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A Negative Donor Center Trapped by a Spherical Quantum Dot*

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Abstract *The properties of the low-lying states of a negative donor center trapped by a spherical quantum dot, which is subjected to a parabolic potential confinement, are investigated in the absence of magnetic field. The calculations have been performed by means of the exact diagonalization of the Hamiltonian matrix within the effective-mass approximation. We find that there is only one bound state the D^- center in a spherical parabolic quantum dot in the absence of magnetic field. The binding energy of the ground state is obtained as a function of the dot size. Moreover, the critical confined potential radius value at which the negative donor center changes from unbound to bound is obtained.*

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Key words: quantum dots, donor

1 Introduction

During the last decade, the subject of a negatively charged donor (D^-) in low-dimensional systems has been studied extensively both experimentally and theoretically. A D^- center in semiconductors is an analog of a hydrogen ion (H^-) in atomic physics,[1] which is formed by a neutral donor trapping an extra electron. A D^- center is one of the simplest many-body systems that cannot be solved exactly. This system is very interesting in the study of electron-electron interaction,[2] because we can expect that one of the electrons can screen the positive ion for the other one and this would not be affected by the Coulombic interaction. On the other hand, impurities in semiconductors influence both transport and optical properties so that the topics like confined D^- centers in low-dimensional space has been extensively investigated. Since the existence of D^- centers in center-doped GaAs/Al_xGa_{1-x}As multiple quantum wells (QWs) was first reported by Huant, Najda, and Etienne[3] in 1990, many experimental[4−6] and theoretical[7−21] investigations for D^- systems in QWs, quantum dots (QDs) with and without magnetic fields have been carried out.

In order to achieve a better understanding of the dimensional characteristics of the D^- centers, a number of theoretical investigations of the D^- center in spherical QDs have been performed.[16,22−24] According to the Hill theorem,[22] the D^- center in a bulk crystal possess only one bound state with the spin-singlet configuration. However, the calculations show that there are more than one bound states in presence of a magnetic field. The binding energies of the low-lying excited states of the D^- center in QWs have also been calculated as a function of magnetic field.[7,25] Hence, in this paper, to obtain a better understanding of the features of the D^- center in a spherical QD, we will calculate the energy spectrum of the low-lying states of the D^- center in a spherical parabolic QD by using the exact diagonalization of the Hamiltonian matrix. Moreover, in the absence of magnetic field, the binding energy of the ground state and the critical confined potential radius value at which the D^- changes from unbound to bound are obtained.

2 Theoretical Framework

The D^- center in a semiconductor spherical parabolic QD can be described as a system composed of two electrons and an ionized donor located at the center of the spherical potential-well region. Within the effective mass approximation, the Hamiltonian of the system has the form

$$H = \sum_{i=1,2} \Big(\frac{p_i^2}{2m_e^*} + \frac{1}{2} m_e^* \omega_0^2 r_i^2 \Big) + V_c \tag{1}$$

with

$$V_c = \frac{e^2}{\epsilon} \Big(\frac{1}{r_{12}} - \frac{1}{r_1} - \frac{1}{r_2} \Big) , \tag{2}$$

where m_e^* is the effective mass of an electron, $\vec{p}_i$ and $\vec{r}_i$ denote the momentum and position of the i-th electron, respectively, $r_{12} = |\vec{r}_1 - \vec{r}_2|$ is the electron-electron separation, ω_0 is the strength of the confinement, and ϵ is the dielectric constant of the medium in which the electrons are moving.

Introducing the coordinates

$$\vec{\xi}_1 = \vec{r}_2 - \vec{r}_1, \quad \vec{\xi}_2 = \frac{1}{2}(\vec{r}_1 + \vec{r}_2) , \tag{3}$$

equation (1) can be rewritten as a sum of the unperturbed and the interacting part,

$$H = H_0 + V_c \tag{4}$$

with

$$H_0 = \sum_{\nu=1,2} \Big(\frac{p_\nu^2}{2\mu_\nu} + \frac{1}{2} \mu_\nu \omega_0^2 \xi_\nu^2 \Big) , \tag{5}$$

where $\mu_1 = m_e^*/2$ and $\mu_2 = 2m_e^*$.

