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# Energy Spectra of Three-Electron Quantum Dots*

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**Abstract** *By making use of the method of few-body physics, the energy spectra of three electrons confined by two-dimensional and three-dimensional quantum dots (QDs) are investigated. Using the present results, the size and shape effects of QDs on the spectra are revealed.*

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**Key words:** few-body physics, quantum dot, three-electron system

## I. Introduction

With recent advances in nanofabrication technology it has become possible to confine electrons in all three spatial dimensions in semiconductors called quantum dots (QDs).[1,2] These QDs are often referred to as artificial atoms in which the atomic potential is replaced by the artificial dot potential. In a typical structure the number of electrons can be well controlled and a small number $N_e$ ($N_e = 1, 2, 3, \cdots$) of electrons per dot has been achieved experimentally.[3,4] The number of electrons is increased by changing the gate voltage and charging the dot with an additional single electron. The experimental study of semiconductor QDs is expanding rapidly, and electron-electron interaction and correlation effects are shown to be of great importance in such systems.[5–7] In the meantime, a large number of theoretical investigations of electronic structures and related magnetic and optical properties in QDs have been performed to explain the experimental observations.[8–12]

Semiconductor QDs are quite idealistic quasi-zero-dimensional structures to be studied since the effective-mass theory can be applied in a proper regime of quantum size. As is well known, the study of electronic structures in quantum-well structures with and without strong magnetic fields is an important problem in semiconductor physics. Quantum wells, in fact, under strong magnetic fields can form some kinds of QDs. Therefore, the studies of electronic structures in QDs containing a few electrons are of interest both in their own right and in understanding the role of strong magnetic fields in quantum-well structures.

For QDs, two interesting idealistic models are spherical QDs in three-dimensional (3D) space and circular quantum disks in two-dimensional (2D) space which have been used by a number of authors because of the high symmetry. The previous works have investigated the three-electron systems in circular disk QDs and three-spin-polarized-electron systems in spherical QDs.[13,14] In this paper, we will further study the features of three electrons in spherical and circular QDs with parabolic potentials. The knowledge of these systems is the base for the understanding of many-electron interaction in QDs. For the single-electron or two-electron spectra of QDs, the size and shape effects have been studied and shown in detail.[15,16] In order to further show the size and shape effects of QDs on the three-electron spectra and to understand the characteristics of electron-electron interaction and correlation in confined systems, the energy levels of three electrons in 2D and 3D QDs are calculated by using the method of few-body physics. Based on the present results, the interesting phenomenon is clearly revealed.

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## II. Model and Calculation Method

Typically, the confinement potential seen by electrons in a QD is created by spatially extended charge distributions. For most QDs, a parabolic potential is a very good approximation to describe the confinement of electrons. Hence, within the effective-mass approximation, the forms of the Hamiltonian of three electrons in such parabolic 3D and 2D QDs are, respectively, as follows:

$$H_{3\mathrm{D}} = \sum_{i=1}^{3}\Big(\frac{p_i^2}{2m^*} + \frac{1}{2}m^*\omega_0^2 r_i^2\Big) + \sum_{i<j}\frac{e^2}{4\pi\epsilon_0\epsilon_r r_{ij}} \tag{1}$$

and

$$H_{2\mathrm{D}} = \sum_{i=1}^{3}\Big(\frac{p_i^2}{2m^*} + \frac{1}{2}m^*\omega_0^2 \rho_i^2\Big) + \sum_{i<j}\frac{e^2}{4\pi\epsilon_0\epsilon_r \rho_{ij}}\,, \tag{2}$$

where $\boldsymbol{r}_i$ ($\boldsymbol{\rho}_i$) is the position vector of the $i$th electron $e_i$ originated from the center of the dot; $m^*$ is the effective mass; $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$ ($\rho_{ij} = |\boldsymbol{\rho}_i - \boldsymbol{\rho}_j|$); $\omega_0$ is the strength of the confinement.

Introducing the center-of-mass (c.m.) coordinates and the Jacobi coordinates $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$, $\boldsymbol{R} = \boldsymbol{r}_3 - (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2$ ($\boldsymbol{\rho} = \boldsymbol{\rho}_1 - \boldsymbol{\rho}_2, \boldsymbol{\eta} = \boldsymbol{\rho}_3 - (\boldsymbol{\rho}_1 + \boldsymbol{\rho}_2)/2$) helps to simplify Eqs (1) and (2). The motion of the c.m. can be separated from the internal motion and thus be omitted. The Hamiltonians of the internal motion are

$$H_{3\mathrm{DI}} = \frac{p_r^2}{2\mu_r} + \frac{p_R^2}{2\mu_R} + \sum_{i<j} u(r_{ij})\,, \tag{3}$$

