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ARTICLE

Variational Calculations of the Exchange Energy of a Two-Electron Quantum Dot in a Magnetic Field

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Abstract: The ground-state energies of a two-electron quantum dot are calculated using the variational calculation method to solve the relative part Hamiltonian of a two-dimensional quantum dot presented in a uniform magnetic field. We have shown the dependence of the exchange energy of the two-electron quantum dot on the confining frequency and strength of the magnetic field. The transitions in the angular momentum and spin of the quantum dot ground state are also shown. Based on comparisons with different works, the variational method gives very good results.
Keywords: Quantum dots; Variational method; Magnetic field; Exchange energy.
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Introduction

Quantum dots (QDs), or artificial atoms, have been the subject of intense research studies over the past few years. The growing interest is motivated by the physical effects and potential device applications. Different experimental [1-5] and theoretical [6-31] studies have been conducted to investigate the energy spectrum and the correlation effects of the interacting electrons confined in a quantum dot in the presence of an applied uniform magnetic field. One of the most interesting features of electron correlation is the change of the spin and angular momenta structure in the ground state of the QD system in the presence of the magnetic field. The QD, in this case, has the potential to serve as a qubit of a quantum computer, since the magnetic field can be used to tune the transition in the spin of the ground state of the quantum dot from singlet (S=0) to triplet (S=1) state [28-30]. In this work, we shall use the variational method to solve the relative part Hamiltonian of a two-dimensional (2D) quantum dot under the effect of a magnetic field. We shall compare our computed results against the corresponding ones produced by different authors [29-31].

The Quantum Dot Hamiltonian

The effective-mass two-dimensional Hamiltonian for two interacting electrons confined in a quantum dot-helium by a parabolic potential in a uniform magnetic field of strength B is given as:

$$H = \left\{ \sum_{i=1}^{2} \left\{ \frac{p_i^2}{2m^*} + \frac{1}{2} m^* \left[\omega_0^2 + \frac{\omega_c^2}{4} \right] r_i^2 + \frac{\omega_c}{2} \hat{L}_{i_z} \right\} + \frac{e^2}{\kappa |\vec{r}_2 - \vec{r}_1|} \right\} ; \qquad (1)$$

where ω_0 is the confining frequency and κ is the dielectric constant for the GaAs medium. $\vec{r}_1$ and $\vec{r}_2$ describe the positions of the first and second electrons in the xy-plane. $\omega_c = \frac{eB}{m^* c}$ is the cyclotron frequency and the symmetric

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gauge $\vec{A}_i = \frac{1}{2}\vec{B} \times \vec{r}_i$ is used in Eq.(1). Upon introducing the center-of-mass (cm) $\vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{2}$ and the relative coordinates $\vec{r} = \vec{r}_1 - \vec{r}_2$, the Hamiltonian in Eq.(1) can be decoupled to a center-of-mass (H_R) and a relative (H_r) parts. The cm-part is a harmonic oscillator type with well-known eigenenergies [27, 29, 30]:

$$\left.\begin{aligned} E_{cm} &= \left(2n_{cm} + |m_{cm}| + 1\right)\hbar\left[\omega_0^2 + \frac{\omega_c^2}{4}\right]^{1/2} \\ &\quad + m_{cm}\frac{\hbar\omega_c}{2} \end{aligned}\right\}; \quad (2)$$

where $n_{cm} = 0,1,2,\ldots$ and $m_{cm} = 0 \pm 1, \pm 2, \ldots$.

The main task in this work is to solve the relative two-dimensional Hamiltonian part,

$$\left.\begin{aligned} H_r &= \frac{p^2}{2\mu} + \frac{1}{4}\left[\omega_0^2 + \frac{\omega_c^2}{4}\right]r^2 \\ &\quad + \frac{e^2}{\kappa|\vec{r}|} + m\frac{\hbar\omega_c}{2} \end{aligned}\right\} \quad (3)$$

by using the variational calculation method.

