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Two Interacting Electrons in a Spherical Gaussian Confining Potential Quantum Well*

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Abstract *Two-electron states of a three-dimensional spherical GaAs quantum dot (QD) with a Gaussian confining potential confinement are studied. Calculations are made by using the method of few-body physics within the effective-mass approximation. We have calculated the energy levels of single and triplet states as functions of the range and depth of the confining potential well in the spherical QDs. The same calculations performed with the parabolic approximation of the Gaussian potential lead to the results, which are qualitatively and quantitatively different.*

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Semiconductor quantum dots (QDs) are widely considered as artificial atoms, and are uniquely suited to study fundamental electron-electron interactions and quantum effects.[1,2] They are fabricated by modern semiconductor nanotechnology and possess various shapes, for example, a disk-like (cylindrical) shape[3] and a spherical shape.[4] Studies of QDs confined by different forms of external potentials have attracted the attention of both physicists and quantum chemists since the early days of quantum mechanics. The experimental study of semiconductor QDs is expanding rapidly,[5−8] and electron-electron interaction and correlation effects are shown to be of great importance[9−11] in such systems. In the meantime, a large number of theoretical investigations[12−14] of electronic structures and related magnetic and optical properties in QDs have been performed to explain the experimental observations.

In recent years, various theoretical approaches have been employed to calculate the energy spectra of the two interacting electrons in QDs. In 1996 Zhu *et al.*[15] studied the quantum-size effects on the energy spectra of two electrons by using of the expansion in a power series. Reference [16] calculated the energy levels of a disk containing two electrons as a function of an external magnetic field. Analytic expressions are given for the energy spectrum of the two interacting electrons in a harmonic oscillator potential under a perpendicular homogeneous magnetic field by Dineykhan and Nazmitdinov.[17] In 1998 Garcia-Castelan *et al.*[18,19] studied the energies for two interacting electrons in a harmonic QD using the WKB approximation. However, most of the previous studies are concerned with two-electron systems in a two-dimensional parabolic potential QD which possesses infinite depth and range. It is inappropriate to describe the experimentally measured charging of the QD by the finite number of excess electrons.[20] Some experimental results suggest that the real confining potential is nonparabolic and possesses a well-like shape. When a QD is small (i.e., when its radius is comparable to the characteristic length of the variation of the lateral potential near the edge), a good approximation offers simple smooth potentials, such as a Gaussian well, $V(r) = -V_0 \exp(-r^2/2L^2)$.[21] Recently a numerical exact calculation for the energy spectra of two electrons in a finite height cylindrical QD was given by a coupled-channel method.[22] In the present letter, we extend our previous work on the two-electron dot by a two-dimensional Gaussian confining potential well[23] to the case of three-dimensional spherical (3D) QDs. This potential possesses the finite depth and range.

The Hamiltonian describing the pair of interacting electrons in a spherical QD under the confined Gaussian potential within the effective-mass approximation can be written as

$$H = \sum_{i=1,2} \Big[\frac{\vec{p}_i^{\,2}}{2m_e^*} + V(r_i) \Big] + \frac{e^2}{\epsilon r_{12}} \tag{1}$$

with

$$V(r_i) = -V_0 \exp\Big(\frac{-r_i^2}{2R^2} \Big) , \tag{2}$$

where $\vec{r}_i$ ($\vec{p}_i$) is the position vector (the momentum vector) of the i-th electron originating from the center of the dot; m_e^* is the effective mass of an electron; $r_{12} = |\vec{r}_1 - \vec{r}_2|$ is the electron-electron separation, ϵ is the effective dielectric constant of the QD, V_0 is the height of the potential well, $V_0 > 0$; and R is the range of the confinement potential, which corresponds to a radius of the QD. For $r/R \ll 1$, Gaussian potential (2) can be approximated by the parabolic potential,

$$V(r_i) = -V_0 + \gamma^2 r_i^2 , \tag{3}$$

where $\gamma^2 = V_0/2R^2$.