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The Hamiltonian has spherical symmetry, which implies that the total orbital angular momentum L is a conserved quantity, i.e., the corresponding quantum number is a good one. Let $^{2S+1}L^{\pi}$ denote the quantum state because the total angular momentum L, the parity π (in the following e and o represent the even parity and odd parity, respectively), and the total spin of two electrons S are the good quantum numbers. As we know, the two electrons obey Fermi–Dirac statistics, which means that the electronic part of the total wave function must be anti-symmetric, i.e., when $S = 0$ the spatial part of the electronic wave function must be symmetric and when $S = 1$ the spatial part of the electronic wave function must be anti-symmetric. To obtain the eigenfunction and the eigenenergy associated with the D^- center in a spherical QD, we diagonalized H. The better the basis describes the Hamiltonian, the faster the convergence. The most common basis chosen is the one that describes the Hamiltonian at zero order. The Hamiltonian of the D^- center is diagonalized in model space spanned by translational invariant harmonic product states

$$\Phi^{LS\pi}_{[K]} = \sum_{[K]} \tilde{A}\{[\varphi^{\omega}_{n_1\ell_1}(\vec{\xi}_1)\varphi^{\omega}_{n_2\ell_2}(\vec{\xi}_2)]_{L\pi}\chi_S\}\,, \tag{6}$$

where

$$\chi_S = [\eta(1)\eta(2)]_S\,, \tag{7}$$

$\eta(i)$ is the spin state of the i-th electron and the spins of two electrons are coupled to S. $\varphi^{\omega}_{n\ell}$ is a three-dimensional harmonic oscillator state with a frequency ω and an energy $(2n + \ell + 3/2)\ \hbar\omega$, and $\tilde{A}$ is the antisymmetrizer. $[K]$ denotes the whole set 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 the spin $S = 0$ such that the wave function is antisymmetrized. In practice calculations, ω serves as a variational parameter to minimize the eigenvalues. Since the whole set of eigenstates of the harmonic product basis forms a complete basis in the Hilbert space, the procedure of increasing the number of linearly independent eigenstates is converging to the exact result. The limits are set only by the capacity of the computer to diagonalize $N \times N$ Hermitian matrices. On the other hand, we interested only in the low-lying states and in the qualitative aspects, the model space adopted is neither very large to facilitate numerical calculation nor very small to ensure qualitative accuracy. This is achieved by extending the dimension of the model space step by step; in each step the new results are compared with previous results from a smaller space, until satisfactory convergence is achieved. The matrix elements of H are then given by the following expressions

$$\langle\Phi^{LS\pi}_{[K]}|H_0|\Phi^{LS\pi}_{[K']}\rangle = [2(n_1+n_2)+\ell_1+\ell_2+3]\hbar\omega\delta_{[K],[K']}\,, \tag{8}$$

$$\begin{aligned}\langle\Phi^{LS\pi}_{[K]}|V_c|\Phi^{LS\pi}_{[K']}\rangle = {} & (U^{I}_{n_1n_1'}\delta_{n_2,n_2'} + U^{II}_{n_2n_2'}\delta_{n_1,n_1'})\delta_{\ell_1,\ell_1'}\delta_{\ell_2,\ell_2'} \\ & - \sum_{[K''][K''']} B_{[K][K'']}B_{[K'][K''']}(U^{III}_{n_1''n_1'''}\delta_{n_2'',n_2'''} + U^{III}_{n_2''n_2'''}\delta_{n_1'',n_1'''})\delta_{\ell_1'',\ell_1'''}\delta_{\ell_2'',\ell_2'''}\end{aligned} \tag{9}$$

with

$$U^{I}_{n_1n_1'} = \int_0^{\infty} R_{n_1\ell_1}(\xi_1)\Big[\frac{1}{2}\mu_1(\omega_0^2-\omega^2)\xi_1^2 + \frac{e^2}{\epsilon\xi_1}\Big]R_{n_1'\ell_1}(\xi_1)\xi_1^2\,\mathrm{d}\xi_1\,, \tag{10}$$

$$U^{II}_{n_2n_2'} = \int_0^{\infty} R_{n_2\ell_2}(\xi_2)\frac{1}{2}\mu_2(\omega_0^2-\omega^2)\xi_2^4 R_{n_2'\ell_2}(\xi_2)\,\mathrm{d}\xi_2\,, \tag{11}$$

$$U^{III}_{nn'} = \frac{e^2}{\epsilon}\int_0^{\infty} R_{n\ell}(\xi)R_{n'\ell}(\xi)\xi\,\mathrm{d}\xi\,, \tag{12}$$

$$B_{[K][K']} = \int \Phi^{LS\pi}_{[K]}(\vec{\xi}_1,\vec{\xi}_2)\Phi^{LS\pi}_{[K']}(\vec{\xi}_1',\vec{\xi}_2')\,\mathrm{d}^3\vec{\xi}_1\,\mathrm{d}^3\vec{\xi}_2\,, \tag{13}$$

where $R_{n\ell}(\xi)$ is the radial part of three-dimensional harmonic oscillator function, $B_{[K][K']}$ is the transformation bracket of three-dimensional 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 $\Phi^{LS\pi}_{[K]}(\vec{\xi}_1,\vec{\xi}_2)$ and $\Phi^{LS\pi}_{[K']}(\vec{\xi}_1',\vec{\xi}_2')$ have exactly the same eigen-energy and eigen-angular momentum. Analytical expression for $B_{[K][K']}$ has already been derived in Ref. [26]. The set of canonical coordinates $(\vec{\xi}_1',\vec{\xi}_2')$ are defined by $\vec{\xi}_1' = \vec{r}_1$, $\vec{\xi}_2' = -\vec{r}_2$.

