Hydrogenic impurity in double quantum dots

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Abstract

The ground state binding energy and the average interparticle distances for a hydrogenic impurity in double quantum dots with Gaussian confinement potential are studied by the variational method. The probability density of the electron is calculated, too. The dependence of the binding energy on the impurity position is investigated for GaAs quantum dots. The result shows that the binding energy has a minimum as a function of the distance between the two quantum dots when the impurity is located at the center of one quantum dot or at the center of the edge of one quantum dot. When the impurity is located at the center of the two dots, the binding energy decreases monotonically.
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A three-dimensional confinement of charge carriers in semiconductor quantum dots (QDs) results in a quantization of energy levels. Among the various types of QDs, self-assembled QDs have been the subject of extensive study [1–4] because of their possible applications in semiconductor lasers. Strained self-assembled InAs/GaAs QDs grown on subsequent layers stack spontaneously one above the other [5–7], forming artificial molecules with a spatially extended state due to the tunnel interdot coupling. The coupled QDs can be treated as artificial molecules [8–16]. The coupling between the QDs should be useful in optical applications because it leads to the appearance of additional spectral lines. The positions of these lines can be changed by choosing different interdot distances through technological processes. Since this discovery, there have been plenty of experimental data and theoretical studies on double QDs. Liu et al. [17] studied the oscillator strengths of the optical transitions of vertically stacked self-assembled InAs quantum disks. Dong et al. [18] studied single-electron and two-electron vertically assembled quantum disks in an axial magnetic field using the effective mass approximation. Borri et al. [19] measured the exciton dephasing time in InAs/GaAs QD molecules having different interdot barrier thicknesses in the temperature

range from 5 to 60 K. Their results show that the quantum-mechanical coupling of the electronic wave functions in the molecules affects both the exciton radiative lifetime and the exciton-acoustic phonon interaction. Janssens et al. [20] theoretically investigated the influence of strain on the exciton properties in self-assembled two and three vertically coupled InP/GaInP dots. All the investigations show that the effects of the image charges in the double QDs are more pronounced than in the single QD. Double QDs are interesting because they represent a bridge between isolated QDs and super lattices.

Studies of the hydrogenic shallow impurity state in double QDs have recently attracted considerable attention. In determining the impurity binding energy, Bastard [21] was the first to theoretically treat the hydrogenic impurity state in a GaAs quantum well, assuming infinite barrier height. Since then, many authors [22–25] have taken the finite height of the barrier into account. However, most of them have only considered the case in which the impurity is located inside the GaAs well. It is well known that the reduction of dimensionality can increase the effective strength of the Coulomb interaction and affect the binding energy. Extensive theoretical work on hydrogenic impurity states in QDs has been reported [26–29]. Zhu [26] and Zhu, Xiong, and Gu [27] studied the hydrogenic impurity binding energies in spherical QDs by using a series expansion for the wave function. The binding energy was cal-
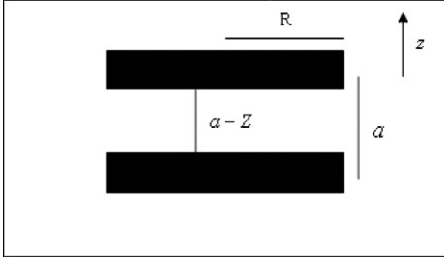
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Fig. 1. Schematic of the double self-assembled QDs of radius R, height Z.

culated as a function of the disk radius, for infinite and finite confining potentials. Chuu, Hsiao, and Wei [28] have calculated the binding energy of the ground state of a hydrogenic impurity located at the center of a QD by using a perturbation-variational approach. Such studies, however, have not yet been performed in double QDs. As in the case of bulk semiconductors and QDs, the study of the behavior of shallow impurity states in double QDs will lead to a better understanding of their electronic and optical properties.

We study the effect of the vertical coupling between the QDs on the impurity states. Fig. 1 shows two vertically self-assembled disk-shaped QDs, both of which have the same height Z, and the same radius R. In order to determine how the impurity's location will influence the binding energy of the donor, our calculations include three different locations of the impurity: (A) at the center of one dot, (B) at the center of the lower edge of the upper dot, (C) at the center of the two QDs.

