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CONFINED DIRAC ELECTRON IN COULOMB AND UNIFORM MAGNETIC FIELDS: THE HILL DETERMINANT APPROACH

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Abstract

The 2+1 dimensional Dirac equation is solved for electron in an oscillator potential together with external fields. Approximate eigenenergies are determined from a second order recurrence relation using the Hill determinant technique. In addition the technique is shown to generate wavefunctions for the quasi-exactly solvable problem. Finite analytic closed form for the recurrence relation derived using the recursive-sum plus discrete dimensional-convolution techniques is shown to be in agreement with the analytic result from the finite Hill determinant.

1. Introduction

Recent technological advances in the microfabrication of low dimensional systems and the consequent measurement of their transport properties as well as the manipulation of their electron density with tunable gate potentials and external fields have generated lots of experimental and theoretical research interests [1]. Low dimensional systems are found to possess novel quantum effects and thus provide fertile ground for testing quantum mechanical concepts such as the Aharonov-Bohm effects, edge-state properties etc [1]. Motion of the unbound electrons in these quantum structures are restricted in one, two or three dimensions resulting to planar, linear and zero dimensional systems widely accepted to have potential applications in nanodevices like single electron transistors and nanoelectromechanical systems etc[1,2].

Theoretically, the dynamics of the confined electrons has been studied using the nonrelativistic Schroedinger equation [3,4], and more recently with low dimensional Dirac equations yielding results that do not only explain the experimental data but also guide future experimental efforts. For systems with restricted motion in one dimension the planar motion of the electrons with lateral confinement, such as in the two dimensional electron gas (2DEG) may appropriately be described by 2+1 dimensional Dirac equation. In the relativistic regime the energies and wavefunction of the electrons in a confining oscillator potential in the presence of uniform magnetic field perpendicular to the plane has been studied [5,6]. The dynamics of the electrons with respect to varying strength of the confining interaction was discussed. The quasi-exact solution of the combined effect of an external Coulomb potential together with only the constant magnetic field perpendicular to the plane containing the electron has also been studied[7,8]. In graphene quantum dots (QDs) the possibility of electrostatic and non-homogenous magnetic confinement of the Dirac fermions which avoids the problem of Klein tunnelling in graphene have been investigated[9,10]. The electrostatically confined graphene QDs in external magnetic field has been shown to generate important controllable physical properties that may be exploited in the development of future miniaturised devices [11]. Similar consideration of the elecronic properties of QDs with defects also shows that the energy levels can be controlled by the QDs geometrical parameters and by the uniform field strength [12].

In this work the problem of a confined particle in a parabolic interaction in the presence of a constant magnetic field and a Coulomb potential was considered. Rather than solving the problem by adding the oscillator interaction as a Lorentz scalar we use the minimally coupled Dirac oscillator approach. The 2+1 dimensional Dirac-oscillator in the presence of the external fields was then solved using the series expansion of the wavefunction. The resulting recurrence relation from the first order coupled Dirac equations belongs to the newly discovered class of quasi-exactly solvable problem in which a general solution for the eigenvalue and state wavefunctions are difficult to construct in closed form [3,7,8,13]. The Hill determinant technique [14,15] was used to solve for a more general approximate eigenvalue equation. In addition, and contrary to the popular opinion in the Literatures, we present finite expressions for the coefficients of the wavefunctions of the Dirac problem. An appropriate finite and compact analytic form for the coefficients of the wavefunctions was further constructed using the results of [16]derived from a combination of recursive-sum technique with discrete dimensional-convolution procedure.

