

ENERGY SPECTRUM OF THE GROUND STATE OF A TWO-DIMENSIONAL RELATIVISTIC HYDROGEN ATOM IN THE PRESENCE OF A CONSTANT MAGNETIC FIELD

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We compute the energy spectrum of the ground state of a 2D Dirac electron in the presence of a Coulomb potential and a constant magnetic field perpendicular to the plane where the the electron is confined. With the help of a mixed-basis variational method we compute the wave function and the energy level and show how it depends on the magnetic field strength. We compare the results with those obtained numerically as well as in the non-relativistic limit.

Keywords: Two-dimensional relativistic hydrogen atom; variational methods; Dirac equations.

1. Introduction

Over the past years the study of systems of non-relativistic electrons confined to a plane in an electromagnetic field background has attracted much attention in view of possible applications. This problem is of practical interest because of the technological advances in nanofabrication technology that have made the creation of low-dimensional structures like quantum wells, quantum wires and quantum dots possible.¹ The relativistic extension of this problem has also turned out to be of importance in the description of quantum two-dimensional phenomena such as the quantum Hall effect and high-temperature superconductivity.² Different condensed matter physics phenomena point to the existence of (2+1)-dimensions with

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an energy spectrum determined by the Dirac equation Hamiltonian.^{3,4} In particular, the degenerate planar semiconductor with low-energy electron dynamics is assumed to admit an adequate description in terms of (2+1)-dimensional relativistic Dirac theory.⁵ In conclusion, the study of physical effects occurring in (2+1)-dimensional systems of charged particles in strong external fields is an interesting problem from the theoretical point of view as well from the viewpoint of its practical applications.^{6–10}

In order to analyze relativistic quantum effects in the presence of strong electromagnetic fields, one should be able to compute the Green's function or to find exact solutions of the Dirac equation. Regrettably, the Dirac equation is exactly solvable only in a very restricted family of electromagnetic configurations.¹¹

The non-relativistic two-dimensional Hamiltonian describing the Coulomb interaction $-Z/r$, between a conduction electron and donor impurity center when a constant magnetic \mathbf{B} field is applied perpendicular to the plane of motion has been thoroughly discussed in the literature.^{14–18} Despite its simple form, its solutions cannot be expressed in terms of special functions. An analogous situation occurs when we deal with the (2+1) Dirac equation; therefore one has to apply numerical and approximate techniques in order to compute the energy spectrum and the corresponding wave functions.

In order to compute the energy spectrum of the relativistic hydrogen atom we have at our disposal different numerical and semi-analytic methods. The Kato and Lehman–Maelhy methods have also been applied to solve the Dirac equation without variational collapse.¹² A large finite-basis-set method has been applied in order to calculate in 3D relativistic and non-relativistic binding energies of an electron in a Coulomb magnetic field.¹³

It is the purpose of the present paper to compute the energy spectrum of the ground state of the (2+1) Dirac equation in the presence of a Coulomb interaction and a constant magnetic field perpendicular to the plane where the electron moves. For this purpose, we use a two-term mixed-basis variational approach.¹⁶ We also compute the non-relativistic limit with the help of the Pauli equation. Finally, we compare the results with those obtained numerically with the help of the Schwartz method,¹⁹ which is a generalization of the mesh point technique.

The paper is arranged as follows: In Sec. 2 we write the (2+1) Dirac equation in the presence a constant magnetic field and a Coulomb potential; we construct a two-term mixed-basis in order to compute the energy spectrum. In Sec. 3, we solve the Pauli equation and show how the energy spectrum depends on the spin orientation. In Sec. 4, with the help of a mesh method we solve the Dirac equation numerically. We compare the numerical result with those obtained in the non-relativistic limit and with the the help of the variational method. Finally, we briefly discuss the validity of our approach and further applications.