Variational Calculation Method

Dyblaski, in a recent work [31], has used successfully the variational method to study the electronic structure of the quantum dot. Encouraged by the accuracy of the variational method used in Ref. [31], we apply the variational technique to calculate the complete eigenenergy spectra of the QD Hamiltonian and the exchange energy (J) as a function of confining frequency and magnetic field strength. In this work, we adopted a one- variation parameter wave function as:

$$\psi(r) = \sqrt[4]{\alpha}\,\frac{u_m(\rho)e^{im\phi}}{\sqrt{2\pi}\,\sqrt{\rho}}; \quad (4)$$

where:

$$u_m(\rho) = \rho^{1/2+|m|}(1+\beta\rho)e^{-\left(\frac{\rho^2}{2}\right)}; \quad (5)$$

$$\rho = \sqrt{\alpha}\,r. \quad (6)$$

The first power term and the third exponential term in the wave function $u_m(\rho)$ in Eq. (5) both give the correct asymptotic behaviors as $\rho \to 0$ and $\rho \to \infty$, respectively. In addition, these states are a very good choice, because they are the eigenstates of parabolically confined electrons in a magnetic field, and the parabolic form is a successful potential model used by many authors in different works to study and explain the behavior of electronic, thermal and magnetic properties of the quantum dot.

The Schrödinger equation, with complete two-dimensional Hamiltonian form and full variational wave function can be written as:

$$\left(-\frac{\hbar^2}{m}\left(r^{-1/2}\frac{\partial^2}{\partial r^2}r^{1/2} + \frac{1}{r^2}\left(\frac{\partial^2}{\partial\phi^2} + \frac{1}{4}\right)\right) + 4\,mr^2\alpha^2 - \frac{1}{2}i\hbar\frac{\partial}{\partial\phi}\,\omega_c + \frac{e^2}{\epsilon|r|}\right)\sqrt[4]{\alpha}\,\frac{u_m(\rho)e^{im\phi}}{\sqrt{2\pi}\,\sqrt{\rho}} = E_r\,\sqrt[4]{\alpha}\,\frac{u_m(\rho)e^{im\phi}}{\sqrt{2\pi}\,\sqrt{\rho}} \quad (7)$$

In our calculations, we have used the following atomic Rydberg units:

$e^2 = 2, \hbar = 1, m = 1, \epsilon = 1$.

Finally, the relative Hamiltonian part is:

$$-2\frac{d^2}{dr^2} + 2\left(m^2 - \frac{1}{4}\right)\frac{1}{r^2} + \frac{1}{2}\omega_c m + 2r^2\alpha^2 + \frac{2}{r} \quad (8)$$

We have normalized our wave function:

$$u_m(\rho) = C_m\,\rho^{1/2+|m|}(1+\beta\rho)e^{-\left(\frac{\rho^2}{2}\right)} \quad (9)$$

by calculating the normalizing constant as:

$$C_m^2 = \frac{2\sqrt{\alpha}}{(1+\beta^2)\Gamma[1+|m|] + \beta^2|m|\Gamma[1+|m|] + 2\beta\Gamma\left[\frac{3}{2}+|m|\right]} \quad (10)$$

The above normalization constant can be expressed in terms of new parameters,

$$C_m^2 - \frac{\sqrt{\alpha}}{d + e\beta + f\beta^2}; \quad (11)$$

where:

$$d = \frac{1}{2\,\Gamma[1+|m|]}; \quad (12)$$

$$e = \Gamma\left[\frac{3}{2}+|m|\right]; \quad (13)$$

$$f = \frac{1}{2\Gamma[2+|m|]}. \quad (14)$$

We have found the energy spectra of the relative part Hamiltonian:

$$\frac{1}{2}\omega_c m+\frac{C_m^2\times 2\alpha}{\sqrt{\alpha}}\Big(\frac{1}{2}m^2\Gamma[|m|]+\frac{1}{2}|m|\Gamma[|m|]+\frac{5}{8}\beta^2|m|\Gamma[|m|]+\frac{1}{2}m^2\beta^2\Gamma[|m|]+\frac{\Gamma\left[\frac{1}{2}+|m|\right]}{2\sqrt{\alpha}}-\frac{1}{4}\beta\Gamma\left[\frac{1}{2}+|m|\right]+m^2\beta\Gamma\left[\frac{1}{2}+|m|\right]+\frac{\beta^2\Gamma\left[\frac{1}{2}+|m|\right]}{4\sqrt{\alpha}}+\frac{\beta^2|m|\Gamma\left[\frac{1}{2}+|m|\right]}{2\sqrt{\alpha}}+\frac{\beta\Gamma[1+|m|]}{\sqrt{\alpha}}-\frac{1}{8}\beta^2\Gamma[1+|m|]+\frac{1}{2}m^2\beta^2\Gamma[1+|m|]+\beta\Gamma\left[\frac{3}{2}+|m|\right]+\frac{1}{2}\Gamma[2+|m|]+\beta^2\Gamma[2+|m|]+\frac{1}{2}\beta^2|m|\Gamma[2+|m|]+\beta\Gamma\left[\frac{5}{2}+|m|\right]\Big) \tag{15}$$