Throughout the present paper, we use the donor Rydberg $\mathrm{Ry}^* = m_e^* \mathrm{Ry}/\epsilon^2$ as a unit of energy, and the donor

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Bohr radius $a^* = \epsilon a_B/m_e^*$ as a unit of length, where Ry is the atomic Rydberg, a_B is the atomic Bohr radius, respectively. The Hamiltonian has spherical symmetry, which implies that the total orbital angular momentum L is a conserved quantity, i.e., a good quantum number. The total spin of two electrons, S, is also a conserved quantity. Hence, the eigenstates of the two electrons in spherical QDs can be classified according to the total orbital angular momentum and the total spin momentum of the electrons, i.e., after solving our Hamiltonian, these states can be indicated by a series of energy levels with quantum numbers (L, S). To obtain the eigenfunction and the eigenenergy associated with the two electrons in a spherical Gaussian potential QD, we diagonalize H. The exact diagonalization method consists in spanning the total Hamiltonian for a given basis and extract the lowest eigenvalues (energies) of the matrix generated. The better the basis describes the Hamiltonian, the faster the convergence will be. The most common basis chosen is the one that describes the Hamiltonian at zero order.

As we know, the two electrons obey Fermi–Dirac statistics, which means that the electronic part of the total wavefunction must be anti-symmetric, i.e., when $S = 0$ the spatial part of the electronic wavefunction must be symmetric and when $S = 1$ the spatial part of the electronic wavefunction must be anti-symmetric.

For the Gaussian confinement potential, the two-electron eigenvalue problem is not separated into center-of-mass and relative coordinates, which leads to the simple Hamiltonian for the relative motion. In order to obtain the corresponding eigenfunction and the eigenenergy, we diagonalize H in a model space spanned by the translational-invariant 3D harmonic product bases

$$\Phi^{\pi}_{[K]} = \tilde{A}\{[\phi^{\omega}_{n_1\ell_1}(\vec{r}_1)\phi^{\omega}_{n_2\ell_2}(\vec{r}_2)]_L\chi_S\}\,,$$

where $\chi_S = [\zeta(1)\zeta(2)]_S$, $\zeta(i)$ is the spin state of the i-th electron and the spins of two electrons are coupled to S, $\phi^{\omega}_{n\ell}$ is a 3D harmonic oscillator state with frequency ω (ω is considered as an adjustable variational parameter) and an energy $(2n + \ell + 3/2)\hbar\omega$, and $\tilde{A}$ is the antisymmetrizer. $[K]$ denotes the whole set of quantum numbers $(n_1, \ell_1, n_2, \ell_2)$ in brevity, $\ell_1 + \ell_2 = L$ is the total angular momentum. The angular momentum $L =$ odd if the spin $S = 1$, and $L =$ even if $S = 0$, so that the wave function is antisymmetrized. The matrix elements of H are then given by the following expressions

$$\begin{aligned}\langle\Phi_{[K]}|H|\Phi_{[K']}\rangle &= [2(n_1+n_2)+\ell_1+\ell_2+3]\hbar\omega\delta_{[K],[K']} + U^I_{n_1n_1'}\delta_{\ell_1,\ell_1'}\delta_{n_2,n_2'}\delta_{\ell_2,\ell_2'}\\ &\quad + U^I_{n_2n_2'}\delta_{\ell_1,\ell_1'}\delta_{n_1,n_1'}\delta_{\ell_2,\ell_2'} + \sum_{[K''][K''']} B_{[K][K'']}B_{[K'][K''']}U^{II}_{n_1''n_1'''}\delta_{n_2'',n_2'''}\delta_{\ell_1,\ell_1'}\delta_{\ell_2,\ell_2'} \qquad (4)\end{aligned}$$

with

$$U^I_{nn'} = \int_0^{\infty} R_{n\ell}(r)\Big[-V_0\exp(-r^2/2R^2) - \frac{1}{2}m_e^*\omega^2r^2\Big]R_{n'\ell}(r)r^2\,\mathrm{d}r\,, \qquad (5)$$

$$U^{II}_{nn'} = \int_0^{\infty} R_{n\ell}(r)\frac{e^2}{\epsilon r}R_{n'\ell}(r)r^2\,\mathrm{d}r\,, \qquad (6)$$