3 Results and Discussions

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 mass of the free electron. Thus we find that the effective Bohr radius (the length unit) becomes $a_B^* = \hbar^2\epsilon/(m_e^*e^2) = 9.8$ nm, and the effective Rydberg (the energy unit) is $\mathrm{Ry}^* = e^2/(2a_B^*\epsilon) = 5.93$ meV. In this study we define the confined potential radius $r_c = \sqrt{\hbar/m_e^*\omega_0}$ as the characteristic length associated with the confining potential.

We restrict our study to the $L = 0$ (S states) for the

even parity and the $L = 1$ (P states) for the odd parity with the spin-singlet and the spin-triplet states of two electrons, which are denoted by ${}^1S^e$, ${}^3S^e$, ${}^1P^0$ and ${}^3P^0$. To demonstrate the dependence of the energy on the range of the confinement potential radius we plotted in Fig. 1 the energy spectrum of the low-lying states of the D^- center confined in a spherical parabolic QD as a function of the dot radius r_c. As illustrated in Fig. 1, the energies of the low-lying states of the D^- centers increase as the confined potential radius decreases, i.e., the stronger the confinement is, the higher the energies of the low-lying states are.

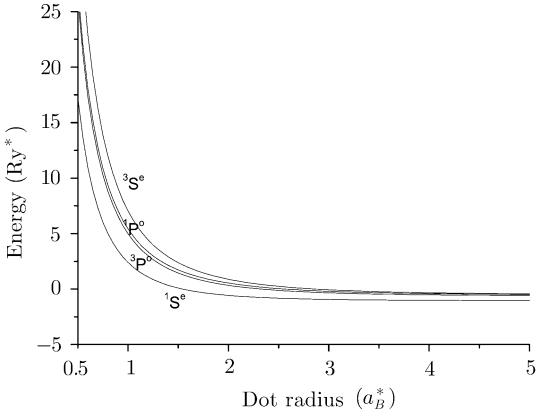

Fig. 1 The energy spectrum of the low-lying states of the D^- centres confined in a spherical parabolic QD as a function of dot radius r_c. The levels are labeled with the quantum state ${}^{2S+1}L^{\pi}$. Energy is expressed in the effective Rydberg Ry^* and length in effective Bohr radius a_B^*.

From Fig. 1, it is readily seen that the energy values of two states with $L = 1$, i.e., ${}^1P^0$ and ${}^3P^0$ states, are very much closer together and the energy difference of them is almost identical with increasing the confinement potential radius. On the other hand, from Fig. 1, we also find that the energy values of the $L+S =$ even states are lower than those of the adjacent $L + S =$ odd states. Our present results are qualitatively in good agreement with those of the two-electron systems in the low-dimensional space. This feature is a consequence of quantum mechanics symmetry as a few-electron system in QDs.[27] Obviously, the equilibrium configuration of the present system is a linear chain (LC) with electrons 1 and 2 on the two ends. Though in quantum mechanics, a system cannot possess a definite geometrical shape as its classical correspondent does, the distribution of the wave function of low-lying states should be smoothly (without nodal surfaces) peaked at the LC in order to minimize the interacting energy. However, a rotation about the positively charged ion by 180° is equivalent to an interchange of electrons 1 and 2. Let $\Psi_{[K]}^{LS\pi}$ (LC) be the probability amplitude for the D^- centre to form an LC. Then this can be expressed as

$$R_{180^\circ}\Psi_{[K]}^{LS\pi}(\mathrm{LC}) = P_{(12)}\Psi_{[K]}^{LS\pi}(\mathrm{LC})\,. \tag{14}$$

The former operator produces a factor of $(-1)^L$, while the latter produces a functor of $(-1)^S$. This implies that the LC configuration would be completely prohibited (i.e., $\Psi_{[K]}^{LS\pi}(\mathrm{LC}) = 0$) by quantum mechanics symmetry unless L takes the numbers fulfilling $(-1)^L = (-1)^S$, i.e., $L =$ even if $S = 0$, and $L =$ odd if $S = 1$. The internal motion of these states is just a small oscillation around the LC as an equilibrium shape to minimize the potential energy. In the case of $(-1)^L \neq (-1)^S$, we have $\Psi_{[K]}^{LS\pi}(\mathrm{LC}) = 0$. Thus an inherent nodal surface appears at the LC, and the binding of the $\Psi_{[K]}^{LS\pi}$ states is spoiled. Hence, the energy values of the states fulfilling $(-1)^L = (-1)^S$, i.e., the $L + S =$ even states, are lower than those of the adjacent $L + S =$ odd states.