The energy matrix element in Eq. (15) can be rewritten in a closed form as:

$$E_r(\beta)=-\frac{1}{2}m\omega_c+2\alpha\frac{a+b\beta+c\beta^2}{d+e\beta+f\beta^2}\ ; \tag{16}$$

where:

$$a=\frac{e}{(2|m|+1)\sqrt{\alpha}}+2f\ ; \tag{17}$$

$$b=\frac{2d}{\sqrt{\alpha}}+2(|m|+1)e\ ; \tag{18}$$

$$c=\frac{e}{2\sqrt{\alpha}}+(2|m|^2+4|m|+3)d\ . \tag{19}$$

The constants: d, e and f are as defined previously in Eqs. (12-14).

The energy eigenvalues of H_r can be obtained by minimizing the energy expression in Eq. (16) with respect to the variational parameter (β); namely,

$$\frac{\partial E}{\partial \beta}=0,\ \frac{\partial^2 E}{\partial \beta^2}>0\ . \tag{20}$$

The value of the parameter β which satisfies the minimum energy requirement is:

$$\beta_{min,m}=\frac{2cd-2af-\sqrt{(2cd-2af)^2-4(bd-ae)(ce-bf)}}{2(-ce+bf)} \tag{21}$$

So, the final energy expression in terms of the variational parameter value which satisfies the minimization condition is:

$$E_r(\beta_{min})=-\frac{1}{2}m\omega_c+2\alpha\frac{a+b\beta_{min}+c\beta_{min}^2}{d+e\beta_{min}+f\beta_{min}^2} \tag{22}$$

Having obtained the eigenenergies for the QD system for any state labeled by quantum numbers: n, m, we are able to calculate the exchange energy (J) defined as:

$$J=E_{triplet}-E_{singlet} \tag{23}$$

for any range of magnetic field strength and parabolic potential confining frequency.

2. Results and Discussion

Our computed results for 2e quantum dot are presented in Figs. 1 to 4 and Tables 1 to 3. In Fig. 1, we have displayed the computed eigenenergies of the relative part 2D-Hamiltonian for two interacting electrons at a confining frequency of $\omega_0=\frac{2}{3}R^*$ in a QD system. The figure clearly shows the transitions in the angular momentum of the ground state energy as the magnetic field increases. The origin of these transitions is due to the effect of the Coulomb interaction energy in the QD Hamiltonian. For this purpose, we have plotted, in Fig. 2, the energy spectra of two independent (zero Coulomb interaction) QDs. The figure shows no energy level crossings, and the state with $m=0$ is always the ground state.On the other hand, the ground state of the interacting electron model of the QD oscillates with the angular momentum m as we have mentioned.For example, the angular momentum changes from $m=0\ to\ m=-1\ and\ m=-2$....Since the total spin of the two electrons is $S=\frac{[1-(-1)^m]}{2}$, this leads to an exchange in the sequence of the singlet (S) and triplet (T) states. These transitions in the angular momentum of the QD system are expected to manifest themselves as cusps in the spectra of thermodynamic quantities of the QD: like heat capacity, magnetization and magnetic susceptibility [7, 9,10]. Our computed results by the present variational method are also listed in Table 1 for the sake of comparison. The underlined energy values show the angular momentum transitions of the ground state of the QD. These underlined ground state transitions agree very well with the corresponding ones shown in Fig. 1 of Ref. [31]. We have also compared, in Table 2, the present computed results against the data of Ref. [29, 30]. The tabulated results (up to six significant figures) show excellent agreement between both works. In Fig. 3, we have plotted the exchange energy (J), defined in Eq. (23), as a function of magnetic field strength (ω_c) and confining frequency: $\omega_0 = 0.4\,R^*$ (solid line —) and $\omega_0 = 0.8\,R^*$ (dashed line – – –) .