$$B_{[K][K']} = \int \Phi_{[K]}(\vec{r}_1,\vec{r}_2)\Phi_{[K']}(\vec{r}_1',\vec{r}_2')\,\mathrm{d}^3\vec{r}_1\,\mathrm{d}^3\vec{r}_2\,, \qquad (7)$$

where $R_{n\ell}(r)$ is the radial part of 3D harmonic oscillator function, $B_{[K][K']}$ is the transformation bracket of 3D harmonic product states with two different sets of coordinates, which allows us to reduce the otherwise multi-integral into single-integral. Nonvanishing $B_{[K][K']}$ occurs only when both the states $\Phi_{[K]}(\vec{r}_1,\vec{r}_2)$ and $\Phi_{[K']}(\vec{r}_1',\vec{r}_2')$ have exactly the same eigenenergy and eigenangular momentum. Analytical expression for $B_{[K][K']}$ has already been derived in Ref. [24]. The set of canonical coordinates $(\vec{r}_1', \vec{r}_2')$ are defined by $\vec{r}_1' = \vec{r}_1 - \vec{r}_2$, $\vec{r}_2' = (\vec{r}_1 - \vec{r}_2)/2$. The dimension of the model space is constrained by $0 \le N = 2(n_1 + n_2) + \ell_1 + \ell_2 \le 26$. If N is increased by 2, the ratio of the difference in energy is less than 0.01%.

Our numerical computation is carried out for one of the typical semiconducting materials, GaAs, as an example with the material parameters shown in the following: $\epsilon = 12.4$, and $m_e^* = 0.067m_e$, where m_e is the single electron bare mass. The potential-well depth is taken to be $V_0 = 5.0\mathrm{Ry}^*$ corresponding to the GaAs QDs, for which $\mathrm{Ry}^* = 6$ meV and $a^* = 10$ nm.

We plotted in Fig. 1(a) the energy spectrum of two-electron systems confined in the 3D spherical Gaussian (solid curves) and parabolic (dashed curves) potentials as a function of the dot radius R which corresponds to the QDs with the strong and intermediate confinement, i.e., $R \le 5.0\ a^*$. The singlet and triplet states of the two-electron states with the total angular momentum $L = 0$ (S state) are denoted by ^1S and ^3S, respectively. Figure 1(a) shows that the qualitative properties of energy levels for the spherical Gaussian potential and the parabolic

potential are similar. However, the quantitative differences are also obvious. In the strong confinement case, i.e., $R \leq 2.0\ a^*$, the energies in the spherical Gaussian potential are obviously lower than those in the spherical parabolic potential. The energy difference between the spherical Gaussian potential and the spherical parabolic potential rapidly increases as the dot radius decreases. When R/a^* is larger, the calculation values of both the spherical Gaussian potential and the spherical parabolic potential are reaching consistent, i.e., only for a larger QD the parabolic can be regarded as a fairly good approximation of the nonparabolic Gaussian potential. It is obvious that the energy differences of the ground state are less than those of the excited states.

