Double hydrogenic impurities in double quantum dots

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The ground states and degree of entanglement of double hydrogenic impurities in a pair of vertically stacked InGaAs/GaAs quantum dots are studied with a proposed diagonalization technique. It is found that at short barrier widths, the entanglement is small due to the coupling between the intra- and interdot orbitals. At large barrier widths, large entanglement occurs. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2781323]

I. INTRODUCTION

Two vertically[1,2] or laterally[3] coupled quantum dots (QDs) containing electrons, holes, or an exciton constitute the simplest solid structure proposed for the basic gate operations of quantum computing.[4,5] Quantum computation has become an intensively studied field in the last couple of years,[6] and many different ways to realize an entangled system have been proposed, including schemes in atomic physics, quantum optics, nuclear and electron magnetic resonance spectroscopy, and superconducting electronics.[7] Electronic states in artificial atomic and molecular devices, such as semiconductor single and coupled QDs, have been studied theoretically and experimentally for the past two decades.[8] Semiconductor QDs are regarded as artificial atoms due to their characteristic discrete energy spectra and controllable physical properties. Corresponding to the similarity between a QD and an atom, a pair of vertically or laterally coupled QDs is called a quantum molecule. Recently, with the development of the indium flush growth technique,[9] vertically stacked QDs of high quality have been fabricated and a large interaction-induced energy splitting of exciton states has been observed in the photoluminescence spectra.[4] Double QDs are interesting because they represent a bridge between isolated QDs and superlattices, and there have been plenty of experimental data and theoretical studies on double QDs.[10–17]

Studies of the hydrogenic shallow impurity state have recently attracted considerable attention. In determining the impurity binding energy, Bastard[18] was the first to theoretically treat the hydrogenic impurity state in a GaAs quantum well, assuming infinite barrier height. It is well known that the reduction of dimensionality can increase the effective strength of the Coulomb interaction and affect the binding. Extensive theoretical work on hydrogenic impurity states in QDs[19–21] and in double QDs[13] has been reported.

Quantum entanglement in single and double QDs has attracted even more attention.[15,22] Exciton states and optical spectra in a pair of vertically stacked InGaAs/GaAs QDs have been studied with a proposed variation-diagonalization technique.[12] The results show that the entanglements of qubits in coupled QDs may be influenced by many factors, such as composition fluctuations, dot size differences, and applied external fields. Starting with a pseudopotential description of the single-particle states, and followed by a configuration-interaction treatment of correlated electrons in vertically coupled, self-assembled InAs/GaAs QDs, He[23] depicted the basic physical characteristics including the singlet-triplet splitting, degree of entanglement, and correlation. Studying double hydrogenic impurities in double QDs is important for us to better study entanglement in double QDs.

In this article we study double impurities in vertically coupled QDs. Under the framework of the effective mass approximation, we provide a diagonalization method to efficiently calculate the states of double impurities.

II. THEORETICAL FRAMEWORK

The Hamiltonian of two impurities in vertically coupled InGaAs/GaAs QDs when the two impurities are located at the centers of the two quantum dots can be written as

$$H=\sum_{i=1,2}\left(\frac{\mathbf{P}_i^2}{2m_i^*}+\mathbf{U}_i\right)+\frac{e^2}{4\pi\varepsilon_0\varepsilon_r}\left(\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}-\frac{1}{|\mathbf{r}_1-\mathbf{r}_{i1}|}-\frac{1}{|\mathbf{r}_1-\mathbf{r}_{i2}|}-\frac{1}{|\mathbf{r}_2-\mathbf{r}_{i1}|}-\frac{1}{|\mathbf{r}_2-\mathbf{r}_{i2}|}\right), \tag{1}$$

where m_i^* is the electron conduction-band effective mass, $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of the two electrons, and $\mathbf{r}_{i1}$ and $\mathbf{r}_{i2}$ denote the coordinates of the two impurities. The confining potential $\mathbf{U}_i$ is written as

$$\mathbf{U}_i=\begin{cases}0 & \text{in QDs},\\ V_i & \text{in surrounding matrix}.\end{cases} \tag{2}$$