The figure clearly shows the effect of the strength of the confining frequency ω_0 on the transition of the angular momentum of the ground state energy. As the confining frequency increases, the transiton (J =0) shifts to hihger magnetic field. For example, the first transition occurs at $\omega_c = 0.35$ for $\omega_0 = 0.4$, while for $\omega_0 = 0.8$ the trasition occurs at a higher confining frequency value, $\omega_c = 0.9$. This shows that as the parabolic confinement increases, more magnetic energy is needed to make the ground state transition. In Table 3, we have listed the values of the calculated exchange energy (J) as a function of ω_c for different values of confining frequency. Furthermore, we have displayed, in Fig. 4, the singlet-triplet phase diagram ($\omega_0 - \omega_c$) of the QD showing the singlet – triplet regions separated by J=0-lines.

TABLE 1. The ground state eigenenergies, in (R^*) , calculated by using the variational method for various values of magnetic field strength (ω_c) and different angular momentum values (m=0, 1, 2, 3 and 4) of a QD system with a confining frequency, $\omega_0 = \frac{2}{3} R^*$. The underlined energy values show the angular momentum transitions of the QD ground state

	m				
ω_c	0	1	2	3	4
0.0	1.6998	2.000	2.5219	3.10835	3.7226
0.4	1.7566	1.8743	2.2218	2.6356	3.0780
0.8	1.9119	**1.8788**	2.0975	2.3876	2.7082
1.2	2.1341	1.9751	2.0992	2.3015	2.5371
1.6	2.3954	2.1286	2.1813	2.3200	2.4950
2.0	2.6708	2.3164	**2.3131**	2.4039	2.5341
2.4	2.9715	2.5246	2.4758	2.5292	2.6251
2.8	3.2702	2.7453	2.6583	2.6815	2.7502
3.2	3.5707	2.9737	2.8538	**2.8518**	2.8983
3.6	3.8714	3.2068	3.0580	3.0346	3.0624
4.0	3.2462	3.2381	3.2781	3.3348	3.4022

TABLE 2. The present ground state energies (in R^*) of QD as a function of dimensionless Coulomb coupling parameter $\lambda - \frac{e^2\alpha}{\hbar\omega}$ obtained from exact diagonlization method (second column) compared with reported work (third column) taken from Ref. [29, 30]. The parameter $\alpha = \sqrt{\frac{m\omega}{\hbar}}$ has the dimension of inverse length

λ	E(Present work)	E(Ref. [29, 30])
0	2.00000	2.00000
1	3.000969	3.00097
2	3.721433	3.72143
3	4.318718	4.31872
4	4.847800	4.84780
5	5.332238	5.33224
6	5.784291	5.78429
7	6.211285	6.21129
8	6.618042	6.61804
9	7.007949	7.00795
10	7.383507	7.38351

TABLE 3. The exchange energy (J), in meV, listed against the magnetic field strength ω_c for different QD confining frequencies: $\omega_0 = 0.4 \quad and \ 0.8 \ R^*$

ω_c	ω_0=0.4 R^*	ω_0=0.8 R^*
0.0	0.1492	0.3807
0.2	0.0558	0.2845
0.4	-0.0255	0.1959
0.6	-0.07852	0.1144
0.8	- 0.0346	0.0394
1.0	0.0009	-0.0295