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2. Theoretical Formalism

The minimally coupled Dirac Hamiltonian in 2+1 dimension with $\hbar = c = 1$is

$$[\gamma^{\mu}(i\partial_{\mu} - eA_{\mu}) - m]\Psi = 0, \quad (1)$$

where$A_{\mu} = (A_0, \boldsymbol{A})$ represents the external potentials, e and m are respectively the electric charge and rest mass of an electron. The Dirac matrices $\gamma^{\mu} = (\gamma^0, \gamma^i), i = 1,2$is taken to satisfy the algebra

$$\{\gamma^{\nu}, \gamma^{\mu}\} = 2g^{\nu,\mu} \quad (2)$$

with the metric defined as $g^{\nu,\mu} = diag(+1,-1,-1)$for $\nu,\mu = 0,1,2$ so that $\gamma^0 = \beta$and $\boldsymbol{\alpha} = \beta\vec{\gamma}$. Eq. (1) may therefore be recastedinto the form

$$i\frac{\partial}{\partial t}\Psi = [\boldsymbol{\alpha}\cdot\boldsymbol{p} + e\boldsymbol{\alpha}\cdot\boldsymbol{A} + \beta m + eA_0]\Psi, \quad (3)$$

where$\boldsymbol{p}$is the momentum operator. Introducing the nonminimal coupling $\boldsymbol{p} \to \boldsymbol{p} - im\omega\beta\boldsymbol{r}$in Eq. (3) gives [5,6]

$$i\frac{\partial}{\partial t}\Psi = [\boldsymbol{\alpha}\cdot\boldsymbol{p} - im\omega\beta\boldsymbol{\alpha}\cdot\boldsymbol{r} + e\boldsymbol{\alpha}\cdot\boldsymbol{A} + \beta m + eA_0]\Psi, \quad (4)$$

which may be written in the condensed form as

$$i\frac{\partial}{\partial t}\Psi = H\Psi, \quad (5)$$

with$H$ denoting Hamiltonian which, in the cylindrical coordinate system, is given by

$$H = -i\boldsymbol{\alpha}\cdot\hat{\boldsymbol{\rho}}(p_\rho - m\omega\beta\rho + ieA_\rho) - i\boldsymbol{\alpha}\cdot\hat{\boldsymbol{\varphi}}(p_\varphi + ieA_\varphi) + \beta m + eA_0, \quad (6)$$

where the polar coordinates (ρ,φ)has been used for the 2-D plane containing the electron so that $p_\rho = \frac{\partial}{\partial\rho}andp_\varphi = \frac{1}{\rho}\frac{\partial}{\partial\varphi}$. The scalar products $\boldsymbol{\alpha}\cdot\hat{\boldsymbol{\rho}}$and $\boldsymbol{\alpha}\cdot\hat{\boldsymbol{\varphi}}$are defined, using the Pauli matrices $\gamma^0 = \sigma_3$, $\gamma^i = i\sigma_i$and $\boldsymbol{\alpha} = i\sigma_3\sigma_i$, as

$$\boldsymbol{\alpha}\cdot\hat{\boldsymbol{\rho}} = \begin{bmatrix} 0 & ie^{-i\varphi} \\ -ie^{i\varphi} & 0 \end{bmatrix}, \boldsymbol{\alpha}\cdot\hat{\boldsymbol{\varphi}} = \begin{bmatrix} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{bmatrix},$$

and hence

$$H = \begin{bmatrix} m + eA_0 & e^{-i\varphi}(p_\rho + m\omega\rho + ieA_\rho - ip_\varphi + eA_\varphi) \\ -e^{i\varphi}(p_\rho - m\omega\rho + ieA_\rho + ip_\varphi - eA_\varphi) & -m + eA_0 \end{bmatrix}. \quad (7)$$

For$\varphi = 0$ the scalar products $\boldsymbol{\alpha}\cdot\hat{\boldsymbol{\rho}} = -\sigma_2and\boldsymbol{\alpha}\cdot\hat{\boldsymbol{\varphi}} = \sigma_1$. Hence the spinor equation (5) reduces to the form

$$i\frac{\partial}{\partial t}\Psi = [i\sigma_2(p_\rho - m\omega\beta\rho + ieA_\rho) - i\sigma_1(p_\varphi + ieA_\varphi) + \beta m + eA_0]\Psi \quad (8)$$

with Ψ being a time-dependent two components wavefunction in consistent with earlier works [5, 6]. Introducing the Coulomb potential$eA_0 = \frac{k}{\rho}$ and the vector potential $\boldsymbol{A} = \frac{1}{2}\boldsymbol{B}\times\boldsymbol{r}$with components