As shown in Fig. 1, W_b is the barrier width, R_0 and W_d are the dot radii and height, respectively, and V_i are the conduction and valence band offsets, respectively. To efficiently solve the Hamiltonian H of Eq. (1), a diagonalization method is used. H can be rewritten as

$$H=H_0+H', \tag{3}$$

where

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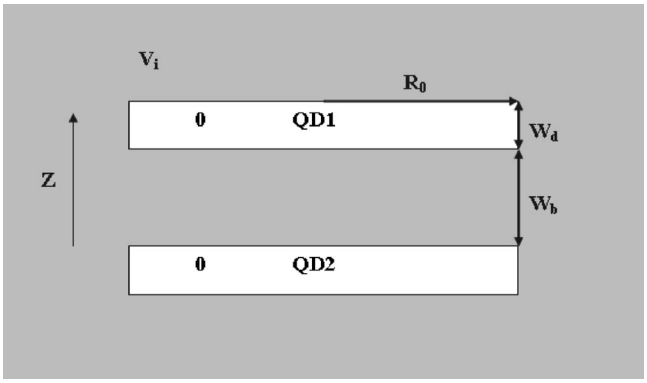

FIG. 1. Schematic illustration of the InGaAs/GaAs coupled quantum dots of radii R_0 with height W_d and interdot barrier width W_b.

$$H' = \frac{e^2}{4\pi\varepsilon_0\varepsilon_r}\left(-\frac{1}{|\rho_1-\rho_2|}+\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}-\frac{1}{|\mathbf{r}_1-\mathbf{r}_{i1}|}-\frac{1}{|\mathbf{r}_1-\mathbf{r}_{i2}|}-\frac{1}{|\mathbf{r}_2-\mathbf{r}_{i1}|}-\frac{1}{|\mathbf{r}_2-\mathbf{r}_{i2}|}\right). \tag{4}$$

In polar coordinates, H_0 can be written as

$$H_0 = H_{0z} + H_{0\rho}, \tag{5}$$

where

$$H_{0z} = \sum_{i=1,2}\left(\frac{\mathbf{P}_{zi}^2}{2m_i^*}+\mathbf{U}_{zi}\right) \tag{6}$$

and

$$H_{0\rho} = \sum_{i=1,2}\left(\frac{\mathbf{P}_{\rho i}^2}{2m_i^*}+\mathbf{U}_{\rho i}\right)+\frac{e^2}{4\pi\varepsilon_0\varepsilon_r}\frac{1}{|\rho_1-\rho_2|}, \tag{7}$$

where $\mathbf{P}_{zi}$ and $\mathbf{P}_{\rho i}$ are as follows:

$$\mathbf{U}_{zi} = \begin{cases} 0 & 0.5W_b \le |z_i| \le W_d + 0.5W_b, \\ V_i & \text{else}, \end{cases} \tag{8}$$

and

$$\mathbf{U}_{\rho i} = \begin{cases} 0 & \rho \le R_0, \\ V_i & \text{else}. \end{cases} \tag{9}$$

Then $H_{0\rho}$ can be separated into center-of-mass and relative motion terms:

$$H_{0\rho} = H_{0CM} + H_{0rel}, \tag{10}$$

with $H_{0CM} = = \frac{\mathbf{P}_{\rho_{CM}}^2}{4m^*}$ and $H_{0rel} = = \frac{\mathbf{P}_{\rho_{rel}}^2}{m^*}+\frac{e^2}{4\pi\varepsilon_0\varepsilon_r\rho_{rel}}+\mathbf{U}_{\rho i}$. Using the method of series expansion, we can obtain the solutions of H_{0CM}, H_{0rel}, and H_{0z}. Once the zeroth-order wave functions of H_0 are obtained, we then diagonalize the Hamiltonian (3) numerically. The secular equation is given by

$$\det\|(E_i^0 - E)\delta_{ij} + H'_{ij}\| = 0, \quad i,j = 1,2,\ldots,f, \tag{11}$$

where E_i^0 is the energy eigenvalue of H_0, and H'_{ij} are the matrix elements of the Hamiltonian H',

$$H'_{ij} = \langle\phi_i^0|H'|\phi_j^0\rangle, \quad i,j = 1,2,\ldots,f. \tag{12}$$

