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Binding energies of an exciton in a Gaussian potential quantum dot*

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In this paper, an exciton trapped by a Gaussian confining potential quantum dot has been investigated. Calculations are made by using the method of numerical diagonalization of Hamiltonian in the effective-mass approximation. The dependences of binding energies of the ground state and the first excited state on the size of the confining potential and the strength of the magnetic field are analysed explicitly.

Keywords: quantum dot, exciton
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1. Introduction

The investigation of artificial few-body systems is an attractive topic for both application and interest in basic research. In these systems usually an external field is introduced so that particles can be trapped and quantum states can be manipulated. Quantum dots (QDs) are structures in which charge carriers (electrons or holes) are confined in three dimensions.[1,2] In such QDs, some novel physical phenomena and potential electronic device applications have aroused a great deal of interest of many researchers. The spatial confinement of carriers leads to a discrete energy structure with sharp optical absorption lines. This is referred to as quantum size effect. In QDs excitons may be confined in all spatial dimensions, and if the exciton Bohr radius is comparable to the QD size, quantum confinement effects can be observed. Recently, very fine structures were observed in exciton photoluminescence from GaAs quantum wells (QWs).[3−5] These sharp lines are interpreted as luminescence from localized excitons at island structures in the QW. These island structures can be regarded as zero-dimensional QDs.

Quantum confinement effects of excitons in QDs have been studied extensively in the past few years. Since the pioneering work by Efros and Efros[6] and Brus,[7] many theoretical studies have been devoted to exciton states in microcrystals.[8−30] Most of them are related to variational studies of the excitonic ground state in spherical dots or to calculations in some limiting cases.[6−14,23,24] Typically, infinite barriers are considered. A full numerical analysis of this problem is done by Hu and co-workers,[15,16] expanding the excitonic wavefunctions in terms of solutions of the single-particle Schrödinger equations. There are also papers studying nonspherical dots, e.g. boxes,[17] square flat plates,[18] and cylindrical quantum dots.[19,20] Effects of, such as, dielectric confinement and electron–hole exchange interaction on exciton states in semiconductor QDs are also studied.[21] In 1998 Marfn *et al*[25] performed variational calculation of the ground state energy of excitons confined in spherical quantum dots with a finite-height potential wall. These studies have shown a strong competition among the QD size, Coulomb interaction, and magnetic confinement.

Since QDs are created mainly through producing a lateral confinement restricting the motion of the charged particles, which are initially confined in a very narrow quantum well, they usually have the shape of flat discs, with transverse dimensions considerably exceeding their thickness. The energy of single-particle excitations across the disc exceeds other characteristic energies in the system, and the confined electrons

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and holes can be considered to be two-dimensional. In most studies, a harmonic oscillator potential is used to describe the lateral confinement of carriers. However, the parabolic potential possesses an infinite depth and range. It is inappropriate to a description of the experimentally measured charging of the QD by the finite number of excess electrons.[26] Some experimental results suggest that the real confining potential is nonparabolic and possesses a well-like shape. Without defining the type of a QD (i.e. deciding on the simplified but universal model), we assume that the potential of a QD can be modelled in the form of a Gaussian potential well, $V(r) = V_0 \exp(-r^2/2R^2)$.[1] This model potential is smooth and possesses a finite depth V_0 and a characteristic finite radius R. It is obvious that the Gaussian potential does not exhibit the discontinuity at the QD boundary, which is the undesirable property of the rectangular potential, since it leads to the discontinuity of the second derivative of the wavefunction. Due to its continuity and finite depth and range, the Gaussian potential fairly well approximates the real confinement potential in QDs. In 2000 Adamowski *et al*[27] studied two electrons confined in QDs on the assumption of a Gaussian confining potential well and its parabolic approximation. Later, we calculated the energies of the low-lying states of an exciton in a Gaussian potential well in the absence of a magnetic field.[31] More recently, Gu and Liang[32] investigated the energy spectra of an exciton in a Gaussian potential using numerical matrix diagonalization in the presence of a magnetic field. In the present paper, to obtain a better understanding of the feature of the exciton confined in a Gaussian potential QD, we calculate the binding energies of the ground state and the first excited state of an exciton in a QD with a Gaussian potential by using the method of numerical matrix diagonalization. This model is based on the assumption of the Gaussian distribution of indium concentration in the QD. This potential possesses a finite depth and range and, in the vicinity of the dot centre it can be approximated by a parabolic potential. Contrary to the rectangular potential well, the Gaussian potential well is smooth at the QD boundaries, which permits us to model a compositional modulation within the QDs.[33]