$$A_\rho = 0, \quad A_\varphi = \frac{1}{2}B\rho \quad (9)$$

for uniform magnetic field$\boldsymbol{B} = B\hat{k}$perpendicular to the plane containing the particle the equation of motion for the system reduces to the matrix form

$$\begin{bmatrix} m + eA_0 - E & e^{-i\varphi}(p_\rho + m\omega\rho - ip_\varphi + eB\rho/2) \\ -e^{i\varphi}(p_\rho - m\omega\rho + ip_\varphi - eB\rho/2) & -m + eA_0 - E \end{bmatrix}\begin{bmatrix}\psi_1(\rho,\varphi) \\ \psi_2(\rho,\varphi)\end{bmatrix} = 0, \quad (10)$$

where$E$is the energy eigenvalue and the time-dependent wavefunction is defined as $\Psi(\rho,\varphi,t) = \psi(\rho,\varphi)e^{-iEt}$with the stationary solution taken as a two components spinor[7, 5, 17].

$$\psi(\rho,\varphi) = \begin{bmatrix}\psi_1(\rho,\varphi) \\ \psi_2(\rho,\varphi)\end{bmatrix}.$$

Defining$\psi_1(\rho,\varphi) = \rho^{-1/2}G_j(\rho)e^{i(j-1/2)\varphi}$ and $\psi_2(\rho,\varphi) = \rho^{-1/2}F_j(\rho)e^{i(j+1/2)\varphi}$for the upper and lower components, with $j = \pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}$ ….., and the total angular momentum$j \pm \frac{1}{2}$, Eq. (10) reduces to the following coupled radial equations

$$\frac{dF_j}{d\rho} + \frac{j}{\rho}F_j + Q\rho F_j = \left(E - m - \frac{k}{\rho}\right)G_j \quad (11)$$

$$-\frac{dG_j}{d\rho} + \frac{j}{\rho}G_j + Q\rho G_j = (E + m - \frac{k}{\rho})F_j \quad (12)$$

The symbol $Q = m(\omega + \omega_c)$ and $\omega_c = \frac{eB}{2m}$is the cyclotron frequency. In the limit $\rho \to \infty$ the coupled equations reduce to the nonrelativistic harmonic oscillator equation

$$F_j'' + (\lambda^2 - Q^2\rho^2)F_j = 0 \quad (13)$$

where$\lambda^2 = E^2 - m^2 + Q$ so that$F_j \sim e^{-Q\rho^2/2}$. For $\rho \to 0$, the coupled equations reduce to the form

$$F_j'' + \frac{1}{\rho}F_j' + \frac{\tau^2}{\rho^2}F_j = 0 \tag{14}$$

where $\tau^2 = j^2 - k^2$ with solution of the form $F_j \sim \rho^\tau$. Combining the asymptotic solutions together with the series expansions gives the following ansatzs

$$F_j = \rho^\tau e^{-Q\rho^2/2}\sum_{l=0}^{\infty} a_l\rho^l \tag{15}$$

$$G_j = \rho^\tau e^{-Q\rho^2/2}\sum_{l=0}^{\infty} b_l\rho^l \tag{16}$$

which upon substitution in Eqs (11) and (12) gives the recurrence relations

$$(\tau + j)a_0 = -kb_0 \tag{17}$$

$$(\tau + j + 1)a_1 + kb_1 = (E - m)b_0 \tag{18}$$

$$(\tau + j + n + 1)a_{n+1} + kb_{n+1} = (E - m)b_n;\ n \geq 1 \tag{19}$$

and

$$(\tau - j)b_0 = ka_0 \tag{20}$$

$$(\tau - j + 1)b_1 - ka_1 = -(E + m)a_0 \tag{21}$$

$$(\tau - j + n + 1)b_{n+1} - ka_{n+1} = 2Qb_{n-1} - (E + m)a_n;\ n \geq 1 \tag{22}$$