Here ϕ_i^0 is the eigenvalue wave function of the Hamiltonian H_0. By diagonalizing Eq. (11), we can obtain the energy level and the corresponding wave function of the system. The ground state binding energy of the double impurity state is given by $E_b = 2E^{D_0} - E^{2D_0}$, that is, twice the ground state energy of a single hydrogenic impurity minus the ground state energy of the double hydrogenic impurity.

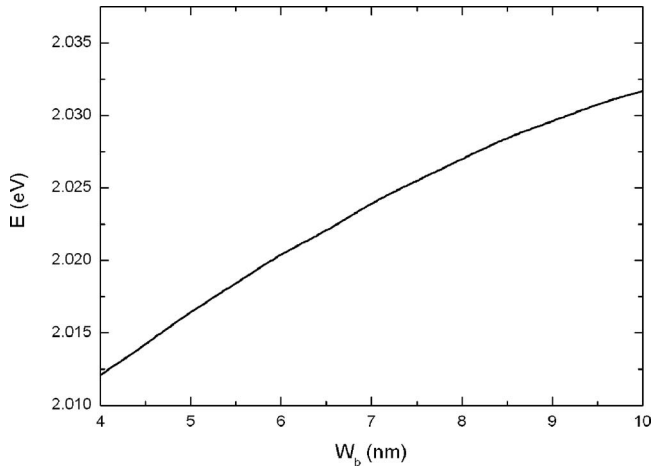

FIG. 2. The ground state energy versus the barrier width W_b in coupled QDs with $R_0 = 10$ nm and $W_d = 2$ nm.

The entanglement is characterized by the fact that the many-particle wave functions cannot be factorized as a direct product of single-particle wave functions. The degree of entanglement (DOE) is one of the most important quantities for successful quantum gate operations. An alternative way to define the DOE for the two electrons in the system is through a Schmidt decomposition, where the wave functions of the two hydrogenic impurities are written in a biorthogonal basis,

$$\psi(1,2) = \sum_i c_i|n_1\rangle \otimes |n_2\rangle, \tag{13}$$

where $|n_1\rangle$ and $|n_2\rangle$ are the basis wave functions of a single hydrogenic impurity state in a double QD. With $c_i \ge 0$ and $\Sigma_i c_i^2 = 1$, the number of nonzero c_i is called the Schmidt rank. The DOE for the system can be obtained by

$$S = -\sum_i c_i^2 \log_2 c_i^2. \tag{14}$$

III. RESULTS AND DISCUSSION

We have performed a numerical calculation for InGaAs/GaAs coupled QDs for $R_0 = 10$ nm, $W_d = 2$ nm, $m^* = 0.043m_0$, $\varepsilon_r = 13.5$, and $V1 = V2 = 0.53$ eV.

Figure 2 shows the dependence of the ground state energy on the barrier width W_b. With the increase of the barrier width, the energies increase. This is because a large interdot distance can reduce the coupling between the two dots. At the same time we have calculated the ground state binding energy of double hydrogenic impurities in coupled QDs. As can be seen in Fig. 3, the result increases with the increasing of the barrier width W_b. For large W_b, the system is the same as a single QD, so the binding energy approaches a constant.