2. Model and formulation

Here we consider localized excitons at quantum dot-like islands in QW structures that are formed by the lateral fluctuations of the QW thickness. In these island-like structures, the confinement in the direction of the crystal growth is strong, whereas the confinement in the lateral direction is rather weak. In order to facilitate the calculation, the lateral confinement potential in the xy-plane is assumed to be a Gaussian potential. Hence, we make the generalization that the Hamiltonian in the system within the effective-mass approach is given by

$$H = \frac{1}{2m_{\rm e}}\left(\boldsymbol{p}_{\rm e} + \frac{e}{c}\boldsymbol{A}_{\rm e}\right)^2 + V_{\rm e} + \frac{1}{2m_{\rm h}}\left(\boldsymbol{p}_{\rm h} - \frac{e}{c}\boldsymbol{A}_{\rm h}\right)^2 + V_{\rm h} - \frac{e^2}{\epsilon\,|\boldsymbol{r}_{\rm e} - \boldsymbol{r}_{\rm h}|}, \quad (1)$$

where $m_{\rm e}$ and $m_{\rm h}$ are the effective electron and hole masses, $\boldsymbol{p}_{\rm e}$, $\boldsymbol{p}_{\rm h}$, $\boldsymbol{r}_{\rm e}$, $\boldsymbol{r}_{\rm h}$ and $\boldsymbol{A}_{\rm e}$, $\boldsymbol{A}_{\rm h}$ denote respectively the momenta, positions and the vector potentials of an electron and a hole, ϵ is the dielectric constant of the medium in which the electron and the hole are moving. $V_{\rm e}$ and $V_{\rm h}$ are the bare single-particle potentials of an electron and a hole in the QD, respectively, which are of Gaussian potential,

$$V_i = -V_i^0 \exp(-r_i^2/2R^2), \quad i = {\rm e}, {\rm h}, \quad (2)$$

where $V_{\rm e}^0$ and $V_{\rm h}^0$ denote the heights of the potential wells of the electron and the hole respectively, and R is the range of the confinement potential, which corresponds to a radius of the QD. The last term of the above Hamiltonian describes the electron–hole Coulomb attraction. For simplicity, we omit here the Zeeman spin energy (negligible for GaAs). For $r/R \ll 1$, the Gaussian potential (2) can be approximated by the parabolic potential

$$V_i = -V_i^0 + \gamma_i^2 r_i^2, \quad i = {\rm e}, {\rm h}, \quad (3)$$

where $\gamma_i^2 = V_i^0/2R^2$.

With the symmetric gauge for the vector potential $\boldsymbol{A} = \frac{1}{2}B(-y, x, 0)$, the Hamiltonian then reads

$$H = \frac{p_{\rm e}^2}{2m_{\rm e}} + \frac{1}{8}m_{\rm e}\omega_{\rm ce}^2 r_{\rm e}^2 + \frac{1}{2}\omega_{\rm ce} l_{\rm e} + V_{\rm e} + \frac{p_{\rm h}^2}{2m_{\rm h}} + \frac{1}{8}m_{\rm h}\omega_{\rm ch}^2 r_{\rm h}^2 - \frac{1}{2}\omega_{\rm ch} l_{\rm h} + V_{\rm h} - \frac{e^2}{\epsilon\,|\boldsymbol{r}_{\rm e} - \boldsymbol{r}_{\rm h}|}, \quad (4)$$

where $\omega_{\rm ce} = eB/(cm_{\rm e})$ and $\omega_{\rm ch} = eB/(cm_{\rm h})$ stand for the cyclotron frequencies of the electron and hole, and $l_{\rm e}$ and $l_{\rm h}$ are the orbital angular momenta of the electron and the hole along the z direction, respectively.