2. Dirac Equation

The covariant Dirac equation^{7,20} in atomic units, $\hbar = M = e = 1$, in the presence of an external electromagnetic field A_μ can be written as

$$\left(\tilde{\gamma}^\mu \left(\frac{\partial}{\partial x^\mu} - \Gamma_\mu - i \frac{A_\mu}{c} \right) + c \right) \Psi = 0, \quad (1)$$

where the Dirac matrices $\tilde{\gamma}^\mu$ satisfy the commutation relation $\{\tilde{\gamma}^\mu, \tilde{\gamma}^\nu\}_+ = 2g^{\mu\nu}$. The metric tensor $g_{\alpha\beta}$ written in polar coordinates (t, ρ, ϑ) has the form:

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

and Γ_μ are the spinor connections.²¹ The vector potential A^α associated with a 2D Coulomb potential and a constant magnetic field interaction is

$$A^\alpha = \left(-\frac{Z}{\rho}, 0, -\frac{B\rho^2}{2} \right). \quad (3)$$

Choosing to work in the diagonal tetrad gauge, we have that the $\tilde{\gamma}$ matrices take the form:

$$\tilde{\gamma}^\rho = \gamma^1, \quad \tilde{\gamma}^\vartheta = \frac{\tilde{\gamma}^2}{\rho}, \quad \tilde{\gamma}^t = \gamma^0, \quad (4)$$

where γ^μ are the standard constant Dirac matrices, satisfying the anticommutation relations $\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}$.

In the diagonal tetrad gauge,²⁰ the spinor connections take the form:

$$\Gamma_0 = 0, \quad \Gamma_1 = 0, \quad \Gamma_2 = \frac{1}{2}\gamma^1\gamma^2. \quad (5)$$

Since we are working in 2+1 dimensions, it is convenient to introduce the following representation of the Dirac matrices in terms of the Pauli matrices:

$$\gamma^1 = \sigma_1, \quad \gamma^2 = \sigma_2, \quad \gamma^0 = \sigma_3. \quad (6)$$

The Dirac equation (1) expressed in the diagonal tetrad gauge commutes with the operators $i\frac{\partial}{\partial t}$ and $-i\frac{\partial}{\partial \vartheta}$; therefore the spinor Ψ can be written as

$$\Psi(t, \rho) = \frac{1}{\sqrt{2\pi\rho}} \exp(-iEt + ik_\vartheta\vartheta)\psi(\rho), \quad (7)$$

with

$$\psi = \begin{pmatrix} \psi_1(\rho) \\ \psi_2(\rho) \end{pmatrix}, \quad (8)$$

where the $\sqrt{\rho}$ factor has been introduced in order to eliminate the spinor contribution $\gamma^\mu\Gamma_\mu$ in the Dirac equation (1). Substituting Eq. (7) into Eq. (1) and taking into account Eq. (5), we obtain

$$\left[\frac{E}{c} + \frac{Z}{c\rho} + i\sigma^2\partial_\rho + \sigma^1 \left(\frac{k_\vartheta}{\rho} + \frac{B\rho}{2c} \right) + \sigma^3c \right] \psi = 0. \quad (9)$$

After substituting the Pauli matrices into Eq. (9) we reduce our problem to the following system of coupled differential equations:

$$\frac{d\psi_2}{d\rho} + \left(\frac{k_\vartheta}{\rho} + \frac{B\rho}{2c}\right)\psi_2 + \left(\frac{E}{c} + c + \frac{Z}{c\rho}\right)\psi_1 = 0, \tag{10}$$

$$\frac{d\psi_1}{d\rho} - \left(\frac{k_\vartheta}{\rho} + \frac{B\rho}{2c}\right)\psi_1 - \left(\frac{E}{c} - c + \frac{Z}{c\rho}\right)\psi_2 = 0. \tag{11}$$

In order to analyze the nature of the eigenvalues k_ϑ of the $-i\frac{\partial}{\partial\vartheta}$ operator, we notice that the spinor Ψ expressed in the (rotating) diagonal tetrad gauge is related to the Cartesian (fixed) spinor Ψ_c by means of the transformation²⁰:

$$\Psi = S(\vartheta)^{-1}\Psi_c, \tag{12}$$

where the matrix $S(\vartheta)$ can be written as

$$S(\vartheta) = \exp\left(-\frac{\vartheta}{2}\gamma^1\gamma^2\right) = \exp\left(-i\frac{\vartheta}{2}\sigma_3\right). \tag{13}$$

