$\begin{aligned} & -Z \int \frac{1}{|x|} \langle \psi_\lambda, \psi_\lambda(x) \rangle dx + \frac{1}{8\pi\alpha^2} \int |B_\lambda(x)|^2 dx \\ & = \lambda \left(-Z \int \frac{1}{|x|} \langle \psi, \psi(x) \rangle dx + \frac{1}{8\pi\alpha^2} \int |B(x)|^2 dx \right) . \end{aligned}$$

Hence, we see that if $Z\alpha^2$ is too large we get an arbitrarily negative energy by letting $\lambda \rightarrow \infty$.

Thus the main question is, are there any zero modes? Examples are hard to come by although people have discovered infinitely many of them so far. We give an idea how to construct such zero modes. Consider

$$\psi(x) = \frac{1 + i\sigma \cdot x}{(1 + |x|^2)^{3/2}} \phi$$

where ϕ is a constant spinor of length 1.

A straightforward calculation leads to

$$\sigma \cdot \frac{\nabla}{i} \psi = \frac{3}{(1 + |x|^2)} \psi .$$

Next, we note that every normalized spinor η satisfies the eigenvalue equation

$$[\sigma \cdot \langle \eta, \sigma \eta \rangle] \eta = \eta$$

(PROOF: We have the general formula

$$\sigma \cdot a \sigma \cdot b = a \cdot b + i\sigma a \times b .$$

Hence

$$[\sigma \cdot \langle \eta, \sigma \eta \rangle]^2 = |\langle \eta, \sigma \eta \rangle|^2 = 1 ,$$

Further which means that the eigenvalues of the matrix $[\sigma \cdot \langle \eta, \sigma \eta \rangle]$ are ± 1 . Further

$$\langle \eta, [\sigma \cdot \langle \eta, \sigma \eta \rangle] \eta \rangle = 1$$

and hence by the minmax principle η is the eigenvector with eigenvalue 1.) Hence we know that

$$\sigma \cdot \frac{\langle \psi, \sigma \psi \rangle}{\langle \psi, \psi \rangle} \psi = \psi$$

and if we define

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

the spinor ψ is a zeromode.

A straightforward calculation yields

$$A(x) = \frac{3}{(1 + |x|^2)^2} ((1 - |x|^2)w + 2w \cdot xx + 2w \wedge x) .$$

A further calculation shows that

$$B(x) = \frac{12}{(1 + |x|^2)^3} ((1 - |x|^2)w + 2w \cdot xx + 2w \wedge x)$$

which is clearly square integrable.

The field lines form closed Euclidean circles that sit on a family of nested tori and are linked once. In fact the field lines are given by pulling the Hopf-fibration from the three sphere to R^3 .