Note that Eq. (18) is derived from Eq. (19) using $n = 0$. Eliminating b_0 from Eq. (18) using Eq. (17) and combining the resulting equation with Eq. (21) to eliminate b_1 gives

$$a_1 = \frac{k^2(E+m) - (\tau + j - k^2)(E - m)}{k(2\tau + 1)}a_0 \tag{23}$$

Similarly b_1 may be expressed in terms of b_0 by using Eq. (18) together with the equation obtained by eliminating a_0 from Eqs. (20) and (21) as

$$b_1 = \frac{k^2(E-m) - (\tau - j - k^2)(E + m)}{k(2\tau + 1)}b_0 \tag{24}$$

Thus for the case $a_0 \neq 0$ ($b_0 \neq 0$) and $a_1 = 0$($b_1 = 0$) corresponding to the case $n = 0$ the eigenvalue

$$E = \frac{m(\tau \pm j)}{j \pm \tau \mp 2k^2} \tag{25}$$

is seen to depend on the Coulomb factor with no explicit contribution from both the magnetic field and the confining interaction suggesting $b_{-i} = 0$ ($i = 1,2\cdots$). We next eliminate a_{n+1} and a_n (with $n \to (n-1)$) from Eq. (22) using Eq. (19) to deduce the recurrence relation for the coefficients valid for $n \geq 1$

$$\frac{(n+1)(2\tau + n + 1)}{D_n + 1}b_{n+1} = \left[\frac{k(E+m)}{D_n} + \frac{k(E-m)}{D_n + 1}\right]b_n + \left[2Q - \frac{E^2 - m^2}{D_n}\right]b_{n-1} \tag{26}$$

where $D_n = \tau + j + n$. The three-term recurrence relation is a characteristic of quasi-exactly solvable problem whose complex nature does not permit complete analytical solution as is common for physical problems leading to two-term recurrence relation. Therefore rather than solve for the complete spectrum together with a closed analytic form for the wavefunction only parts of the eigenvalue and the corresponding eigenstates are possible. However once the solution for the expansion coefficients b_n is achieved the solution for the coefficients a_n follows easily from Eq. (19).

For the case $b_{n+1} = 0$ in which the series is assumed to terminate at a particular $n \geq 1$, the coefficients of b_n and b_{n-1} may trivially be taken to be identically zero thus giving the energies

$$E = m \pm \sqrt{-2Q(\tau + j + n + 1)} \tag{27a}$$

$$E = -m \pm \sqrt{\frac{-2Q(\tau + j + n)^2}{(\tau + j + n + 1)}} \tag{27b}$$

when solved simultaneously for the energy E, where $Q = m(\omega_c + \omega)$. The eigenvalues in Eq. (27) are seen to be complex valued corresponding to the possible existence of a quasibound state. This is an important phenomenon suggesting that the confined particle may be trapped for a finite lifetime.

For an exact solution the second-order recurrence relation may be solved using the continued fraction or the Hill determinant approach [14, 15, 18]. The latter which is more mathematically tractable, especially in the lowest order approximations, has been successfully used to yield global analytical or numerical eigenvalues for nonrelativistic anharmonic oscillator problems [15,18,19,20]. Contrary to the misconceptions about the technique its validity had been supported with rigorous mathematical proofs requiring the imposition of the necessary physical conditions to yield the correct eigenvalues [21, 22].

The nonperturbative Hill determinant technique was used to deduce the approximate eigenvalues. Whether this technique is suitable for the present relativistic problem will be justified a posteriori by the degree of its agreement with known results within an appropriate limit. Rewriting Eq. (26) in the form

$$f_n b_{n+1} - g_n b_n - h_n b_{n-1} = 0, \tag{28}$$

where the coefficients

$$f_n = (n+1)(\tau+j+n)(2\tau+n+1) \quad (29)$$
$$g_n = [Ek(2\tau+2j+2n+1)+km] \quad (30)$$
$$h_n = (\tau+j+n+1)[2Q(\tau+j+n)+m^2-E^2] \quad (31)$$

