Analytic Solution of a Relativistic Two-dimensional Hydrogen-like Atom in a Constant Magnetic Field

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Abstract

We obtain exact solutions of the Klein-Gordon and Pauli Schrödinger equations for a two-dimensional hydrogen-like atom in the presence of a constant magnetic field. Analytic solutions for the energy spectrum are obtained for particular values of the magnetic field strength. The results are compared to those obtained in the non-relativistic and spinless case. We obtain that the relativistic spectrum does not present $s$ states.
The study of the two-dimensional Hydrogen atom in the presence of homogeneous magnetic fields has been a subject of active research during the last years. Much work has been done in the framework of non-relativistic quantum mechanics, computing the energy spectrum for different magnetic field strengths. This problem is of practical interest in discussing single and multiple-quantum well (superlattice) systems in semiconductor Physics.

The two-dimensional Schrödinger equation, with a Coulomb potential $-\frac{Z}{r}$ and a constant magnetic $\vec{B}$ field, perpendicular to the plane where the particle is, can be written in atomic units as follows

$$H\varphi = \frac{1}{2}(-i\nabla + \frac{1}{2}\vec{B} \times \vec{r})^2\varphi - \frac{Z}{r}\varphi = i\partial_t\varphi = E\varphi \quad (1)$$

Since we are dealing with a two-dimensional problem, we choose to work in polar coordinates $(r, \vartheta)$. The angular operator $-i\partial_\vartheta$ commutes with the Hamiltonian (1), consequently we can introduce the following ansatz for the eigenfunction

$$\varphi(\vec{r}) = \exp(im\vartheta) u(r) \sqrt{\frac{2}{\pi r}} \quad (2)$$

Substituting (2) into (1), we readily obtain that the radial function $u(r)$ satisfies the second order differential equation

$$\left[ -\frac{1}{2} \frac{d^2}{dr^2} + \left( m^2 - \frac{1}{4} \right) \frac{1}{r^2} + \frac{\omega_L^2 r^2}{2} - \frac{Z}{r} + m\omega_L - E \right] u(r) = 0 \quad (3)$$

where $\omega_L = B/2c$ is the Larmor frequency, $E$ is the energy, and $m$ the eigenvalue of the angular momentum. A general closed-form solution to (3) in terms of special functions does not exist. There are analytic expressions for the energy for particular values of $\omega_L$ and $m$ as, pointed out by Lozanskii and more recently by Taut. The advantage of having exact values of the energy spectrum for some values of the magnetic field strength and the angular momentum becomes clear when we use numerical methods for computing the energy for any value $B$ and $m$, in particular for higher excited states (Rydberg states) and high magnetic fields, as pointed out by Taut.

In this article we solve the two-dimensional hydrogen atom with an homogeneous magnetic field (perpendicular to the plane in which the electron is located) when relativistic corrections are considered. We obtain analytic solutions of the 2D Klein-Gordon and we also compute the relativistic energy spectrum for some particular values of the angular momentum $m$ and the magnetic field strength $B$. Finally, we solve the nonrelativistic problem when spin corrections are included.

The covariant generalization of the Klein-Gordon equation in the presence of electromagnetic interactions takes the form

$$\left( g^{\alpha\beta} (\nabla_\alpha - \frac{i}{c} A_\alpha) (\nabla_\beta - \frac{i}{c} A_\beta) - c^2 \right) \Psi = 0 \quad (4)$$

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1In this paper we adopt the atomic units $\hbar = M = e = 1$ in the CGS system.
where $g^{\alpha\beta}$ is the contravariant metric tensor, and $\nabla_\alpha$ is the covariant derivative. Since we are working in a 2+1 spacetime, the metric tensor $g_{\alpha\beta}$ written in polar coordinates ($t, r, \vartheta$) takes the form:

$$g_{\alpha\beta} = \text{diag}(-1, 1, r^2)$$

(5)

and the vector potential $A^\alpha$ associated with a Coulomb and a constant magnetic field interaction is

$$A^\alpha = (-\frac{Z}{r}, 0, -\frac{Br^2}{2}).$$

(6)

With the help of the vector potential (6), it is straightforward to verify that the corresponding magnetic and electric fields satisfy the invariant relations

$$F_{\alpha\beta}F^{\alpha\beta} = 2(\mathcal{B}^2 - \mathcal{E}^2) = 2(\mathcal{B}^2 - \frac{Z^2}{r^4})$$

(7)

$$^*F_{\alpha\beta}F^{\alpha\beta} = 0 \rightarrow \vec{E} \cdot \vec{B} = 0$$

(8)

where $F^{\alpha\beta}$ is the electromagnetic field strength tensor, which in a (2+1) spacetime has three independent components.