We may rewrite the Hamiltonian, for convenience, as

$$H = H_0 + U + V_{\rm c}, \quad (5)$$

where

$$H_0 = \frac{p_e^2}{2m_e} + \frac{1}{8}m_e\omega^2 r_e^2 + \frac{1}{2}\omega_{ce}l_e + \frac{p_h^2}{2m_h} + \frac{1}{8}m_h\omega^2 r_h^2 - \frac{1}{2}\omega_{ch}l_h, \quad (6)$$

$$U = \sum_{i=e,h}\left[V_i^0\exp(-r_i^2/2R^2) + \frac{1}{2}m_i(\omega_{ci}^2/4 - \omega^2)r_i^2\right], \quad (7)$$

$$V_c = -\frac{e^2}{\epsilon\,|\boldsymbol{r}_e - \boldsymbol{r}_h|}. \quad (8)$$

To obtain the eigenenergies and eigenstates, H is diagonalized in model space expanded by translational invariant harmonic product states

$$\Phi_L = \sum_{[K]}\varphi^{\omega}_{n_e l_e}(\boldsymbol{r}_e)\varphi^{\omega}_{n_h l_h}(\boldsymbol{r}_h), \quad (9)$$

where φ^{ω}_{nl} is a two-dimensional harmonic oscillator state with a frequency ω and an energy $(2n + |l| + 1)\ \hbar\omega$, and $[K]$ denotes the set quantum numbers(n_e, l_e, n_h, l_h) in brevity. At the same time, we must take into account the fact that the total angular momentum of an exciton is a good quantum number because of the cylindrical symmetry of the Hamiltonian in the expression (4). The angular momenta of the electron, the hole, and the pair are denoted by l_e, l_h, and $L = l_e + l_h$, respectively. In practical calculation, ω serves as a variational parameter to minimize the eigenvalues. Throughout the present paper, we use the donor Rydberg $R_d = e^2/(2\epsilon a_d)$ as a unit of energy, and the donor Bohr radius $a_d = \hbar^2\epsilon/(m_e e^2)$ as a unit of length.

The exact diagonalization method consists in expanding the Hamiltonian for a given basis and extracting 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 consists of oscillator harmonics which are the eigenfunctions of the Hamiltonian when the electron–hole interaction is switched off. The matrix elements of H are then given by the following expressions:

$$\langle\Phi_{[K]}|H_0|\Phi_{[K']}\rangle = \left\{[2(n_e + n_h) + |l_e| + |l_h| + 2]\hbar\omega + \frac{1}{2}\omega_{ce}l_e - \frac{1}{2}\omega_{ch}l_h\right\}\delta_{[K],[K']}, \quad (10)$$

$$\langle\Phi_{[K]}|U|\Phi_{[K']}\rangle = U^e_{n_e n'_e}\delta_{l_e,l'_e}\delta_{n_h,n'_h}\delta_{l_h,l'_h} + U^h_{n_h n'_h}\delta_{l_h,l'_h}\delta_{n_e,n'_e}\delta_{l_e,l'_e}, \quad (11)$$

$$\langle\Phi_{[K]}|V_c|\Phi_{[K']}\rangle = -\sum_{[K'']}\sum_{[K''']} B_{[K][K'']}B_{[K'][K''']} \times U^c_{n''_e n'''_e}\delta_{n''_h,n'''_h}\delta_{l_e,l'_e}\delta_{l_h,l'_h}, \quad (12)$$

with

$$U^i_{n_i n'_i} = \int_0^\infty R_{n_i l_i}(r_i)[V_i^0\exp(-r_i^2/2R^2) + \frac{1}{2}m_i(\omega_{ci}^2/4 - \omega^2)r_i^2]R_{n'_i l_i}(r_i)r_i\mathrm{d}r_i, \quad (13)$$

$$U^c_{nn'} = \int_0^\infty R_{nl}(r)\frac{e^2}{\epsilon r}R_{n'l}(r)r\mathrm{d}r, \quad (14)$$

$$B_{[K][K']} = \int \Phi_{[K]}(\boldsymbol{r}_e, \boldsymbol{r}_h)\,\Phi_{[K']}(\boldsymbol{r}, \boldsymbol{r}')\mathrm{d}\boldsymbol{r}_e\mathrm{d}\boldsymbol{r}_h, \quad (15)$$

where $R_{nl}(r)$ is the radial part of 2D harmonic oscillator function, $B_{[K][K']}$ is the transformation bracket of 2D 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 $\Phi_{[K]}(\boldsymbol{r}_e, \boldsymbol{r}_h)$ and $\Phi_{[K']}(\boldsymbol{r}, \boldsymbol{r}')$ have exactly the same eigenenergy and eigenangular momentum. The set of canonical coordinates $(\boldsymbol{r}, \boldsymbol{r}')$ are defined by $\boldsymbol{r} = \boldsymbol{r}_e - \boldsymbol{r}_h$, $\boldsymbol{r}' = (m_e\boldsymbol{r}_e + m_h\boldsymbol{r}_h)/(m_e + m_h)$.