For calculating the impurity ground-state energy in double QDs, we adopt the Gaussian model of the confinement potential [30,31], which was successfully applied to a quantitative interpretation of the exciton spectra in $In_xGa_{1-x}As$ self-assembled QDs. The confinement potential in $In_xGa_{1-x}As$ QDs embedded in the GaAs matrix can be derived from the spatial distribution of indium concentration within the QDs. We assume that this distribution can be described by a cylindrically symmetric Gaussian function [32],

$$X(\rho, z; R, Z) = X_0 \exp(-\rho^2/R^2 - z^2/Z^2), \tag{1}$$

where $\rho^2 = x^2 + y^2$ and X_0 is the concentration of indium at the center of the QD. In accordance with Eq. (1), we take the confinement potential for electrons to be

$$V_e^c(\rho, z; R, Z)$$
$$= V_e(\rho, z - a/2; R, Z) + V_e(\rho, z + a/2; R, Z), \tag{2}$$

where $V_e(\rho, z; R, Z) = -\Delta E_g X(\rho, z; R, Z)$, ΔE_g is the energy-gap difference between GaAs and InAs, and a is the distance between the centers of the two QDs. The confinement potential has the shape shown in Fig. 2. The thickness of the barrier between the QDs can be expressed in terms of the distance between the QDs centers and the height of the QDs as follows: $t = a - Z$. The calculations have been performed for $\Delta E_g = 1.11$ eV [31], $X_0 = 0.67$ and the material parameters of GaAs, i.e., the static dielectric constant $\varepsilon = 12.5$ and the effective mass of the electron $m_e = 0.0667 m_0$. The material parameters of QDs enter through the effective Rydberg $R_y = m_e e^4 / 2\varepsilon^2 \hbar^2$
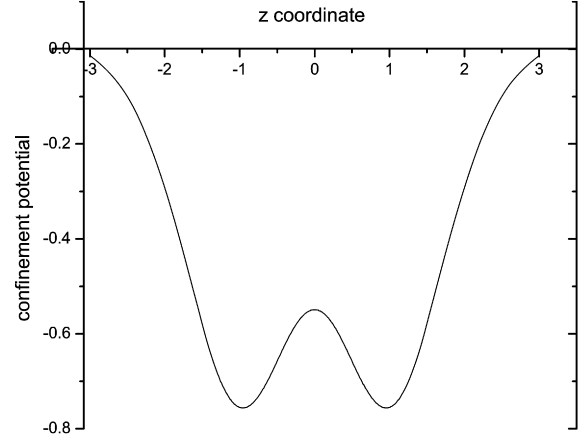

Fig. 2. The confinement potential vs the z coordinate at $x = y = 0$.

and the effective Bohr radius $a_B = \varepsilon \hbar^2 / m_e e^2$. Throughout this work a_B and R_y will be used as units of length and energy, respectively.

The ground-state wave function of the system confined in potential (2) possesses an even parity with respect to the change of sign of the z coordinate. Using the effective-mass approximation for electrons, the ground-state energy of a hydrogenic impurity confined in a double QDs with radius R and height Z is determined by the variational method with a trial-wave-function

$$\Psi_2 = N \cdot \left[\Phi_e\left(\rho_e, z_e + \frac{a}{2}, R, Z\right) + \Phi_e\left(\rho_e, z_e - \frac{a}{2}, R, Z\right) \right]$$
$$\times \exp(-\alpha_{ed}\rho_{ed}^2 - \beta_{ed}z_{ed}^2), \tag{3}$$

where N is the normalization constant, $\rho_{ed} = \rho_e - \rho_d$, $z_{ed} = z_e - z_d$ are relative coordinates between the electron and the impurity, and $\Phi_e(\rho_e, z_e, R, Z) = \exp(-\alpha_e\rho_e^2 - \beta_e z_e^2)$ is the wave function of the ground state of the electron confined in the single isolated QD. In Eq. (3), the interdot correlations are introduced via the two-center localization of the products of one-particle functions Φ_e. Wave function (3) is a good approximation of the ground state wave function for the double QDs. When $0 \leqslant a \leqslant Z$, the system can be seen as a single QD, and wave function Eq. (3) cannot be used directly. When $a \to \infty$, the electron cannot transfer to the other QD, so the system is the same as a single QD, too. Therefore, we select the wave function

$$\Psi_3 = \left(1 - \frac{1}{(a - Z)^2 + 1}\right) \cdot N_1 \cdot \Phi_e(\rho_e, z_e, R, Z)$$
$$\times \exp(-\alpha_{ed}\rho_{ed}^2 - \beta_{ed}z_{ed}^2)$$
$$+ \frac{a}{(a - Z)^2 + 1} \cdot N_2$$
$$\times \left[\Phi_e\left(\rho_e, z_e + \frac{a}{2}, R, Z\right) + \Phi_e\left(\rho_e, z_e - \frac{a}{2}, R, Z\right) \right]$$
$$\times \exp(-\alpha'_{ed}\rho_{ed}^2 - \beta'_{ed}z_{ed}^2), \tag{4}$$