Noticing that $S(\vartheta)$ satisfies the relation:

$$S(\vartheta + 2\pi) = -S(\vartheta), \tag{14}$$

we obtain

$$\Psi(\vartheta + 2\pi) = -\Psi(\vartheta), \tag{15}$$

and we have $k_\vartheta = N + 1/2$, where N is an integer. The rotating Dirac spinor Ψ can be written in terms of Ψ_c as

$$\Psi = \begin{pmatrix} e^{i\vartheta/2}\Psi_{1c} \\ e^{-i\vartheta/2}\Psi_{2c} \end{pmatrix} \quad \text{with} \quad \Psi_c = \begin{pmatrix} \Psi_{1c} \\ \Psi_{2c} \end{pmatrix}. \tag{16}$$

Taking into account the relation (12) between Ψ and Ψ_c as well as Eq. (7) we readily obtain

$$\Psi_c(\mathbf{r}) = \frac{1}{\sqrt{2\pi\rho}} \begin{pmatrix} e^{i(k_\vartheta-1/2)\vartheta}\psi_1(\rho) \\ e^{i(k_\vartheta+1/2)\vartheta}\psi_2(\rho) \end{pmatrix}. \tag{17}$$

The system of equations (10) and (11) does not admit an exact solution in terms of special functions, therefore we proceed to compute energy eigenvalues with the help of variational techniques.

In non-relativistic quantum mechanics, variational methods provide a powerful technique for the construction of approximate eigenvalues and eigenfunctions and for calculations involving sums over the complete energy spectrum. The variational method cannot be extended to the Dirac case in a straightforward manner because the Hamiltonian associated with Eq. (1) is not bounded from below. Any positive-energy eigenvalue can collapse into a negative-energy eigenvalue as the basis set is increased or as the nonlinear parameters of the basis are varied.²²

The earliest attempts at the solution of the relativistic basis set problem revealed a tendency for any variational approach to a bound-state of positive energy to

collapse into the negative-energy region of the spectrum. This effect, which was first noticed by Kim,²³ has since become known as variational collapse or finite basis set disease.

Among the possible ways to circumvent the problems related to a finite basis and the variational collapse, we have chosen to work with a quadratic Dirac equation:

$$\left[\frac{d^2}{d\rho^2} + \left(\frac{E}{c} + \frac{Z}{c\rho} \right)^2 + i\sigma^2 \frac{Z}{c\rho^2} - \left(\frac{k_\vartheta}{\rho} + \frac{B\rho}{2c} \right)^2 - c^2 + \frac{k_\vartheta\sigma^3}{\rho^2} - \frac{B\sigma^3}{2c} \right] \psi = 0, \quad (18)$$

which can be obtained after squaring Eq. (9). It is worth noticing that Eq. (18) is a second order differential equation and therefore it does not present the problems associated with variational collapse.

In order to solve Eq. (18) we propose a mixed-basis variational approach that has been successfully applied in the non-relativistic case as well as in computing the energy eigenvalues of the (2+1) Klein–Gordon equation. We introduce the following trial function:

$$\psi = c_1\psi_1 + c_2\psi_2 = c_H\psi_H + c_O\psi_O, \quad (19)$$

where $\psi_1 = \psi_H$ and $\psi_2 = \psi_O$ are the corresponding hydrogen and oscillator wave functions associated with the ground state, and c_O and c_H are constants to be calculated. It is worth mentioning that our basis is not orthogonal under the inner product $\langle \psi_i | \psi_j \rangle = \int_0^\infty \psi_i^\dagger \psi_j d\rho$. Substituting Eq. (19) into Eq. (18), and performing variation on the basis coefficients c_j , we readily obtain the following matrix equation:

$$\begin{aligned} & \left(\left\langle \psi_i(\rho), \frac{d^2\psi_j(\rho)}{d\rho^2} \right\rangle + \left(\frac{Z^2}{c^2} - k_\vartheta^2 \right) A_{ij} - \frac{B}{2c} F_{ij} + k_\vartheta G_{ij} + i \frac{Z}{c} H_{ij} \right) c_j \\ & + \left(\left(\frac{mB}{c} - c^2 + \frac{E^2}{c^2} \right) \delta_{ij} - \frac{1}{4} \frac{B^2}{c^2} D_{ij} + \frac{2EZ}{c^2} C_{ij} \right) c_j = 0 \end{aligned} \quad (20)$$