The accuracy of the solutions depends on how large the model space is. Since we are interested only in the ground state and the first excited state and in qualitative aspect, 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. In this paper, the dimension of the model space is constrained by $0 \le N = 2(n_e + n_h) + |l_e| + |l_h| \le 20$. If N is increased by 2, the ratio of the difference in energy is less than 0.01%.

3. Numerical results

Our numerical computation is carried out for one of the typical semiconducting materials, GaAs, as an example with the material parameters shown as follows: $\epsilon = 12.58$, m_e=0.067m_0, where m_0 is the mass of the free electron, and m_h=0.340m_0. The potential-well depths are taken as $V_e^0 = 216$meV and V_h^0=163meV corresponding to the GaAs QDs, for which R_d=5.79meV and a_d=9.97nm, respectively.

We define the binding energy of an exciton as

$$E_{\rm B}(X) = E(e) + E(h) - E(X), \qquad (16)$$

where $E(X)$ is the energy of an exciton, $E(e)$ and $E(h)$ are the lowest energies of an electron and a hole in the QDs, respectively.

To demonstrate the dependence of the binding energies on the range of the confinement potential we plot in Fig.1 the binding energy spectra of the ground state and the first excited state of an exciton in the Gaussian (solid curves) and the parabolic (dashed curves) potential QDs as a function of the dot radius R which corresponds to the QDs with the strong and intermediate confinement, i.e. $0.2a_{\rm d} \leq R \leq 5.0a_{\rm d}$. We first took the magnetic field B=0T. Although the $L = 0$ excitons have been extensively discussed in the literature, there exists little experimental or theoretical information on $L \geq 1$ exciton states. The $L = 1$ excitons are especially interesting since these may be excited in infrared spectroscopy as well as in two-photon spectroscopy. Both of the phenomena have received some experimental attention.[34,35]

Figure 1 shows that the qualitative properties of the binding energies for the Gaussian potential and the parabolic potential are similar. However, the quantitative differences are also obvious. In the ground state case, as expected, the binding energy increases with the decrease of dot radius. The physical origin is that, with dot radius decreasing, the spatial overlap between an electron and a hole is increased, leading to the increase in the Coulomb binding energy. We find that, when $R \geq 0.5a_{\rm d}$, the binding energy of the ground state for the Gaussian potential QD is in good agreement with that for the parabolic potential QD, and when $R < 0.5a_{\rm d}$, the increase in the binding energy of the Gaussian potential QD is faster than that for the parabolic potential QD. Hence, the binding energy of the ground state for the parabolic potential QD is lower than that for the Gaussian potential QD in $R < 0.5a_{\rm d}$ case, and the binding energy difference increases with the decrease of dot radius. This is obviously different from the energy level cases of the Gaussian potential QD and the parabolic potential QD.[31,32] It is the competition between the single particle energy and the interaction energy that finally determines the binding energy. Obviously the increase in the single particle energy in the parabolic potential QD is faster than that in the Gaussian potential QD with dot radius decreasing when R is smaller.

From Fig.1 we find that the binding energies of the first excited state ($L = 1$) are different from those of the ground state with the increase of dot radius. The binding energies of the first excited state decrease with dot radius decreasing. As the dot radius decreases further, we find that the binding energy becomes negative, i.e. there exists a critical radius $R_{\rm c}$, such that if $R < R_{\rm c}$ the first excited state of the exciton is unstable. As is well known, the energy of the low-lying states in a QD is determined by a competition between kinetic energy and Coulomb interaction energy. We note that as the dot size reduces, the Coulomb attractive interaction increases, thus the confinement kinetic energy increases. For the ground state, an increase in the confinement energy can be compensated for by an increase in the Coulomb attractive interaction with the decrease of dot radius, thus the binding energy increases. For the $L = 1$ state, since there exists the rotation kinetic energy, the increase in the confinement energy cannot compensated for by the increase in the Coulomb attractive interaction with the decrease of dot radius, thus the binding energy decreases. It is obvious that, when $R \geq 1.5a_{\rm d}$, the binding energy of the first excited state for the Gaussian potential QD is in good agreement with that for the parabolic potential QD.