Expression (7) and (8) tell us that in fact $A^\alpha$ is associated with a 2D Coulomb atom in a constant magnetic field perpendicular to the plane where the particle is located. The corresponding $\vec{E}$ and $\vec{B}$ can be written in polar coordinates as follows:

$$\vec{E} = -\frac{Z}{r^2}\hat{e}_r$$

(9)

$$\vec{B} = B\hat{e}_z.$$  

(10)

Since the vector potential components do not depend on time or the angular variable $\vartheta$, we have that the wave function $\Psi$, solution of the Klein-Gordon equation (4) can be written as

$$\Psi(r, \vartheta, t) = \frac{u(r)}{\sqrt{r}}\exp(im\vartheta - Et),$$

(11)

where the function $u(r)$ satisfies the second order ordinary differential equation

$$\frac{d^2 u(r)}{dr^2} + \left(\frac{1}{r} - \frac{m^2}{r^2} + \frac{Z^2}{c^2} - \frac{mc}{c^2} - \frac{E^2}{c^2} - \frac{1}{4} \frac{r^2B^2}{c^2} + 2EZ \right) u(r) = 0$$

(12)

Equation (12) does not admit an exact solution in terms of special functions, and therefore approximate methods have to be applied in order to compute the energy spectrum. It is worth noting that the 2+1 relativistic Coulomb problem can be solved in closed form [3] and the energy levels are...
\[ E = c^2 \left[ 1 + \frac{Z^2}{c^2(n - \frac{1}{2} + \sqrt{m^2 - \frac{Z^2}{c^2}})^2} \right]^{-1/2} \] (13)

Also we have that the energy spectrum of a relativistic spinless particle in a constant magnetic field satisfies the relation
\[
\frac{E^2}{c^2} - c^2 = \frac{B}{c} (2n + m + |m| + 1) \] (14)

We look for a series solution of eq. (12). In order to do that, after analyzing the asymptotic behavior of the solution \( u(r) \) at \( r = 0 \) and as \( r \to \infty \), we write \( u(r) \) in the form
\[
u(r) = \exp\left( -\frac{1}{4} \frac{B r^2}{c} \right) r^{\frac{1}{2} + \frac{m^2 - Z^2}{c^2}} \sum_{n=0} a_n r^n \] (15)

substituting (15) into (12) and imposing that
\[ a_0 \neq 0 \] (16)

we obtain
\[ a_1 = -\frac{2EZ}{(2\sqrt{m^2 - \frac{Z^2}{c^2}} + 1) c^2} a_0 \] (17)

and for \( n \geq 2 \) we have
\[
\left[ n^2 + 2n \sqrt{m^2 - \frac{Z^2}{c^2}} \right] a_n + 2a_{n-1} \frac{EZ}{c^2} + a_{n-2} \left[ \frac{E^2}{c^2} - c^2 - \frac{B}{c} (n - 1 + m + \sqrt{m^2 - \frac{Z^2}{c^2}}) \right] = 0 \] (18)

Since only polynomial solutions of eq (12) are bounded as \( r \to \infty \), the series given by the recurrence relation (18) terminates at a certain \( n \) when \( a_n = 0 = a_{n+1} = a_{n+i} = 0 \) for any positive integer value of \( i \). From the recurrence relation (18), we readily obtain the following relation
\[
\frac{E^2}{c^2} - c^2 = (m + \sqrt{m^2 - \frac{Z^2}{c^2}} + n) \frac{B}{c} \] (19)

for those values of the field strength \( B \) for which (15) becomes a polynomial. After substituting (15) into (12), we obtain a system of equations which gives the permitted values of \( B \). It is worth mentioning that the relation (19) makes sense only when
\[ m^2 - \frac{Z^2}{c^2} > 0 \] (20)

a condition that forbids the existence of the \( s \) energy levels \( (m = 0) \), this is in fact a particularity of the relativistic Klein-Gordon solution, which is not present in the standard
Schrödinger framework. Let us obtain the first excited state of the relativistic Klein-Gordon 2+1 hydrogen atom. In this particular case we have that only \( a_0 \) and \( a_1 \) are nonzero, and the recurrence relations (17),(18) give

\[
\frac{2EZ}{c} a_0 + a_1 \left( 1 + 2 \sqrt{m^2 - \frac{Z^2}{c^2}} \right) = 0 \tag{21}
\]

\[
a_0 \frac{B}{c} + \frac{2EZ}{c^2} a_1 = 0 \tag{22}
\]

\[
\frac{E^2}{c^2} - c^2 = \frac{B}{c} \left( 2 + m + \sqrt{m^2 - \frac{Z^2}{c^2}} \right) \tag{23}
\]

from which we obtain that the energy is given by the expression

\[
E = c^2 \left[ 1 - \frac{4Z^2 \left( 2 + m + \sqrt{m^2 - \frac{Z^2}{c^2}} \right)}{c^2 \left( 2\sqrt{m^2 - \frac{Z^2}{c^2}} + 1 \right)} \right]^{-1/2} \tag{24}
\]

for a magnetic field \( B \) that can be obtained after substituting (24) into (19).

