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Solutions to the N-dimensional radial Schrödinger equation for the potential $ar^2 + br - c/r$

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Abstract. Approximate solutions to the N-dimensional radial Schrödinger equation for the potential $ar^2 + br - c/r$ are obtained by employing the formulation described in Ciftci *et al*, *J. Phys. A* **43**, 415206 (2010). The problem, for some special cases, is solved numerically. Using this analysis, the energy spectra of a two-dimensional two-electron quantum dot (QD) in a magnetic field are also obtained. The results of this study are in good agreement with the other studies.

Keywords. N-dimensional radial Schrödinger equation; Coulomb perturbed potential; eigenvalue; eigenfunction; quantum dot.

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1. Introduction

Since its discovery, the radial Schrödinger equation (SE) has been playing a crucial role in devising well-behaved physical models in different branches of physics. It is possible to solve the SE with available tools to get an insight of the underlying dynamics of a physical system provided the form of interaction potential amongst the constituents of the system is known precisely. So depending upon the nature of interactions, there exists various types of interaction potentials. But the solutions of the SE cannot be found exactly for all types of interaction potentials. In fact, the SE can be solved exactly only for a few relatively simpler interaction potentials like hydrogen atom and harmonic oscillator potentials.

In the past, for obtaining the exact or approximate solutions of the SE for various interaction potentials [1–5], a number of analytic and numerical formulations such as the shifted $1/N$ expansion method [6], supersymmetric quantum mechanics [7], the WKB approximation [8], Hill determinant method [9], Nikiforov–Uvarov method [10], the asymptotic iteration method (AIM) [11] and many more [12–15] have been developed.

Here, in the present work, we consider the following interaction potential which is a combination of harmonic, linear and Coulombic potential terms:

$$U(r) = ar^2 + br - \frac{c}{r}, \quad a > 0. \tag{1}$$

The above potential is also known as Coulomb perturbed potential (CPP) and has widely been studied [16–18]. The potential (1) has played a vital role in different branches of physics such as atomic and molecular physics [19,20], particle physics [21,22], plasma physics and solid-state physics [23–25].

Recently, the solutions of the SE in N-dimensional space are reported in a number of works [26–28]. Such higher-dimensional studies of the SE are interesting from the point of view that these give us a general idea about the problem and may provide an easy route for obtaining energy spectra in lower dimensions from the generalized higher-dimensional results. Therefore, to further enhance the scope of such studies, here, we solve the SE for the potential (1) in N-dimensional space using the formulation developed in [29].

The study of quantum dots (QDs) has now become a very active research field due to their promising applications in the design and production of optoelectronic devices. In the past, many authors have used a variety of forms of the confining potentials to study the eigenvalue spectra of QDs employing different techniques [30–35]. Therefore, in view of the technological aspects of QDs, here we calculate the energy spectra of a two-dimensional two-electron QD in a magnetic field. For this pupose, we take the linear term equal to zero ($b = 0$) in eq. (1) and the resultant potential, i.e., Coulomb plus harmonic terms then acts as the confined potential for QDs.

The paper is organized as follows: The solutions of the N-dimensional radial SE for potential (1) are found analytically in §2. In §3, a special case of the given problem is studied both analytically and numerically. Section 4 consists of the study of a two-electron QD in 2D under the influence of magnetic field. Finally, the concluding remarks are presented in §5.

2. Solutions for the interaction potential (1)

The SE in N-dimensional space for the spherically symmetric potential (1) is written as

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{N-1}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+N-2)}{r^2} + \frac{2\mu}{\hbar^2}\left(E - ar^2 - br + \frac{c}{r}\right)\right]\psi(r) = 0, \tag{2}$$

where m, N and μ denote the angular momentum quantum number, dimensionality and reduced mass of the particles. E is the energy eigenvalue corresponding to the radial eigenfunctions $\psi(r)$ in an arbitrary dimensional space.