for $n \geq 1$ generate consistenly[20], by taking the recurrence relation as an infinite set of linear equations in b_n, the matrix elements of the infinite dimensional Hill determinant $\Delta(E)$. The eigenvalues may thenbe taken as the characteristic roots of the determinant $\Delta(E) = 0$. In practice the approximate analytic eigenenergies ($E_n^{(\kappa)}$)are obtained from the roots of $(2\kappa+1) \times (2\kappa+1)$ finite dimensional approximant $\Delta^{(\kappa)}(E)$ of the Hill determinant $\Delta(E)$. Following [15]the first-order $\Delta^{(1)}(E)$approximant from a 3 × 3 matrix constructed around the central term $b_n$was obtained as

$$\Delta^{(1)}(E) = \begin{vmatrix} 2E_n^{(0)}\mathrm{k} & f_{n-1} & 0 \\ -h_n & -g_n & f_n \\ 0 & -h_{n+1} & -2E_n^{(0)}\mathrm{k} \end{vmatrix}, \quad (32)$$

where the zeroth-order energy

$$E_n^{(0)} = \frac{-m}{2(\tau+j+n)+1}, \quad (33)$$

corresponding to the root of $\Delta^{(0)}(E) = 0$ (i.e. the zeros of the central term g_n) has been used in the diagonal terms except in the central term. The purpose of which is to simplify the resulting cubic equation which would otherwise have been obtained withoutusingthe $E_n^{(0)}$. The appearance of the energy E in the non-diagonal matrix elements h_i ($i = n,n+1$) is an uncommon feature characterising the relativistic Dirac problem.The explicit approximate energy $E_n^{(1)}$ obtained from the solution of $\Delta^{(1)}(E) = 0$ is given by

$$E_n^{(1)} = \frac{-mk^2 \pm \sqrt{m^2k^4 + f_{nn}\left[m^2 f_{nn} + 2QD_n f_{nn} + 2Qf_n D_{n+2} + 2E_n^{(0)} mk^2\right]}}{f_{nn}}, \quad (34)$$

where$f_{nn} = f_n D_{n+2} - f_{n-1}D_{n+1}$and recall that $D_n = \tau + j + n$. Higher order approximants representing results with improved accuracy may similarly be deduced by using larger matrix sizes. In the limit $k \to 0$ and $\tau = \pm j$the zeroth and first order approximate eigenenergies reduce to

$$E_n^{(0)} = \begin{cases} \dfrac{-m}{2(2j+n)+1}, & \tau = +j \\ \dfrac{-m}{2n+1}, & \tau = -j, \end{cases} \quad (35)$$

and

$$E_n^{(1)} = \pm m\sqrt{1 + \frac{2Q}{m^2}\left(2j + n + (n+1)\frac{2j+n+2}{2j+4n+2}\right)}, \quad for \quad \tau = +j \quad (36)$$

$$E_n^{(1)} = \pm m\sqrt{1 + \frac{2Q}{m^2}\left(n + (n+2)\frac{n-2j+1}{4n-6j+2}\right)}, \quad for \ \tau = -j \quad (37)$$

respectively. As can be seen Eq. (34) yields the rich spectra in the form of Eqs. (36) and (37) which approximates the well-known expression for the energies [6]in the absence of the Coulomb interaction. Similarly in the absence of the parabolic interaction and the magnetic field ($Q \to 0$), Eq. (34) reduces to the form

$$E_n^{(1)} = \frac{-mk^2}{f_{nn}} \pm m\sqrt{\left(\frac{k^2}{f_{nn}}\right)^2 - \frac{k^2}{D_n + \frac{1}{2}} + 1}, \quad (38)$$

which does not immediately reflect the expected spectrum [7] for electron in the Coulomb potential. It is however possible to show the extent of agreement with the standard form via a simple algebraic manipulation of both the Eq. (38) and the eigenvalue equation for the electron in the Coulomb field.