with

$$\begin{aligned} A_{ij} &= \left\langle \psi_i(r) \left| \frac{1}{\rho^2} \right| \psi_j(r) \right\rangle, & G_{ij} &= \left\langle \psi_i(r) \left| \frac{\sigma_{ij}^3}{\rho^2} \right| \psi_j(r) \right\rangle, \\ C_{ij} &= \left\langle \psi_i(r) \left| \frac{1}{\rho} \right| \psi_j(r) \right\rangle, & H_{ij} &= \left\langle \psi_i(r) \left| \frac{\sigma_{ij}^2}{\rho^2} \right| \psi_j(r) \right\rangle, \\ D_{ij} &= \left\langle \psi_i(r) \left| \rho^2 \right| \psi_j(r) \right\rangle, & F_{ij} &= \left\langle \psi_i(r) \left| \sigma_{ij}^3 \right| \psi_j(r) \right\rangle. \end{aligned} \quad (21)$$

Instead of computing all the matrix terms in Eq. (21) one can use the fact that ψ_H and ψ_O are the corresponding hydrogen and oscillator wave functions associated with the ground state

$$H|\Psi\rangle = c_H E_H |\Psi_H\rangle + c_O E_O |\Psi_O\rangle. \quad (22)$$

Using the expression (22) we reduce Eq. (20) to the following matrix equation:

$$Q_{ij}c_j = 0, \quad (23)$$

where the components of the square matrix Q_{ij} are

$$Q_{11} = \left(\frac{E}{c}\right)^2 + \frac{2(E - E_H)Z}{c^2}C_{11} - \left(\frac{E_H}{c}\right)^2 - D_{11}\left(\frac{B}{2c}\right)^2 - \frac{B}{2c}(k_{\vartheta} + G_{11}) \quad (24)$$

$$Q_{12} = \left[\left(\frac{E}{c}\right)^2 - \left(\frac{E_H}{c}\right)^2 - \frac{Bk_{\vartheta}}{2c}\right]S + \frac{2(E - E_H)Z}{c^2}C_{12} - D_{12}\left(\frac{B}{2c}\right)^2 \quad (25)$$

$$Q_{22} = \left(\frac{E}{c}\right)^2 - \left(\frac{E_O}{c}\right)^2 + \frac{2EZ}{c^2}C_{22} + \left(\frac{Z}{c}\right)^2 A_{22}, \quad (26)$$

where $S = \langle \Psi_H | \Psi_O \rangle$ is the overlap between the hydrogen and oscillator wavefunctions.

The equation $\det(Q_{ij}) = 0$ gives as a result an algebraic equation for E that permits one to obtain the variational estimate for the energy. Among the solutions of the secular equation, we identify the energy as the lowest positive root.

The advantage of the two-term mixed-basis variational approach is two-fold: First, it gives accurate results in the pure-Coulomb as well as in the strong magnetic field regimes and very good estimates for the intermediate region. Second, the variational wave function can be calculated in a closed form. We do not have to handle large term variational basis and the problems related to balancing small and large components of the Hamiltonian.

In this paper we are interested in computing the energy spectrum of the ground s state. The lowest energy configuration corresponds to a state that in the absence of the Coulomb interaction has the electron spin directed opposite to the magnetic field.¹¹

The solution of the Dirac equation in the presence of a constant magnetic field with the electron spin directed opposite to B is

$$\psi_0 = \sqrt{\frac{B}{c}} \begin{pmatrix} 0 \\ \sqrt{\rho} \end{pmatrix} e^{-\frac{B\rho^2}{4c}}, \quad (27)$$

the energy associated with spinor (27) does not depend on the magnetic field strength and it is given by the simple expression:

$$\frac{E_O^2}{c^2} = c^2, \quad (28)$$

which corresponds to a zero non-relativistic energy.