On substituting $\psi(r) = r^{-(N-1)/2}R(r)$ in the above equation, we obtain

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{4l(l+N-2)+(N-1)(N-3)}{4r^2} + \frac{2\mu}{\hbar^2}\left(E - ar^2 - br + \frac{c}{r}\right)\right]R(r) = 0. \tag{3}$$

This equation can further be written in a simplified form as

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\eta^2 - \frac{1}{4}}{r^2} + \left(\xi - a_1 r^2 - b_1 r + \frac{c_1}{r}\right)\right] R(r) = 0, \tag{4}$$

with

$$\eta = l + \frac{N-2}{2}, \quad \xi = \frac{2\mu}{\hbar^2}E, \quad a_1 = \frac{2\mu}{\hbar^2}a, \quad b_1 = \frac{2\mu}{\hbar^2}b$$

and

$$c_1 = \frac{2\mu}{\hbar^2}c.$$

An approximate solution of eq. (4) can be obtained by taking the appropriate choice of the wavefunction as

$$R(r) = \exp(-\alpha r^2 - \beta r) g(r), \tag{5}$$

where α and β are positive parameters whose values are to be determined in terms of potential parameters a, b and c. After substituting eq. (5) in eq. (4), we get

$$\begin{aligned} &r g''(r) + \left[-4\alpha r^2 - 2\beta r + (2\eta + 1)\right] g'(r) + \left[(4\alpha^2 - a_1) r^3\right. \\ &\left. + (4\alpha\beta - b_1) r^2 + (\beta^2 - 4(\eta + 1)\alpha + \xi) r + c_1 - (2\eta + 1)\beta\right] g(r) = 0. \end{aligned} \tag{6}$$

The above equation can be solved by considering $g(r) = \sum_{k=0}^{n} a_k r^k$. To this effect, we follow Theorem 5 of [29] which defines the polynomial solutions of a class of differential equations of the form

$$\begin{aligned} &(a_{3,0}x^3 + a_{3,1}x^2 + a_{3,2}x + a_{3,3})y'' \\ &+ (a_{2,0}x^2 + a_{2,1}x + a_{2,2})y' - (\tau_{1,0}x + \tau_{1,1})y = 0, \end{aligned} \tag{7}$$

where $a_{3,i}, i = 0, 1, 2, 3, a_{2,j}, j = 0, 1, 2$ and $\tau_{1,k}, k = 0, 1$ are arbitrary constant parameters.

The second-order linear differential eq. (7) has a polynomial solution of degree n if

$$\tau_{1,0} = n(n-1)a_{3,0} + n a_{2,0}, \qquad n = 0, 1, 2... \tag{8}$$

along with the vanishing of $(n+1) \times (n+1)$-determinant $\triangle_{n+1}$ given as

$$\triangle_{n+1} = \begin{vmatrix} \beta_0 & \alpha_1 & \eta_1 & & & & \\ \gamma_1 & \beta_1 & \alpha_2 & \eta_2 & & & \\ & \gamma_2 & \beta_2 & \alpha_3 & \eta_3 & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \cdot \\ & & & \gamma_{n-2} & \beta_{n-2} & \alpha_{n-1} & \eta_{n-1} \\ & & & & \gamma_{n-1} & \beta_{n-1} & \alpha_n \\ & & & & & \gamma_n & \beta_n \end{vmatrix} = 0,$$

where the entries of the above determinant are expressed in terms of the parameters of eq. (7) by

$$\begin{aligned}\beta_n &= \tau_{1,1} - n((n-1)a_{3,1} + a_{2,1}),\\ \alpha_n &= -n((n-1)a_{3,2} + a_{2,2}),\\ \gamma_n &= \tau_{1,0} - (n-1)((n-2)a_{3,0} + a_{2,0}),\\ \eta_n &= -n(n+1)a_{3,3}.\end{aligned} \tag{9}$$

Here, $\tau_{1,0}$ is established by eq. (8) for a given value of n, i.e., the degree of the polynomial solution.

Now in order to cast eq. (6) in the form of eq. (7), we take $\alpha = \sqrt{a_1/2}$ and $\beta = b_1/2\sqrt{a_1}$. Thus, using the values of α and β in eq. (6), we get

$$\begin{aligned}&r g''(r) + \left[-2\sqrt{a_1}\, r^2 - \frac{b_1}{\sqrt{a_1}}\, r + (2\eta+1)\right] g'(r)\\ &\quad + \left[\left(\frac{b_1^2}{4a_1} - 2(\eta+1)\sqrt{a_1} + \xi\right) r + c_1 - (2\eta+1)\frac{b_1}{2\sqrt{a_1}}\right] g(r)\\ &\quad = 0.\end{aligned} \tag{10}$$