where N_1 and N_2 are the linear variational parameters, $\Phi_e(\rho_e, z_e, R, Z) = \exp(-\alpha_e\rho_e^2 - \beta_e z_e^2)$, and $\Phi_e(\rho_e, z_e \pm \frac{a}{2}, R, Z) = \exp(-\alpha'_e\rho_e^2 - \beta'_e(z_e \pm \frac{a}{2})^2)$, and α_e, β_e, α_{ed}, β_{ed}, α'_e, β'_e, α'_{ed} and β'_{ed} are the nonlinear variational parameters.
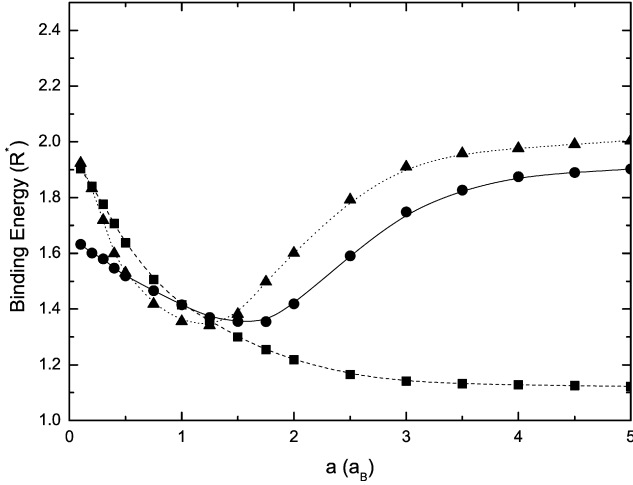
Fig. 3. Binding energies of the ground states of a donor in a double QDs vs the distance between the centers of the two QDs for $Z = 1.0a_B$, $R = 1.0a_B$. The solid curve represents the impurity located at the center of the underside of the upper QD, the dashed curve represents the impurity located at the center of the two QDs, and the dotted curve represents the impurity located at the center of the upper QD.

The Hamiltonian of an impurity confined in the double QDs has the form

$$H = -\nabla_e^2 + \frac{2}{r_{ed}} + V_e(\rho, z, R, Z), \qquad (5)$$

where $r_{ed} = |r_e - r_d|$ is the distance between the electron and the hydrogenic donor impurity. Therefore, the ground-energy of the impurity state is determined by numerically minimizing

$$E^{D^0} = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \qquad (6)$$

The binding energy can be obtained by varying all variational parameters. We obtain the binding energy of the impurity state in double QDs. Fig. 3 shows the binding energy E_B as a function of a for $Z = 1.0a_B$ and $R = 1.0a_B$ when the impurity is located at the center of the two QDs, the center of the underside of the upper QD, and the center of the upper QD. When a is small, the result is the same as for a single QD. As a increases, the binding energy decreases. With the increasing of a to a certain number, the two single QDs separate, while the impurity is located at the center of the underside of the upper QD and the center of the upper QD, the curves have a minimum, when the impurity is located at the center of the two QDs, the curve decreases monotonically as a increases. When $a \geqslant 1a^*$, the system is double QDs, when the impurity is located at the center of the upper QD, the binding energy is larger than for the other two positions. This is because the particle wave functions vanish at the boundaries, and thus their contributions to the energy are smaller when the impurity is at the boundary. For large a, the system is the same as a single QD, so the binding energy approaches a constant. The constant is the same as the result in single QD for $a \to 0$.

The average interparticle distances between the impurity and the electron in double QDs can be obtained by
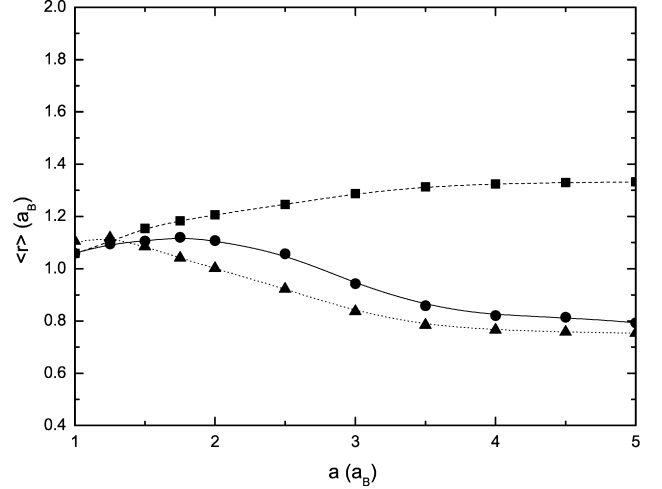