In order to compute the spinor ψ_H , solution of the (2+1) Dirac equation in the presence of the Coulomb interaction, we solve Eqs. (10) and (11) for $B = 0$. The solution can be readily obtained in terms of Laguerre polynomials that for the s state take the simple form:

$$\psi_H = \frac{(2\lambda)^{\nu+\frac{1}{2}}}{\sqrt{\Gamma(2\nu+1)}} \rho^{\nu} e^{-\lambda\rho} \begin{pmatrix} \sqrt{1 - E_H/c^2} \\ \sqrt{1 + E_H/c^2} \end{pmatrix}, \quad (29)$$

where ν and γ are given by

$$\lambda = \sqrt{c^2 - \frac{E_H^2}{c^2}} \tag{30}$$

and

$$\nu = \sqrt{k_\vartheta^2 - \frac{Z^2}{c^2}}. \tag{31}$$

The energy of the ground state is

$$\frac{E_H}{c} = c \left[\sqrt{1 + \left(\frac{Z}{c\nu}\right)^2} \right]^{-1}. \tag{32}$$

Some coefficients of the matrix Q_{ij} are divergent in the hydrogen-oscillator basis. In order to circumvent this problem we replace $\rho^{1/2}$ by $\rho^{1-\nu}$ in Eq. (27). This substitution permits one to compute the coefficients A_{ij} and does not sensitively affect the computation of the energy spectrum.

3. Non-Relativistic Limit

In this section we are interested in computing the energy spectrum of the 2 + 1 Coulomb atom in the presence of a constant magnetic field when one considers spin effects. The non-relativistic limit of the Dirac equation (1) is given by the Pauli equation:

$$H\Psi = \left[\frac{1}{2} \left(\mathbf{P} + \frac{1}{2c} \mathbf{B} \times \mathbf{r} \right)^2 - \frac{Z}{\rho} + \mathbf{s} \cdot \frac{\mathbf{B}}{c} \right] \Psi, \tag{33}$$

where \mathbf{s} is the spin operator. For a constant magnetic field, we have that $\mathbf{s} \cdot \mathbf{B}$ can be written as

$$\mathbf{s} \cdot \mathbf{B} = \frac{1}{2} \sigma_3 B. \tag{34}$$

Since we are dealing with a two-dimensional problem, we choose to work in polar coordinates (ρ, ϑ) . The angular operator $-i\partial_\vartheta$ commutes with the Hamiltonian (33), and consequently we can introduce the following *ansatz* for the eigenfunction:

$$\Psi = \frac{e^{im\varphi}}{\sqrt{2\pi}} \frac{u(\rho)}{\sqrt{\rho}}. \tag{35}$$

Substituting Eq. (35) into Eq. (33), we readily obtain that the radial function $u(\rho)$ satisfies the second order differential equation:

$$-\frac{1}{2} \frac{d^2 u}{d\rho^2} + \left[\frac{1}{2} \left(m^2 - \frac{1}{4} \right) \frac{1}{\rho^2} + \frac{B^2 \rho^2}{8c^2} - \frac{Z}{\rho} \right] u = \left[E - \frac{B}{c} s - m \frac{B}{2c} \right] u. \tag{36}$$

The solution of Eq. (36) cannot be expressed in terms of special functions.¹¹ Taking into account how the spin couples to the magnetic field in the Pauli equation, we can compute the energy eigenvalues of Eq. (36). The energy spectrum of the Pauli

can be computed in a straightforward manner with the help of the solutions of the Schrödinger equation. The presence of the spin introduces a shift in the energy proportional to the magnetic field strength:

$$E_{\text{nonrel}} = E_{\text{Schr}} \pm \frac{B}{2c}, \quad (37)$$

where the positive and negative signs correspond to the a magnetic field oriented along or in the opposite direction to the electron spin, respectively. Since we are interested in a configuration where the spin is in the opposite direction to the magnetic field, which corresponds to the lowest energy configuration, we choose the negative sign in Eq. (37).

The computation of energy spectrum of the (2+1) Schrödinger equation in the presence of the a Coulomb potential and a constant magnetic is a problem that has been widely discussed in the literature and different analytic and numerical techniques are at our disposal.¹⁸

4. Discussion

In this section we proceed to compute the energy spectrum of the Dirac equation with the help of the methods discussed in Secs. 2 and 3. In order to compare the accuracy of the variational approach as well as of the non-relativistic limit, the numerical computations of the relativistic energy spectra are carried out with the help of the Schwartz method,¹⁹ which is a generalization of the mesh point technique for numerical approximation of functions.