\[
B = \frac{4E^2Z^2}{c^3 (1 + 2\sqrt{m^2 - \frac{Z^2}{c^2}})} \tag{25}
\]

also, we have that for \( n=3 \) \( (a_2 \neq 0, \ a_n = 0, \ n > 2) \) the corresponding energy is given by the expression

\[
E = c^2 \left[ 1 - \frac{2Z^2 \left( \sqrt{m^2 - \frac{Z^2}{c^2}} + m + 3 \right)}{c^2 (3 + 4\sqrt{m^2 - \frac{Z^2}{c^2}})} \right]^{-1/2} \tag{26}
\]

for \( B \) given by

\[
B = \frac{2E^2Z^2}{c^3} \left[ (3 + 4\sqrt{m^2 - \frac{Z^2}{c^2}}) \right]^{-1} \tag{27}
\]

In order to obtain the magnetic field for which analytic solutions of eq. (3) are possible, we have to solve the system of equations given by the recurrence relation (18). The following table shows all the allowed magnetic fields for \( 2 \leq n \leq 10 \). Notice that for higher values of \( n \) the number of solutions increases as \( \text{int}(n/2) \).
Table 1 Energy values for all the allowed magnetic fields for $Z = 1, m = -1$, and a comparison with the non relativistic energy spectrum. N is the number of nodes of the radial wavefunction.

| n  | $B$     | $E$     | $E - c^2$ | $E - c^2$ non rel. | $E$ | N |
|----|---------|---------|-----------|---------------------|-----|---|
| 2  | 182.6968| 18770.3334| 3.3336| 1.3336| 1 |
| 3  | 184.1492| 18769.4289| 4.2857| 4.2857| 2 |
| 4  | 15.1057 | 18769.2205| 0.2205| 0.2205| 3 |
| 5  | 4.2611  | 18769.0933| 0.0933| 0.0933| 4 |
| 6  | 13.0381 | 18769.2850| 0.2850| 0.2850| 5 |
| 7  | 28.5767 | 18769.1684| 0.1684| 0.1684| 6 |
| 8  | 32.8207 | 18769.1948| 0.1948| 0.1948| 7 |
| 9  | 3.8206  | 18769.1115| 0.1115| 0.1115| 8 |
| 10 | 1.6310  | 18769.2180| 3.2180| 3.2180| 9 |

A comparison with the non-relativistic energy levels, obtained with the help of the Schwartz method [7], which is a generalization of the mesh point technique for numerical approximation of functions, shows that the relativistic correction to the problem becomes noticeable when $B > 100$. Table 1 shows that the energy correction is smaller than $10^{-3}$ even when $B \approx 100$. From (13) and (14) we can see that for weak as well as for strong magnetic field strengths, the rôle played by the relativistic corrections is to shift down the energy levels.

The inclusion of spin effects can be carried out in a rather simple way with the help of the Schrödinger-Pauli equation. 

$$H \Psi = \left[ \frac{1}{2} \left( \vec{P} + \frac{\vec{A}}{c} \right)^2 + U(r) + \vec{s} \cdot \vec{B} \right] \Psi \quad (28)$$

which, after substituting the vector potential (11) into (28), with $\Psi(r)$ given by (11) we obtain

$$- \frac{1}{2} \frac{d^2 u}{dr^2} + \left[ \frac{1}{2} \left( m^2 - \frac{1}{4} \right) \frac{1}{r^2} + \frac{\omega^2}{2} - \frac{Z}{r} \right] u = [E - 2\omega s - m\omega] u \quad (29)$$

where $\vec{s}$ is the spin operator which satisfies the relations

$$\vec{s} \cdot \vec{s} = 3/4, \quad s_i s_j = \frac{1}{4} (\delta_{ij} + \epsilon_{ijk} s_k) \quad (30)$$

and, for our magnetic field strength, we have that $\vec{s} \cdot \vec{B}$ can be written as

$$\vec{s} \cdot \vec{B} = \frac{1}{2} \sigma_3 B \quad (31)$$
where $\sigma_3$ is the diagonal Pauli matrix. Eq. (29) has essentially the same form as (3). The presence of the spin introduces a shift in the energy proportional to the magnetic field strength. For the allowed magnetic field values reported in [3] we have that the Schrödinger-Pauli spectrum is

$$E = \omega(n + 2\sigma + m + |m|) \tag{32}$$

It is worth noticing that the spin contribution does not introduce any restriction on the allowed values of $m$. It is the relativistic contribution that forbids the existence of the $s$ values. The inclusion of spin correction as well as relativistic effects requires to deal with the 2+1 Dirac equation in the background field given by (9) and (10). This problem will be discussed in a forthcoming publication.

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