$$H_{2\mathrm{DI}} = \frac{p_\rho^2}{2\mu_\rho} + \frac{p_\eta^2}{2\mu_\eta} + \sum_{i<j} u(\rho_{ij}) \tag{4}$$

with

$$u(r_{ij}) = \frac{1}{6}m^*\omega_0^2 r_{ij}^2 + \frac{e^2}{4\pi\epsilon_0\epsilon_r r_{ij}}\,, \tag{5}$$

$$u(\rho_{ij}) = \frac{1}{6}m^*\omega_0^2 \rho_{ij}^2 + \frac{e^2}{4\pi\epsilon_0\epsilon_r \rho_{ij}}\,, \tag{6}$$

where $\mu_r = \mu_\rho = m^*/2$, $\mu_R = \mu_\eta = 2m^*/3$; $u(r_{ij})$ (or $u(\rho_{ij})$) is the effective pairwise interaction.

To obtain the eigen-energies and eigen-states, $H_{3\mathrm{DI}}$ is diagonalized in a model space spanned by a set of basis functions with a total orbital angular momentum $L$ ($L = \ell_1 + \ell_2$), a parity $\pi$ and a total spin $S$ as

$$\Psi_L^\pi = \tilde{A}\{[\varphi_{n_1\ell_1}(\boldsymbol{r})\varphi_{n_2\ell_2}(\boldsymbol{R})]_L \chi_s^S\}\,, \tag{7}$$

where $\chi_s^S = [(\xi(1)\xi(2))_s\xi(3)]_S$, $\varphi(\boldsymbol{r})$ is a 3D harmonic oscillator state with frequency $\omega$ ($\omega$ is considered as an adjustable variational parameter) and energy $(2n+\ell+3/2)\hbar\omega$. $\xi(i)$ is a spin state of $e_i$; the spins of $e_1$ and $e_2$ are coupled to $s$, $s$ and the spin of $e_3$ are coupled to $S$. By taking notice the fact that any permutation of particles just transforms one set of Jacobi coordinates into another, the antisymmetrization can be achieved by using the generalized Talmi–Moshinsky coefficients.

$$\tilde{A} = \frac{1}{6}(P_e - P_{12} - P_{23} - P_{13} + P_{123} + P_{132})$$

is the antisymmetrizer; when $S = 3/2$, an antisymmetrized harmonic oscillator product state with $\ell_1$ = odd can be expressed as

$$\tilde{A}\{[\varphi_{n_1\ell_1}(\boldsymbol{r})\varphi_{n_2\ell_2}(\boldsymbol{R})]_L \chi_1^{3/2}\}$$

$$= \chi_1^{3/2} \sum_{n'_1,n'_2,\ell'_1,\ell'_2} [\delta_{[K][K']} + 2B(n_1\ell_1 n_2\ell_2; n'_1\ell'_1 n'_2\ell'_2)][\varphi_{n'_1\ell'_1}(\boldsymbol{r})\varphi_{n'_2\ell'_2}(\boldsymbol{R})]_L \,, \tag{8}$$

where $[K]$ denotes a set of quantum numbers $(n_1, \ell_1, n_2, \ell_2)$ and the sum runs only over those quantum numbers fulfilling

$$2(n'_1 + n'_2) + \ell'_1 + \ell'_2 = 2(n_1 + n_2) + \ell_1 + \ell_2 \,, \tag{9}$$

$$\ell'_1 + \ell'_2 = \ell_1 + \ell_2 \,, \qquad \ell'_1 = \text{odd} \,, \tag{10}$$

$B(n_1\ell_1 n_2\ell_2; n'_1\ell'_1 n'_2\ell'_2)$ is the generalized Talmi–Moshinsky bracket for three-body systems.[17] When $S = 1/2$, an antisymmetrized wavefunction can be expressed as

$$\begin{aligned} &\tilde{A}\{[\varphi_{n_1\ell_1}(\boldsymbol{r})\varphi_{n_2\ell_2}(\boldsymbol{R})]_L \chi_s^{1/2}\} \\ &= \chi_1^{1/2} \sum_{n'_1,n'_2,\ell'_1,\ell'_2}{}' C^I(n_1\ell_1 n_2\ell_2; n'_1\ell'_1 n'_2\ell'_2)[\varphi_{n'_1\ell'_1}(\boldsymbol{r})\varphi_{n'_2\ell'_2}(\boldsymbol{R})]_L \\ &+ \chi_0^{1/2} \sum_{n'_1,n'_2,\ell'_1,\ell'_2}{}'' C^{II}(n_1\ell_1 n_2\ell_2; n'_1\ell'_1 n'_2\ell'_2)[\varphi_{n'_1\ell'_1}(\boldsymbol{r})\varphi_{n'_2\ell'_2}(\boldsymbol{R})]_L \,, \end{aligned} \tag{11}$$