This method gives highly accurate results given a thoughtful choice of the reference function. For Eqs. (10) and (11) we chose as the interpolation function:

$$f(\rho) = \sum_m f_m \frac{u(\rho)}{(\rho - r_m)a_m}, \quad (38)$$

where

$$u(\rho) = \sin[\pi(\rho/h)^{1/2}]. \quad (39)$$

r_m is a zero of $u(\rho)$, a_m is a zero of its derivative, and h is the step of the quadratic mesh. The use of this scheme for Eqs. (10) and (11) leads to an algebraic eigenvalue problem, giving a non-symmetric matrix to be diagonalized in order to obtain the energy values. This selection gives an overall convergence rate which goes approximately as $\epsilon \approx 10^{(-2/3)N}$ where N is the number of truncations. The accuracy of the technique has been verified by computing the energy spectrum of the 2D Hydrogen atom^{14–16} and reproducing the analytic results obtained by Taut¹⁷ for the excited states.

Figure 1 shows the dependence of the non-relativistic energy $E - c^2$ on the magnetic field strength B . In order to compare the results with those previously reported in the literature,^{14,18} we introduce the parameter $\gamma = B/c$. Figure 1 shows that the two-term variational method gives very good results for

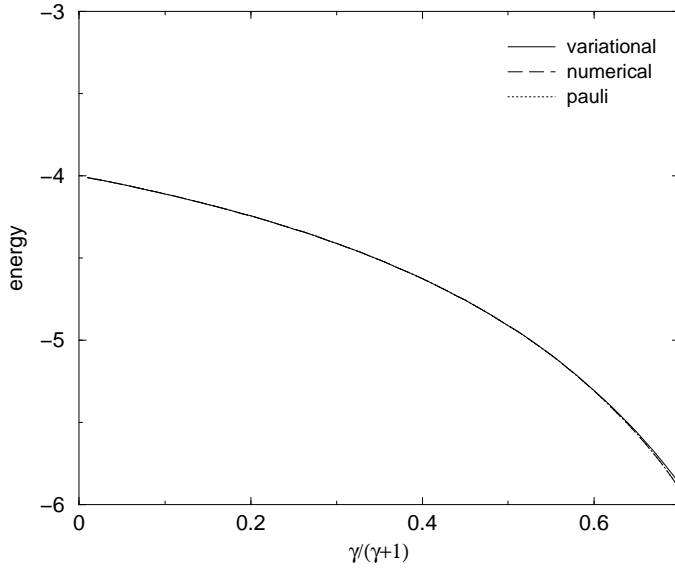


Fig. 1. Energy $E - c^2$ in atomic Rydberg units of the $1s^-$ state as a function of $\gamma' = \gamma/(\gamma+1)$. The long-dashed line is obtained by numerical methods; the solid line corresponds to the mixed-basis variational method. The dotted line is obtained by using the Pauli equation.

Table 1. Relativistic energy values $E - c^2$ in atomic Rydberg units for the s state and a comparison with the non-relativistic energy spectrum. The first column corresponds to the value obtained via the mixed-basis variational method, the second column is the numerical value relativistic energy $E - c^2$, the third column corresponds to the energy obtained after solving the Schrödinger equation, the fourth column is the energy spectrum of the Pauli equation, the fifth column (diff1) is the difference between the the first and second columns, and the sixth column (diff2) is difference between the second a fourth column.