So the polynomial solution of eq. (10), using eq. (8), is given as

$$\xi = 2\sqrt{a_1}(n+\eta+1) - \frac{b_1^2}{4a_1}. \tag{11}$$

The constraint conditions on the potential parameters are decided by the vanishing of the tridiagonal determinant with entries

$$\begin{aligned}\beta_n &= -c_1 + (2n+2\eta+1)\frac{b_1}{2\sqrt{a_1}},\\ \alpha_n &= -n(n+2\eta),\\ \gamma_n &= 2(n-k-1)\sqrt{a_1},\\ \eta_n &= 0,\end{aligned} \tag{12}$$

i.e., the vanishing of the $(n+1)\times(n+1)$-determinant $\triangle_{n+1}$ given by

$$\triangle_{n+1} = \begin{vmatrix} -c_1 + (2\eta+1)\frac{b_1}{2\sqrt{a_1}} & -(1+2\eta) & & & \\ -2k\sqrt{a_1} & -c_1 + (2\eta+3)\frac{b_1}{2\sqrt{a_1}} & -2(2+2\eta) & & \\ & 2(1-k)\sqrt{a_1} & -c_1 + (2\eta+5)\frac{b_1}{2\sqrt{a_1}} & -3(3+2\eta) & \\ & & \cdot & \cdot & \cdot \\ & & & \cdot & \cdot \\ & & & & \cdot \end{vmatrix} = 0,$$

where $k = n$ is fixed by the size of the determinant $\triangle_{n+1} = 0$ and represents the degree of polynomial solution of eq. (10). One can easily obtain the remaining entries of the above determinant using eq. (12).

In particular, for $n = 0$, we have $\triangle_1 = 0$, the ground state energy from eq. (11) becomes

$$\xi = 2\sqrt{a_1}(\eta+1) - \frac{b_1^2}{4a_1} \tag{13}$$

and condition on the potential parameters will be

$$c_1 = (2\eta + 1)\frac{b_1}{2\sqrt{a_1}} \tag{14}$$

when $n = 1$, i.e.,

$$\triangle_2 = \begin{vmatrix} -c_1 + (2\eta+1)\frac{b_1}{2\sqrt{a_1}} & -(1+2\eta) \\ -2\sqrt{a_1} & -c_1 + (2\eta+3)\frac{b_1}{2\sqrt{a_1}} \end{vmatrix} = 0.$$

Then, the first excited state energy becomes

$$\xi = 2\sqrt{a_1}(\eta + 2) - \frac{b_1^2}{4a_1}, \tag{15}$$

and constraint condition is written as

$$c_1^2 - 2(\eta+1)\frac{b_1}{\sqrt{a_1}}c_1 + (4\eta^2 + 8\eta + 3)\frac{b_1^2}{4a_1} - 2(1+2\eta)\sqrt{a_1} = 0. \tag{16}$$

In this way, one can obtain the complete energy spectra as well as accompanying constraint relations in the present system.

3. Special case

With a view to realize the strength and weakness of the present approach, here, we solve the problem for $n = 0$ with $\hbar = \mu = 1$. Under this condition, the analytical solution is obtained from eq. (11), after substituting $\eta = l + (N-2)/2$ and values of other variables as

$$E_{nmN} = \sqrt{\frac{a}{2}}(2l + N) - \frac{b^2}{4a}. \tag{17}$$

For this case the problem is also solved numerically. A comparison of the analytical and numerical results along with the literature results are presented in table 1.

Table 1. Lowest energy eigenvalues for $l = 0, 1, 2$ in two, three and four dimensions.

a	b	c	m	N	From eq. (17)	Numerical results	Results [16–18]
1/32	1	2	0	2	−7.750	−7.750	–
1/32	1	6	1	2	−7.500	−7.500	–
1/32	1	10	2	2	−7.250	−7.250	–
1/32	1	4	0	3	−7.625	−7.625	−7.625
1/32	1	8	1	3	−7.375	−7.375	−7.375
1/32	1	12	2	3	−7.125	−7.125	−7.125
1/32	1	6	0	4	−7.500	−7.500	−7.500
1/32	1	10	1	4	−7.250	−7.250	−7.250
1/32	1	14	2	4	−7.000	−7.000	−7.000

The values of potential parameters a, b and c conform the constraint condition (14). It is apparent that the results of the present study are in good agreement with the other studies [16–18].