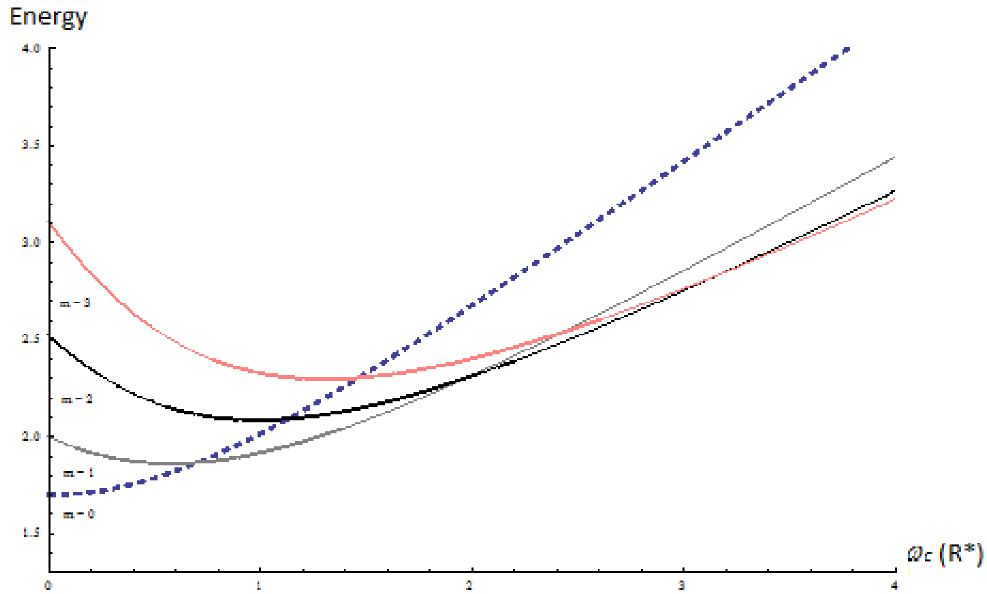

FIG. 1. The computed relative motion energy spectra (in R^*) of two interacting electrons quantum dot against the magnetic field strength ω_c ($in\ R^*$) for a confining frequency $\omega_0 = \frac{2}{3}R^*$ and an angular momentum m = 0, 1, 2 and 3.

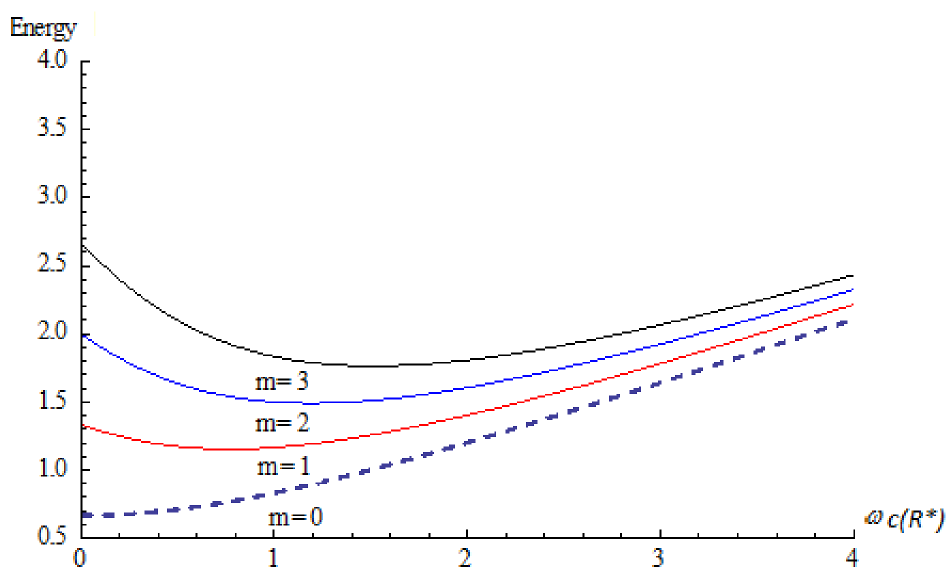

FIG. 2. The energy spectra (in R^*) of two non-interacting electrons (Coulomb=zero) in a quantum dot calculated at $\omega_0 = \frac{2}{3}R^*$ against the confining frequency ω_c ($in\ R^*$).