| γ' | Variational | Numerical | Schrödinger | Pauli | diff1 | diff2 |
|-----------|--------------|--------------|-------------|--------------|--------------------------|-------------|
| 0.01 | -4.010308476 | -4.010303938 | -3.9999905 | -4.01009151 | $-4.5385 \cdot 10^{-6}$ | 0.000212427 |
| 0.05 | -4.052584016 | -4.052582214 | -3.9997404 | -4.052371979 | $-1.80165 \cdot 10^{-6}$ | 0.000210235 |
| 0.10 | -4.110158292 | -4.110161852 | -3.9988434 | -4.109954511 | $3.55978 \cdot 10^{-6}$ | 0.000207341 |
| 0.15 | -4.17375409 | -4.173760085 | -3.9970851 | -4.173555688 | $5.99508 \cdot 10^{-6}$ | 0.000204397 |
| 0.20 | -4.244337352 | -4.244360501 | -3.9941592 | -4.2441592 | $2.31488 \cdot 10^{-5}$ | 0.000201301 |
| 0.25 | -4.32313341 | -4.323172984 | -3.9896419 | -4.322975233 | $3.95743 \cdot 10^{-5}$ | 0.000197751 |
| 0.30 | -4.411646466 | -4.411703859 | -3.9829381 | -4.411509529 | $5.73929 \cdot 10^{-5}$ | 0.00019433 |
| 0.35 | -4.511776714 | -4.511854721 | -3.9732025 | -4.511664038 | $7.8007 \cdot 10^{-5}$ | 0.000190683 |
| 0.40 | -4.625971588 | -4.626065158 | -3.9592116 | -4.625878267 | $9.35697 \cdot 10^{-5}$ | 0.000186891 |
| 0.45 | -4.757387992 | -4.75752472 | -3.9391601 | -4.757341918 | 0.000136728 | 0.000182802 |
| 0.50 | -4.91019842 | -4.910498134 | -3.9103193 | -4.9103193 | 0.000299714 | 0.000178834 |
| 0.55 | -5.089955586 | -5.090843552 | -3.8684466 | -5.090668822 | 0.000887966 | 0.00017473 |
| 0.60 | -5.303980092 | -5.306876432 | -3.806706 | -5.306706 | 0.00289634 | 0.000170432 |
| 0.65 | -5.561460262 | -5.570890138 | -3.7135808 | -5.570723657 | 0.009429876 | 0.000166481 |
| 0.70 | -5.871135116 | -5.902019599 | -3.5685234 | -5.901856733 | 0.030884483 | 0.000162866 |

$\gamma' = \gamma/(\gamma + 1) < 0.7$. The non-relativistic approximation works for all values of the magnetic field strength. Table 1 shows clearly that the variational approach is better suited for small and intermediate values of γ' but the non-relativistic Pauli equation guarantees at least four figures for any value of B and gives reliable results in a range of values not restricted to values $B \ll B_{cr}$ as the semiclassical approximation.⁹

For weak magnetic fields, Ho and Khalilov⁹ have obtained approximate energy values with the help of a semiclassical method; their result, written in atomic Rydberg units, takes the form:

$$E_{sem} = 2 \left(c^2 + \frac{\gamma k_{\vartheta}^2}{2} \right) \left[1 + \frac{1}{c^2(n + \sqrt{k_{\vartheta}^2 - 1/c^2})^2} \right]^{-1/2}. \quad (40)$$

Expression (40) gives good energy estimates for $\gamma' < 0.05$. In fact, for $\gamma' = 0.05$ one obtains $E_{sem} = -4.02649$, a value slightly higher than that obtained numerically with the help of variational techniques. For strong magnetic fields, the authors obtain recursion relations that determine the coefficients of the series expansion of the wave function, the possible energies, and the magnetic fields, showing that the two-dimensional Dirac electron in the presence of an homogeneous magnetic field is a quasi-exactly solvable problem. Unfortunately, just as in the non-relativistic¹⁷ and Klein–Gordon¹⁵ cases, the quasi-exactly solvable energies do not correspond to the ground state.

Since the energy spectrum for the ground state, in the pure magnetic field regime does not depend on B (28), the variational energy slightly deviates from the numerical value for strong magnetic fields. Regarding the methods and results presented in this paper, we have to emphasize that we do not require any special identification between small and large components of the Dirac spinor, a condition that is present in most of the alternative variational methods available in the literature. The electromagnetic configuration given by Eq. (3) presents the interesting feature of combining a Coulomb potential with a magnetic field in a way that makes a single trial-function approach unsuitable. The accuracy of the mixed-basis approach can be improved when one uses a many-terms basis, nevertheless this introduces higher order Q_{ij} matrices and further complications in the computation of the energy eigenvalues.

Regarding the range of validity of variational and non-relativistic approximations, both methods give very good results for values of $\gamma < 1$, which correspond, for the hydrogen atom, to $B < 2.35 \times 10^9$ G, a value that is far from the values of B that one can create in a laboratory.²⁴

However, strong fields can be mimicked in nanomaterials like GaAs or InSb with very small effective masses, where the methods and techniques of quantum effects in the presence of strong fields can be applied.²⁴ In this physical scenario the techniques developed in this paper could be of help.

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