4. Energy spectra of two-electron QD in a magnetic field

In last two decades or so, the quantum nanostructures, like QDs, wire, discs etc., are investigated extensively due to their prospective applications in quantum information processing [30–35]. So, in this section we develop the energy spectra of a two-electron QD of GaAs in a magnetic field within the framework of the methodology developed in §2. The corresponding Hamiltonian for the two-electron QD in a magnetic field is written as

$$H = \frac{1}{2m_e^*}\sum_{i=1}^{2}\left(p_i - \frac{e}{c}A\right)^2 + V(r_1, r_2) + H_{\text{spin}}, \tag{18}$$

with

$$V(r_1, r_2) = \sum_{i=1}^{2}\frac{1}{2}m_e^*\omega_0^2 r_i^2 + \frac{e^2}{\epsilon|r_1 - r_2|} \tag{19}$$

and

$$H_{\text{spin}} = g^*\mu_{\text{B}}(S_1 + S_2)B. \tag{20}$$

Here H_{spin}, μ_{B}, m_e, g^* and ϵ denote the Zeeman energy, the Bohr magneton, the effective mass, the effective Lande factor and the relative dielectric constant of a semiconductor, respectively.

The QD is considered as two-dimensional because the confinement in the z-direction is assumed to be much stronger than the one in the xy-plane. Let us consider the vector potential with a gauge of the form $A = \frac{1}{2}B \times r = \frac{1}{2}B(-y, x, 0)$ and ω_0 constant. The Hamiltonian then becomes

$$H = \sum_{i=1}^{2}\left(\frac{p_i^2}{2m_e^*} + \frac{1}{2}m_e^*\omega^2 r_i^2\right) + \frac{e^2}{\epsilon|r_1 - r_2|} + \frac{1}{2}\omega_c L_z + g^*\mu_{\text{B}}(S_1 + S_2)B, \tag{21}$$

with

$$\omega = \sqrt{\omega_0^2 + \frac{\omega_{\text{c}}^2}{4}} \quad \text{and} \quad \omega_{\text{c}} = \frac{eB}{cm_e^*}$$

is the cyclotron frequency and L_z is the total orbital angular momentum along z-direction. On introducing the relative and center of mass coordinates as $r = r_1 - r_2$, $R = (r_1 + r_2)/2$, eq. (21) is written in the following form:

$$H = H_{\text{cm}} + H_{\text{r}} + H_{\text{spin}}, \tag{22}$$

with

$$H_{\text{cm}} = \frac{P_{\text{cm}}^2}{2M^*} + \frac{1}{2}M^*\omega^2 R^2 + \frac{1}{2}\omega_{\text{c}} L_{z\text{cm}} \tag{23}$$

and

$$H_{\text{r}} = \frac{p_{\text{r}}^2}{2\mu^*} + \frac{1}{2}\mu^*\omega^2 r^2 + \frac{e^2}{\epsilon r} + \frac{1}{2}\omega_{\text{c}} L_z, \tag{24}$$

with $M^* = 2m_e^*$, $\mu^* = m_e^*/2$. $P_{\rm cm}$ and $p_{\rm r}$ are the momenta corresponding to the centre of mass and relative coordinates, respectively.

The total wave function for the Hamiltonian, eq. (22), can be expressed as

$$\Psi(R, r, S) = \psi_{n_1,m_1,n_2,m_2}\exp(im_1\phi)\exp(im_2\phi)\chi(s_1, s_2). \tag{25}$$

The centre of mass Hamiltonian ($H_{\rm cm}$), eq. (23), however, has well-known eigenvalues

$$E_{\rm cm}(n_1, |m_1|) = (2n_1 + |m_1| + 1)\hbar\omega + \frac{1}{2}\omega_{\rm c}m_1\hbar. \tag{26}$$

The radial SE for the Hamiltonian ($H_{\rm r}$), eq. (24), can be written as

$$\left[\frac{{\rm d}^2}{{\rm d}r^2} - \frac{m_2^2 - \frac{1}{4}}{r^2} + \left(\zeta - a_2r^2 + \frac{b_2}{r}\right)\right]R(r) = 0, \tag{27}$$

where

$$\zeta = \frac{2\mu^*}{\hbar^2}(E_{\rm r} - \frac{1}{2}\omega_{\rm c}m_2\hbar), \qquad a_2 = \frac{\mu^{*2}\omega_0^2}{\hbar^2} \quad \text{and} \quad b_2 = -\frac{2\mu^*e^2}{\epsilon\hbar^2}.$$