With known eigenvalue E the Hill determinant technique provides also an analytic expression for the expansion coefficients $b_n$in the form of a determinant, and from which the required solution follows most easily. Following [15]the determinant of an infinite tridiagonal matrix Δ_n was constructed by rewriting Eq. (28) as

$$b_{n+1} - A_n b_n - B_n b_{n-1} = 0 \quad (39)$$

where$A_n = \frac{g_n}{f_n}$and$B_n = \frac{h_n}{f_n}$. The determinant $\Delta_n$given by

$$\Delta_n = \begin{vmatrix} -A_0 & 1 & 0 & 0 & 0 & \cdot & \cdot \\ -B_1 & -A_1 & 1 & 0 & 0 & \cdot & \cdot \\ 0 & -B_2 & -A_2 & 1 & 0 & \cdot & \vdots \\ 0 & 0 & -B_3 & -A_3 & 1 & 0 & \vdots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \vdots & \vdots & \vdots & \vdots & \cdots & -A_n \end{vmatrix}, \qquad (40)$$

may then be used to evaluate the expansion coefficients up to any desired *n*th order by an appropriate truncation of the determinant and using the relation $b_n = (-1^n)\Delta_n$. This gives the first few coefficients

$$b_0 = 1 \qquad (41)$$

$$b_1 = A_0 \qquad (42)$$

$$b_2 = A_0A_1 + B_1 \qquad (43)$$

$$b_3 = A_0A_1A_2 + A_2B_1 + A_0B_2 \qquad (44)$$

$$b_4 = A_3(A_0A_1A_2 + A_2B_1 + A_0B_2) + B_3(A_0A_1 + B_1) \qquad (45)$$

which may then be used in Eq. (16) to express the solution of the wavefunction. The exact finite solution of the second order recurrence relation (Eq. (26)) may thus be expressed in the form [16]

$$b_{n+1} = \prod_{i=0}^{n} A_i \cdot \left[1 + \sum_{p=1}^{[\![\frac{n+1}{2}]\!]} \sum_{q=1}^{Q_n} \prod_{s=1}^{p} \left[d_{t(s,n)} \cdot \Theta\big(t(s,n) - t(s-1,n) - 2\big) \right] \right], \qquad n \geq 1 \quad (46)$$

where the index $Q_n = \frac{n!!(n-2p+2)}{(n-2p+2)!!}$, $d_t = B_t/A_tA_{t-1}$, $\Theta(x)$ is the heaviside function defined as

$$\Theta(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0, \end{cases} \qquad (47)$$

and $t(s,n) = 1 + [\![(n-2p+2s)\{(q-1)/\prod_{j=1}^{s}(n-2p+2j)\}]\!]$ with $t(0,n) = -1$.

The symbols $\{x\} = x - \lfloor x \rfloor$ and $[\![x]\!] = \lfloor x \rfloor$, with the Gauss notation $\lfloor x \rfloor$ being the greatest integer less than or equal to *x*. The corresponding coefficients b_0 and b_1 may be inferred by comparing the b_2 obtained from Eqs. (39) and (46). Remarkably this finite analytic form generates the same coefficients as those found from the Hill determinant technique.

3. Conclusion

Manipulation of the transport properties of charged particles using external fields is a well known standard procedure. Studies have shown that the applications of external magnetic and electric potentials to confined charged particles in nanomaterials generate novel material properties which requires detail experimental and theoretical investigations. In this paper we provide the analytic solution of low dimensional Dirac problem involving the parabolic potential in the presence of Coulomb potential and perpendicular magnetic field. The series expansions of the upper and lower Dirac wavefunctions were used to generate a three term recurrence relation. We obtained the $n = 0$ energy for the system and showed the possible quasibound eigenenergies associated with the system. We also present the energy equation giving an estimate of the possible lifetime for trapped electron in the given configuration. The application of the Hill determinant procedure to the second order recurrence relation is shown to generate novel and more general expressions for the wavefunctions and the eigenenergies. Finally we express the recurrence relation coefficients in a finite closed-form, contrary to the general belief in the Literatures, which agrees with the result obtained from the finite tridiagonal Hill determinant.

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