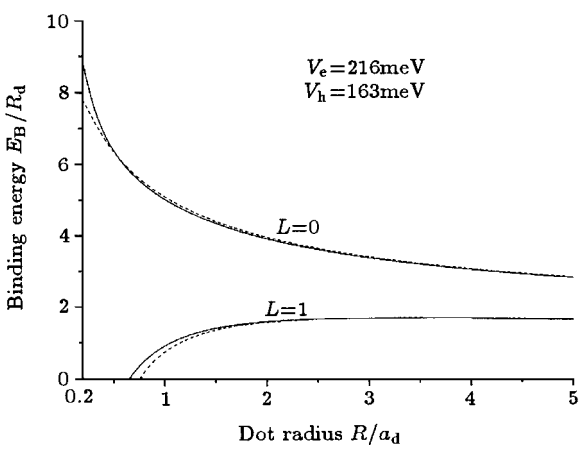


Fig.1. The binding energies of the ground state and the first excited state of the exciton confined in Gaussian (solid curves) and harmonic oscillator (dashed curves) potentials as a function of the dot radius R with $V_{\rm e}^0 = 216$meV, $V_{\rm h}^0 = 163$meV and $B = 0T$. Energy is expressed in the donor Rydberg $R_{\rm d}$ and length in the donor Bohr radius $a_{\rm d}$. The parameters are taken as being appropriate for GaAs.

To illustrate the effect of the magnetic field on an exciton in a Gaussian potential QD, in Fig.2 we plot the binding energies of the ground state and the first excited state as a function of the magnetic field

strength with $R = 1.0a_{\mathrm{d}}$. For the ground state and the first excited state, we observe that the binding energies of the exciton increase slowly with the increase of magnetic field strength. The increase in the binding energy of the first excited state is faster than that of the ground state. This can be interpreted as follows. The orbital radii of the particles are proportional to the QD size. When the magnetic field strength increases, the dot radius will decrease. Hence, the binding energy of the ground state increases. For the first excited state, on the one hand, the binding energy decreases as the magnetic field strength increases. On the other hand, the existence of the term $\frac{1}{2}\omega_{\mathrm{ce}}l_{\mathrm{e}} - \frac{1}{2}\omega_{\mathrm{ch}}l_{\mathrm{h}}$ (negative), which is proportional to the magnetic field strength and therefore would cause a linear increase in the binding energy, enables the binding energy of the first excited state to increase. It is obvious that the increase in the binding energy of the first excited state is faster than that of the ground state.

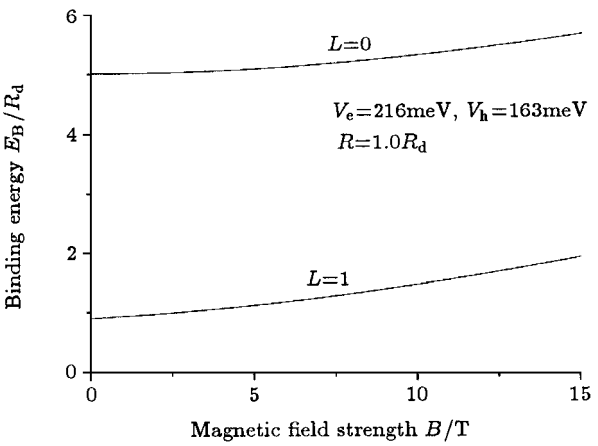


Fig.2. The binding energies of the ground state and the first excited state of the exciton confined in Gaussian potential as a function of the magnetic field strength B with $R = 1.0a_{\mathrm{d}}$. The others are the same as those in Fig.1.

In conclusion, we have applied the Gaussian confining potential to a description of the exciton in semiconductor QDs. We have calculated the binding energies of the ground state and the first excited state as a function of either the dot radius or the magnetic field strength. The same calculations performed in the parabolic approximation of the Gaussian potential lead to the results that are different qualitatively and quantitatively. The results of the present paper show that the Gaussian potential is a good approximation of the real confining potential, which should be especially useful for a description of many-electron systems in QDs with a varying composition. The softness of the Gaussian potential enables us to model the slowly varying confining potential.

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