where $\sum'$ denotes the sum only for $\ell'_1$ = odd, $\sum''$ denotes the sum only for $\ell'_1$ = even, and

$$C^I(n_1\ell_1 n_2\ell_2; n'_1\ell'_1 n'_2\ell'_2) = \begin{cases} \frac{1}{3}[\delta_{[K][K']} - B(n_1\ell_1 n_2\ell_2; n'_1\ell'_1 n'_2\ell'_2)] & \ell_1 = \text{odd} \,, \\ \frac{\sqrt{3}}{3} B(n_1\ell_1 n_2\ell_2; n'_1\ell'_1 n'_2\ell'_2) & \ell_1 = \text{even} \,, \end{cases} \tag{12}$$

$$C^{II}(n_1\ell_1 n_2\ell_2; n'_1\ell'_1 n'_2\ell'_2) = \begin{cases} -\frac{\sqrt{3}}{3} B(n_1\ell_1 n_2\ell_2; n'_1\ell'_1 n'_2\ell'_2) & \ell_1 = \text{odd} \,, \\ \frac{1}{3}[\delta_{[K][K']} - B(n_1\ell_1 n_2\ell_2; n'_1\ell'_1 n'_2\ell'_2)] & \ell_1 = \text{even} \,. \end{cases} \tag{13}$$

It is notable that the basis functions do not form an orthogonal set due to the antisymmetrization, hence, in practical calculation, an additional procedure of orthogonalization is needed to extract linearly independent basis functions.

It is similar for $H_{\rm 2DI}$, let $H_{\rm 2DI}$ be diagonalized in a model space spanned by the 2D antisymmetric translational-invariant basis functions

$$\tilde{\Phi}_i = \tilde{A}\{\varphi_{n_1\ell_1}(\rho)\varphi_{n_2\ell_2}(\eta)\chi_s^S\} \,, \tag{14}$$

where the subscript $i$ denotes the set of quantum numbers $\{n_1\ell_1 n_2\ell_2\}$, $\ell_1+\ell_2$ is the total orbital angular momentum $L$, $\varphi_{n_1\ell_1}$ is a 2D harmonic oscillator state with frequency $\omega$, and energy $(2n + |\ell| + 1)\hbar\omega$. The antisymmetrization is accomplished by using the 2D Talmi–Moshinsky transformation bracket.[18]

The accuracy of the solutions depends on how large the model space is. Since we are interested only in the low-lying states and in qualitative aspect, the model space adopted is neither very large to facilitate numerical calculation, nor very small to assure the qualitative accuracy. This is achieved by expending the dimension of the model space step by step; in each step the new results are compared with the previous results from a smaller space, until satisfactory convergence is achieved.

## III. Results and Discussions

In what follows the energies are in meV, and the lengths are in nm; $m^* = 0.067m_e$, and $\epsilon_r = 12.4$ are assumed (for the GaAs dot). Let the states of 2D and 3D QDs be denoted as $(L, S)$ and $(L, S, \pi)$, respectively.

**Table 1.** Quantum levels of three electrons in 2D QDs with different $\gamma$ ($\gamma = \hbar\omega_0$). The level sequences are in order of increasing magnitude. For the sake of convenience, the short notation, i.e., a, b, c, etc., is used to indicate the quantum number $(L, S)$ and to show the changes of the level order. The energy unit is meV.

| $\gamma$ | 10.0 | 1.0 | 0.01 |
|---|---|---|---|
| a: (1,1/2) | (a) 55.39 | (a) 9.300 | (b) 0.3514 |
| b: (0,3/2) | (b) 59.04 | (b) 9.334 | (a) 0.3512 |
| c: (2,1/2) | (c) 61.12 | (c) 9.596 | (c) 0.3521 |
| d: (0,1/2) | (d) 63.79 | (d) 9.997 | (f) 0.3633 |
| e: (3,3/2) | (e) 67.52 | (e) 10.118 | (d) 0.3532 |
| f: (1,3/2) | (f) 68.72 | (f) 10.342 | (h) 0.3639 |
| g: (3,1/2) | (g) 71.40 | (g) 10.600 | (i) 0.3640 |
| h: (4,1/2) | (h) 75.86 | (h) 10.650 | (e) 0.3548 |
| i: (2,3/2) | (i) 76.50 | (i) 10.796 | (g) 0.3634 |
| j: (4,3/2) | (j) 94.20 | (j) 12.217 | (j) 0.3683 |

**Table 2.** Quantum levels of three electrons in 3D QDs with different $\gamma$. The short notation, i.e., a, b, c, etc., is used to indicate the quantum number $(L, S, \pi)$ and to show the changes of the level order. The energy unit is meV.