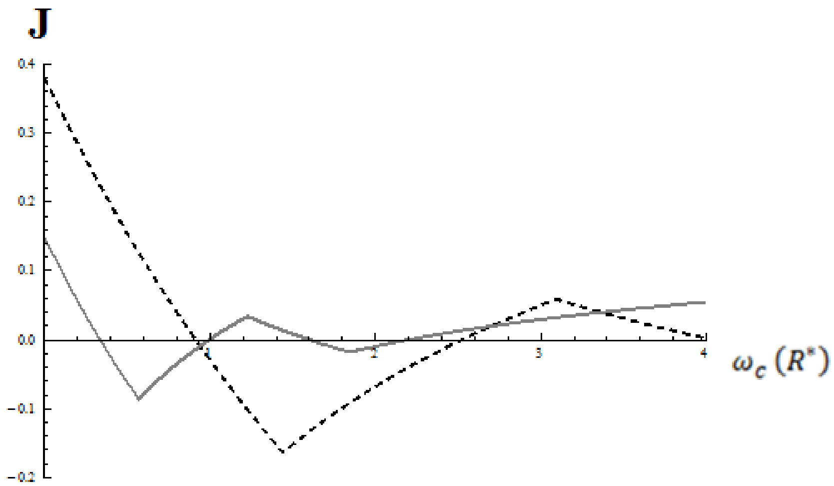

FIG. 3. The exchange energy, J, (in meV) against the magnetic field strength ω_c ($in\ R^*$) for QD confining frequencies $\omega_0 = 0.4\ R^*$ ($solid\ \ line$) and $0.8\ R^*$ ($dashed\ line$).

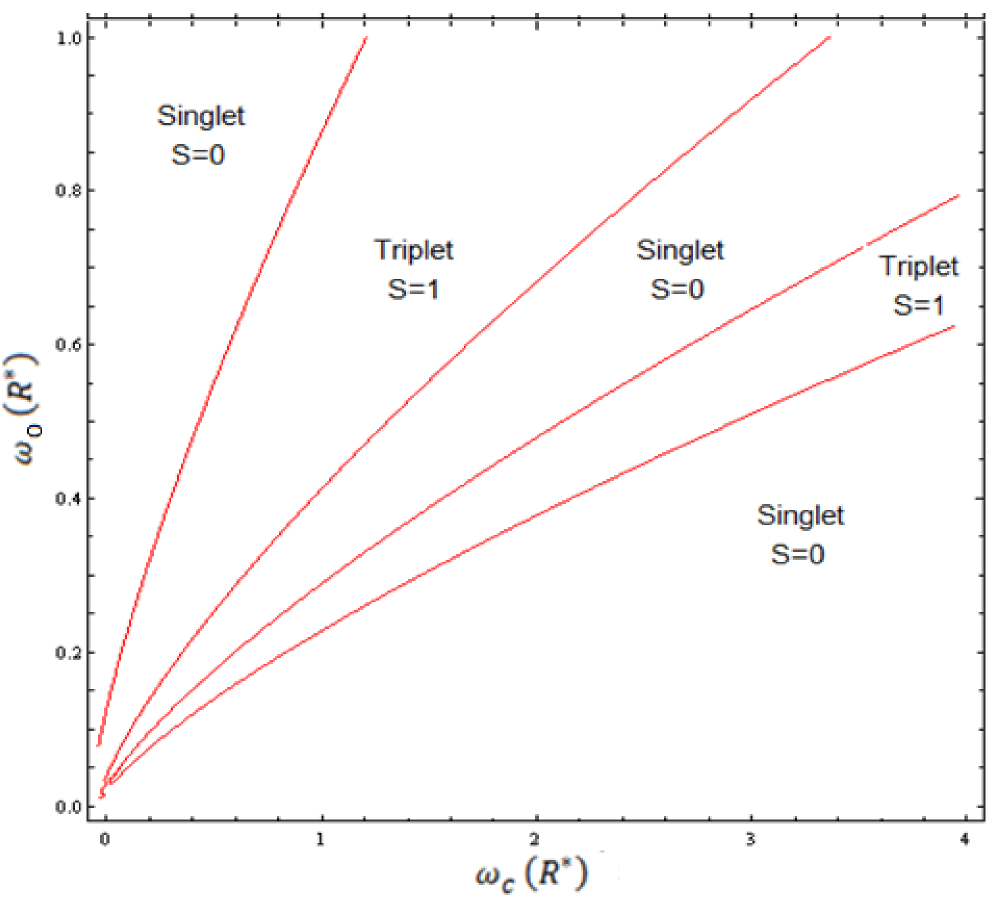

FIG. 4. The QD singlet-triplet phase diagram $(\omega_c - \omega_0)$. S=0, singlet and S=1, triplet states.

3. Conclusion

In conclusion, we have studied the ground state properties of the 2e QD in the presence of an applied uniform magnetic field. The ground state energies of the QD are calculated for various values of field strength and confining frequency. We also have shown the spin single-triplet transition in the ground state of the QD and the phase diagram. The present computed eigenenergy results, given in Figs. 1 and 2 and Tables 1 and 2 are compared with the corresponding ones in References [7, 29-31]. The comparisons give very good results for all ranges of the magnetic field strength and confining frequency of the QD system.

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