In order to solve the problem of the stability of the D^- centre in the QD, we have to determine the binding energy of the system. The binding energy of the ν-th quantum state of the D^- centre is defined as the difference between the continuum threshold energy and the energy of the considered state of the D^- centre, i.e.,

$$W = E(\mathrm{D}^0) + E(e) - E(\mathrm{D}^-)\,, \tag{15}$$

where $E(\mathrm{D}^0)$ is the ground state energy of the D^0 centre in the QD, $E(e)$ is the ground state energy of an electron in the potential-barrier region without the Coulomb interaction, and $E(\mathrm{D}^-)$ is the ν-th state of the D^- centre, i.e., the corresponding eigenvalue of Hamiltonian (1). If $W \geq 0$ (< 0), the D^- center states are the bound (unbound) states.

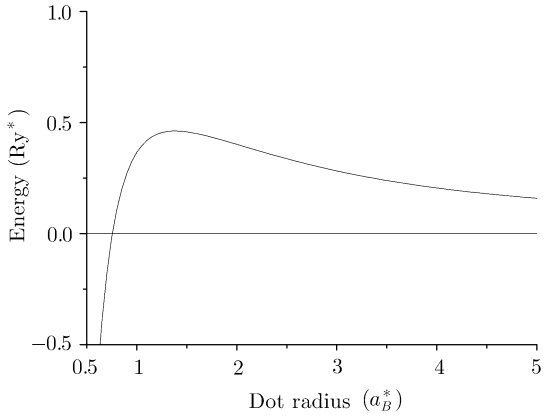

Fig. 2 The binding energy of the ground state of the D^- centres confined in a spherical parabolic QD as a function of dot radius r_c. The units are the same as in Fig. 1.

The binding energy of the ground state of the D^- center in a spherical parabolic QD as a function of dot radius is plotted in Fig. 2 in the absence of magnetic field. From Fig. 2, we observe that the binding energy increases with decreasing the confined potential radius r_c as expected, but it reaches a maximum value at around $r_c \sim 1.4a_B^*$. However, after that, as the confined potential radius r_c

is reduced further, the binding energy begins to decease and eventually becomes negative, i.e., there exists a critical confined potential radius R_c, such that if $r_c > R_c$ ($r_c < R_c$) the configuration of the D^- center is stable (unstable) in a spherical parabolic QD in the absence of magnetic field. This result is qualitatively in good agreement with that of Ref. [22] in a spherical QD with a finite barrier-height potential. From $W = 0$, we can obtain the critical confined potential radius $R_c \approx 0.75a_B^*$. The physical origin is that the increase in the confinement energy becomes predominant and cannot be compensated by the increase of the Coulomb attractive interaction for a smaller confined potential radius. As is well known, the energy of the low-lying states in a QD is determined by a competition of kinetic energy and Coulomb interaction energy. We note that, as the confined potential size is reduced, the Coulomb attractive interaction increases, the confinement kinetic energy increases. When the increase of the confinement energy cannot compensate by the increase of the Coulomb attractive interaction, the D^- center becomes unbound for small confined potential radius. Clearly the confinement kinetic energy increases more quickly than that of the Coulomb attractive interaction for a smaller dot radius. On the other hand, the further calculation shows that there exists only one bound state the D^- center in a spherical parabolic QD in the absence of magnetic field. It is obviously different from those in the presence of magnetic field. We know that, in the presence of magnetic field, the D^- centers in QDs have more than one bound states.[21,25,28,29]

In conclusion, we have applied the spherical parabolic confining potential to a description of the D^- centers in semiconductor QDs. We have calculated the energy levels of $L = 0$ (S states) for the even parity and $L = 1$ (P states) for the odd parity as functions of the confined potential radius. The feature of the low-lying states of the D^- center in a spherical parabolic QD is obtained. The binding energy of the ground state is obtained as a function of the confined potential radius. We find that there is only one bound state the D^- center in a spherical parabolic QD in the absence of magnetic field. Moreover, the critical confined potential radius value at which the negative donor center changes from unbound to bound is obtained. Our results may be important in the quantitative understanding of future experimental work involving D^- centers in a spherical QD.

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