| $\gamma$ | 10.0 | 1.0 | 0.01 |
|---|---|---|---|
| a : $(1, 1/2, -)$ | (a) 59.91 | (a) 9.470 | (a) 0.3517 |
| b : $(1, 3/2, +)$ | (b) 66.55 | (b) 9.796 | (b) 0.3520 |
| c : $(2, 1/2, +)$ | (c) 67.50 | (c) 9.963 | (c) 0.3528 |
| d : $(0, 1/2, +)$ | (d) 69.14 | (d) 10.35 | (l) 0.3630 |
| e : $(3, 3/2, -)$ | (e) 75.39 | (e) 10.44 | (e) 0.3544 |
| f : $(2, 1/2, -)$ | (f) 75.50 | (f) 10.52 | (d) 0.3537 |
| g : $(1, 3/2, -)$ | (g) 76.27 | (g) 10.77 | (m) 0.3641 |
| h : $(3, 1/2, -)$ | (h) 77.06 | (h) 10.85 | (h) 0.3565 |
| i : $(3, 1/2, +)$ | (i) 83.85 | (i) 11.13 | (f) 0.3558 |
| j : $(4, 1/2, +)$ | (j) 84.17 | (j) 11.21 | (g) 0.3564 |
| k : $(3, 3/3, +)$ | (k) 84.18 | (k) 11.27 | (i) 0.3567 |
| l : $(1, 1/2, -)$ | (l) 84.70 | (l) 11.36 | (n) 0.3641 |
| m : $(2, 3/2, +)$ | (m) 84.71 | (m) 11.37 | (o) 0.3642 |
| n : $(4, 3/2, -)$ | (n) 92.93 | (n) 11.89 | (j) 0.3583 |
| o : $(4, 1/2, -)$ | (o) 93.34 | (o) 12.00 | (k) 0.3600 |
| p : $(2, 3/2, -)$ | (p) 94.13 | (p) 12.20 | (p) 0.3668 |
| q : $(4, 3/2, +)$ | (q) 102.89 | (q) 12.89 | (q) 0.3700 |
| r : $(0, 3/2, +)$ | (r) 104.93 | (r) 13.46 | (r) 0.3891 |

We have performed numerical calculations for energy levels of three electrons in 2D and 3D QDs with $\gamma$ between 0.01 meV and 10 meV ($L \leq 4$). As shown in Tables 1 and 2, the three-electron spectra of 2D and 3D QDs vary not only in the values but also in the level ordering as $\gamma$ changes from 0.01 to 10. As illustrated in tables, an important aspect of the quantum effects is the changes of the level ordering and the level differences and then the crossover of two levels with the same or different spins can appear as $\gamma$ is less than 1.0. When $\gamma > 1.0$, the crossover of two levels does not appear. The results of Ref. [14] and this paper show that the changes of the quantum sizes do not change the level orders for the three-spin-polarized-electron ($S = 3/2$) spherical QDs. On the other hand, it is obvious that the changes of energy levels with $\gamma$ are larger for 3D QDs than those for 2D QDs. These mean that the spectra and related properties depend on not only the dot sizes and the total spin of the system but also the dot shapes.

Another notable phenomenon is that the energy level of $(0, 3/2)$ in 2D QDs is basically the lowest but the energy level of $(0, 3/2, +)$ in 3D QDs is the highest. This feature can be explained from quantum-mechanical symmetry.[8,19,20] In general, the states of a microscopic system all obey a basic principle, i.e., they do their best to lower the energy under the condition of being orthogonal with each other. To this end, two important factors should be considered, namely, the lowering of the potential energy and accordingly a pursuit of the geometric symmetry; and the lowering of the kinetic energy of internal motion and accordingly an escape from the inherent nodal lines (INL). The competition of these factors is decisive in determining the structures of quantum states and order of energy levels. The state of $L = 0$ and $S = 3/2$ in 3D QDs contains three INL so that the energy is the highest.[19,20] But, in 2D QDs, the state of $L = 0$ and $S = 3/2$ does not contain any INL so that its energy level is basically the lowest.[8]

In conclusion, we have used the method of few-body physics to calculate the relative motion of three electrons in 2D and 3D QDs with parabolic potentials. The quantum-size effects of 2D and 3D QDs on the spectra are clearly shown. The important aspect of the effects is the crossover of two levels with the same or different spins. It is found that the variation of energy levels with dot size is smaller for 2D QDs than that for 3D QDs, and the positions of crossover points of two levels with the same or different spins between 2D and 3D QDs vary with the strength of the confinement. The present results are useful to understand the optical and magnetic properties of quantum-dot materials since the shape of realistic QDs is usually between spherical and circular ones. The size and shape effects predict a possibility to observe phenomena related to electron-electron interactions in QDs.

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