Entangled double hydrogenic impurity states are important for the realization of quantum computation using

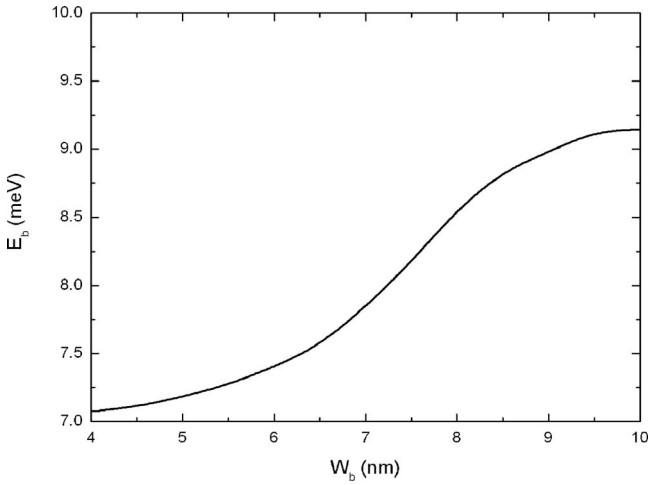

FIG. 3. The ground state binding energy versus the barrier width W_b in coupled QDs with $R_0=10$ nm and $W_d=2$ nm.

coupled QDs. The DOE can be quantified by Eq. (14). The entangled entropy of a maximally entangled state is 1, and that of a completely unentangled state is 0. In Fig. 4, the entanglement entropy is plotted as a function of W_b for double hydrogenic impurity ground states in coupled QDs. We can see that our result is larger than the result in Ref. 12; as W_b is small, the intradot orbital states and the interdot orbital states are all mixed into one state. It leads to large deviation from the Bell states so that in both the double impurities states and the exciton state small entanglements are shown. The coupling of the intra- and interdot orbital depends strongly on both the electron tunneling energy and the difference of Coulomb interaction energies between

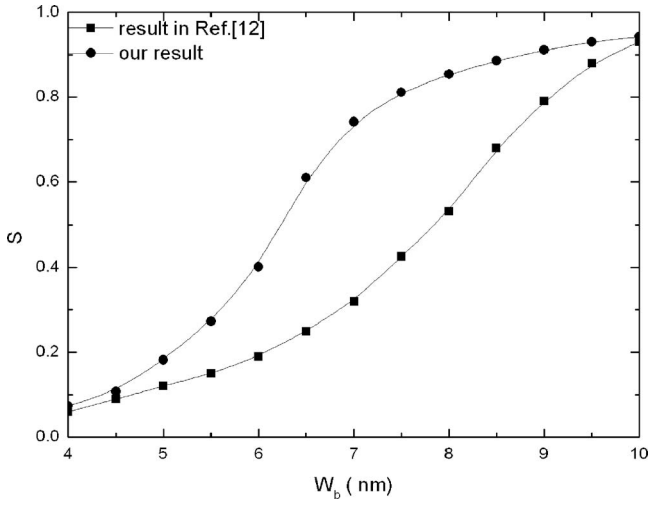

FIG. 4. The ground state entanglement entropy versus the barrier width W_b in coupled QDs with $R_0=10$ nm and $W_d=2$ nm.

them. With increasing W_b, such couplings decrease because of the decrease of tunneling energies and the increase of the differences of Coulomb interaction energies. When the barrier width is close to 7 nm, the electron tunneling energy is equal to the difference of Coulomb interaction energies; because the hole tunneling is weak, the double impurities states have much larger entanglement entropy than the exciton state. When the electron tunneling energy is less than the difference of Coulomb interaction energies, all of the state is close to the Bell states; both the double impurities states and the exciton state have large entanglements.

IV. SUMMARY AND CONCLUSION

To efficiently calculate double hydrogenic impurity states in vertically coupled InGaAs/GaAs QDs, a series expansion method is proposed, and the ground state energy is determined by exact diagonalization with the use of the basis.

The entanglements of double hydrogenic impurity states in coupled QDs are investigated by calculating the entanglement entropies. At small barrier widths, large couplings between the intra- and interdot orbital states exist so that entanglements are small. Large entanglements can occur at large barrier widths.

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