Note that, for $N = 2$ and $b_1 = 0$, eq. (27) has the same form as eq. (4). Therefore, following the procedure of §2, we derive the energy eigenvalues for the above equation as

$$E_{\rm r} = (n_2 + |m_2| + 1)\hbar\omega + \frac{1}{2}\omega_{\rm c}m_2\hbar. \tag{28}$$

The additional Zeeman energy corresponding to the spin of two electrons can be written directly [31] as

$$E_{\rm s} = g^*\mu_{\rm B}BS_z = \frac{\hbar\omega_0}{4}(1 - (-1)^{m_2})g^*\frac{m_e^*\omega_{\rm c}}{m_e\omega_0}. \tag{29}$$

Finally, the expression for energy eigenvalues of two-electron QD is written as $E = E_{\rm cm} + E_{\rm r} + E_{\rm s}$ as

$$\begin{aligned} E_{n_1,m_1,n_2,m_2} = {} & (2n_1 + |m_1| + n_2 + |m_2| + 2) \\ & \times\hbar\omega_0\sqrt{1 + \frac{1}{4}\left(\frac{\omega_{\rm c}}{\omega_0}\right)^2} + \frac{1}{2}\frac{\omega_{\rm c}}{\omega_0}m_1\hbar\omega_0 + \frac{1}{2}\frac{\omega_{\rm c}}{\omega_0}m_2\hbar\omega_0 \\ & + \frac{\hbar\omega_0}{4}(1 - (-1)^{m_2})g^*\frac{m_e^*\omega_{\rm c}}{m_e\omega_0}. \end{aligned} \tag{30}$$

For $n_2 = 0$, the ground-state energy becomes

$$\begin{aligned} E_{n_1,m_1,0,m_2} = {} & (2n_1 + |m_1| + |m_2| + 2) \\ & \times\hbar\omega_0\sqrt{1 + \frac{1}{4}\left(\frac{\omega_{\rm c}}{\omega_0}\right)^2} + \frac{1}{2}\frac{\omega_{\rm c}}{\omega_0}m_1\hbar\omega_0 \\ & + \frac{1}{2}\frac{\omega_{\rm c}}{\omega_0}m_2\hbar\omega_0 + \frac{\hbar\omega_0}{4}(1 - (-1)^{m_2})g^*\frac{m_e^*\omega_{\rm c}}{m_e\omega_0} \end{aligned} \tag{31}$$

and the constraints on ground state is $b_2 = 0$. This implies that in the framework of the present approach the effect of Coulomb term on this state reduces to zero and only harmonic confinement for the electrons in QD is effective.

For $n_2 = 1$, the 1st excited state energy is

$$E_{n_1,m_1,1,m_2} = (2n_1 + |m_1| + |m_2| + 3) \tag{32}$$

$$\times\hbar\omega_0\sqrt{1 + \frac{1}{4}\left(\frac{\omega_c}{\omega_0}\right)^2} + \frac{1}{2}\frac{\omega_c}{\omega_0}m_1\hbar\omega_0$$

$$+\frac{1}{2}\frac{\omega_c}{\omega_0}m_2\hbar\omega_0 + \frac{\hbar\omega_0}{4}(1 - (-1)^{m_2})g^*\frac{m_e^*\omega_c}{m_e\omega_0} \tag{33}$$

and the constraint is $b_2^2 - 2\sqrt{a_2}(2|m_2| + 1) = 0$.

Using the constraint condition, the above equation can be written in a more simplified form as

$$E_{n_1,m_1,1,m_2} = (2n_1 + |m_1| + |m_2| + 2)\hbar\omega_0\sqrt{1 + \frac{1}{4}(\gamma)^2} + \frac{1}{2}\gamma m_1\hbar\omega_0$$

$$+\frac{1}{2}\gamma m_2\hbar\omega_0 + \frac{\lambda^2}{2|m_2| + 1}\hbar\omega_0\sqrt{1 + \frac{1}{4}(\gamma)^2}$$

$$+\frac{\hbar\omega_0}{4}(1 - (-1)^{m_2})g^*\frac{m_e^*}{m_e}\gamma, \tag{34}$$

where $\lambda = e^2\alpha/\epsilon\hbar\omega_0$ is the dimensionless Coulomb correlation parameter, $\alpha = \sqrt{m_e^*\omega_0/\hbar}$ is the harmonic oscillator inverse length and $\gamma = \omega_c/\omega_0$ is the dimensionless magnetic field parameter.