Fig. 4. The interparticle distances of a donor in a double QDs vs the distance between the centers of the two QDs for $Z = 1.0a_B$, $R = 1.0a_B$. The solid curve represents the impurity located at the center of the underside of the upper QD, the dashed curve represents the impurity located at the center of the two QDs, and the dotted curve represents the impurity located at the center of the upper QD.

$$\langle r \rangle = \frac{\int \Psi^* r \Psi \, d\tau}{\int \Psi^* \Psi \, d\tau}. \qquad (7)$$

We calculate the interparticle distances between the impurity and the electron in double QDs when the impurity is located at several different positions. Fig. 4 shows the interparticle distances as a function of a for $Z = 1.0a_B$ and $R = 1.0a_B$. The solid curve represents the impurity located at the center of the underside of the upper QD, the dashed curve represents the impurity located at the center of the two QDs, and the dotted curve represents the impurity located at the center of the upper QD. We calculate the results when $a \geqslant 1.0a_B$. In Fig. 4, the results show that the change tendency of the average interparticle distance is the opposite of that of the binding energy. When the impurity is located at the center of the two QDs, the curves increase monotonically for increasing a. When the impurity is located at the other two positions, the average interparticle distance is much lower than the result for when the impurity is located at the center of the two QDs, and the curve decreases slowly for large values of a.

We have calculated the probability density of the electron for when the donor impurity is located at several different positions. The results are shown in Fig. 5. We can see when the impurity is located at the center of the upper QD and the center of the underside of the upper QD, the probability density in the upper QD is much larger than in the lower QD. At the center of the upper QD, it reaches the maximum. When the impurity is located at the center of the two QDs, the probability density in the two QDs is identical, and at the center of each QD, the result reaches the maximum.

In practice, double QDs are never made of identical dots. Actually, the top dots tend to be a little larger than the bottom dots due to the strain effects. It will influence the properties of the system. While the distance between the centers of the two QDs is small, the system cannot be viewed as a single QD, and
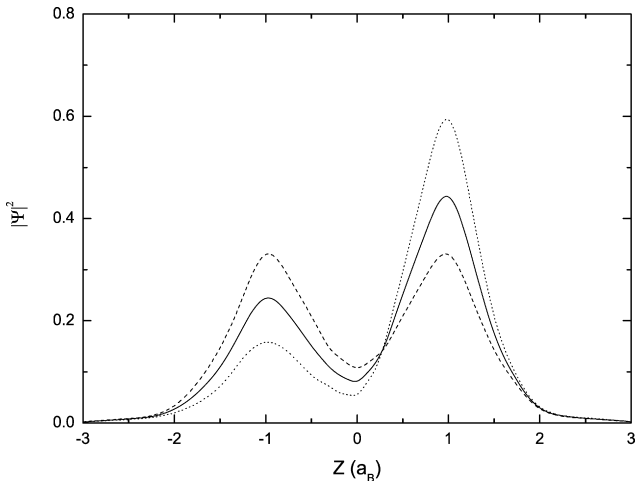
Fig. 5. Probability density of the electron vs the z coordinate for $Z = 1.0a_B$, $R = 1.0a_B$ and $a = 2.0a_B$. The solid curve represents the impurity located at the center of the underside of the upper QD, the dashed curve represents the impurity located at the center of the two QDs, and the dotted curve represents the impurity located at the center of the upper QD.

the discussion will be complex. With the increasing of the distance between the centers of the two QDs to a certain number, the two dots separate. At short inter-dot distances, the difference between two identical QDs and two different QDs will be little. When the inter-dot distance is larger enough, the system is the same as a single QD, and the difference will vanish.

In summary, we have calculated the ground state binding energy and the average interparticle distances of a hydrogenic impurity located at different places in a GaAs double QDs. The probability density of the electron was calculated, too. It has also been seen that the properties of the hydrogenic impurity in the double QDs are more pronounced than in a single QD. Therefore, it would be of interest to extend the problem to double impurities in the double QDs.

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