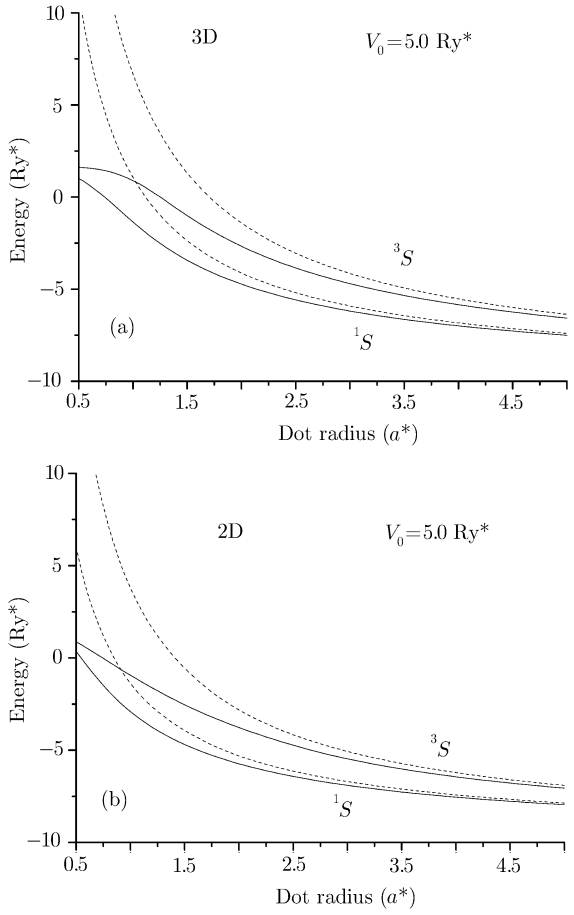

Fig. 1 Energy levels of single (^1S) and triple (^3S) states of two electrons confined in spherical Gaussian (solid curves) and parabolic (dashed curves) potential as a function of the dot radius R with $V_0 = 5.0$ Ry* for the 3D (a) and 2D (b) systems. The levels are labeled by quantum numbers ^{2S+1}L. Energy is expressed in donor Rydbergs Ry* and length in donor Bohr radii a^*.

In order to show better quantum size effects and compare with others, we plot the energy spectrum of two-electron systems confined in the 2D circular Gaussian (solid curves) and parabolic (dashed curves) potentials as a function of the dot radius R in Fig. 1(b). It is readily seen that these results are in good agreement with those of a 3D spherical QD in Fig. 1(a). However, the quantitative differences are also seen. It is obvious that the energy levels for 2D circular QDs are located slightly below the corresponding levels for the 3D spherical QDs. Hence, the electrons in 2D circular QD are easier to form bound states than those in 3D spherical QDs. The physical origin of this effect is related to the enhanced effective confinement of electrons in the 2D nanostructure. On the other hand, the energy difference between the Gaussian potential and the parabolic potential in 2D systems is also obviously lower than that in 3D systems.

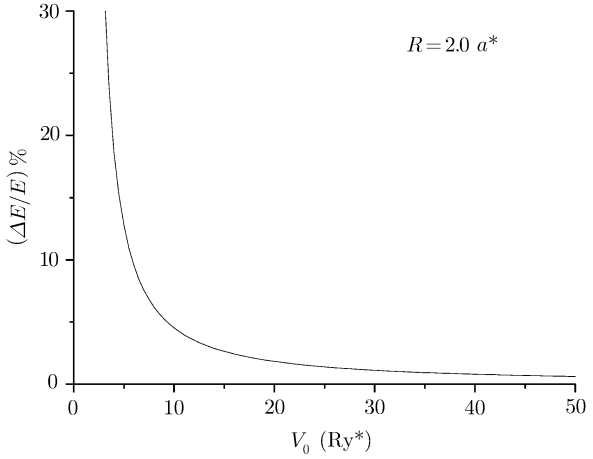

Fig. 2 Energy relative differences of the spherical Gaussian potential and the parabolic potential with the ground state as a function of the potential well depth V_0 with $R = 2.0\ a^*$. The others are the same as in Fig. 1.

Further, we took the dot radius $R = 1.5$ Ry* and plotted in Fig. 2 the energy differences both of the spherical Gaussian potential and the parabolic potential with the ground state, i.e., ^1S state, as a function of the potential depth V_0. We find that the differences of the calculation values of both the spherical Gaussian potential and the parabolic potential decrease as the potential depth increases. We note that when $V_0 \leq 10.0$ Ry* the difference rapidly increases as the potential well depth V_0 decreases. Hence, only, when $V_0 > 10.0$ Ry*, for the ground state the parabolic potential can be regarded as a fairly good approximation of the nonparabolic Gaussian potential for a larger potential depth.

In conclusion, we have applied the spherical Gaussian confining potential to a description of the two-electron systems in semiconductor spherical QDs. We have calculated the energy levels of the single and triplet states as functions of the dot radius and the potential well depth. The same calculations performed with the parabolic approximation of the spherical Gaussian potential lead to the results, which are qualitatively and quantitatively different.

The softness of the spherical Gaussian potential enables us to model the slowly varying confining potential. It may be important in the quantitative understanding of future experimental work involving two-electron systems in QDs. The present results are useful to understanding the optical and magnetic properties of QD material.

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