In a similar way one can obtain the energy spectra for higher states along with the constraints relation of a 2D QD.

In table 2, the energy spectra of 2D QD of GaAs semiconductor is calculated using eq. (30) and some results are compared with other similar studies.

Table 2. Energy spectra of two-electron QD of GaAs. $m_e^* = 0.067m_e$, $g^* = -0.44$ and dielectric constant $\epsilon = 12.5$ in 2D in $\hbar\omega_0$ units.

n_1	n_2	m_1	m_2	γ	From eq. (30)	Variational theory [32]	Results [34]
0	0	0	0	0	2.00000	2.00000	2.00000
0	0	0	0	1	2.23607	2.23607	2.23607
0	0	0	0	2	2.82843	2.82843	2.82843
0	0	0	0	3	3.60555	3.60555	3.60555
0	0	0	0	4	4.47214	4.47214	4.47214
0	0	0	0	5	5.38516	5.38516	5.38516
1	1	0	1	2	9.45580	–	–
2	2	1	1	2	13.28252	–	–
3	3	1	1	2	20.35252	–	–
4	4	1	2	2	27.03800	–	–
4	4	2	2	2	29.45200	–	–

From the above table, we find that some of our analytical results are in good correspondence with the results of other studies.

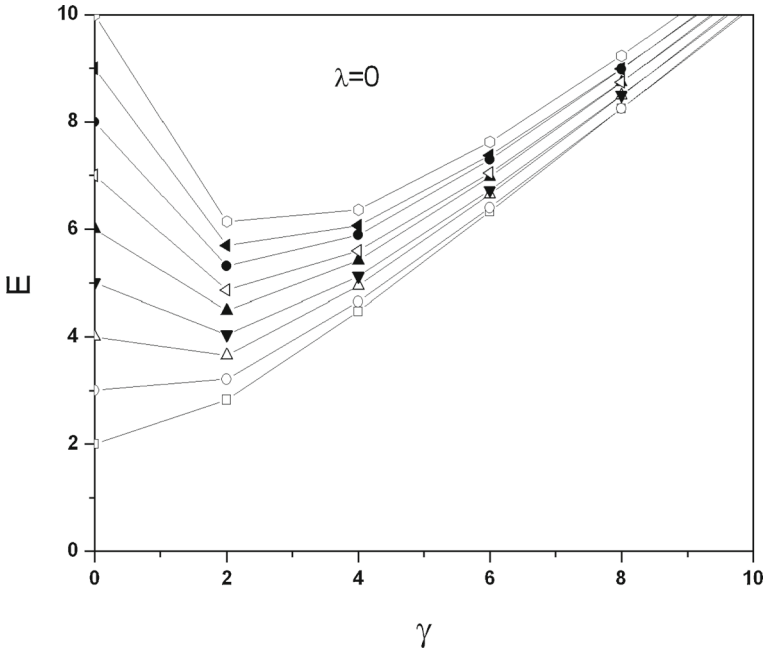

Figure 1. Variation of ground-state energy with magnetic field.

Figure 1 shows the variations of ground-state energy spectrum with magnetic field for angular momentum $m_2 \leq 0$ when both the electrons are free, i.e., there is no Coulomb interaction between them.

5. Conclusions

The quasiexact solutions to the N-dimensional radial SE for the Coulomb perturbed potential were obtained within the framework of the method of [29]. The analytical and numerical energy eigenvalues obtained in different dimensions, are in good agreement with the literature results. Energy spectra for some states in different dimensions were degenerate, and this is called interdimensional degeneracy. We have also derived the energy spectra of a two-electron GaAs QD in a magnetic field and energy spectra for this system were compared with the earlier reported works. The variation of ground-state energy with the magnetic field for different angular momentum values was studied. Some theoretical results of our study are in excellent agreement with the other experimental and theoretical studies.

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