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Calculation of induced electron states in three-dimensional semiconductor artificial molecules

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Abstract

The energy levels calculation of electrons confined in small three-dimensional (3D) coupled quantum $\text{In}_x\text{Ga}_{1-x}\text{As}$ dots embedded in GaAs semiconductor matrix is presented. The quantum dots have disk shapes and are separated (in the disk symmetry axis direction) by a certain distance. Based on the effective one electronic band Hamiltonian, the energy and position dependent electron effective mass approximation, a finite height hard-wall 3D confinement potential, and the Ben Daniel–Duke boundary conditions, the problem is formulated and solved for the disk-shaped coupled quantum dots. To calculate the ground and induced state energy levels, the nonlinear 3D Schrödinger equation (SE) is solved with a developed nonlinear iterative method to obtain the final self-consistent solutions. In the iteration loops, the Schrödinger equation is discretized with a nonuniform mesh finite difference method, and the matrix eigenvalue problem is solved with the balanced and shifted QR method. Our complete 3D approach demonstrates a principal possibility that the number of bound electronic states in the system can be changed when the interdot (vertical) distance is modified. However, it is impossible to produce an additional possibility to manipulate the system electronic properties within only a two-dimensional (2D) simulation. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Semiconductor quantum dots (QDs) are now under extensive study because they have very rich properties of “artificial atoms”. Unlike “natural atoms”, the properties of QD can be controlled technologically [1,2].

In recent years, progress in fabrication technology has made it possible to consider systems of coupled QDs, “artificial molecules”. In this system, the main feature is the electronic structure tunability by dot-to-dot electronic entanglement and charge transfer [3]. This considerably enhances not only physical interest but also practical developments in artificial molecules [3,4]. In self-aligned multilayer $\text{In}_x\text{Ga}_{1-x}\text{As}$ QD structures [5] the electronic coupling between the dots can be observed in photoluminescence spectra if an interlayer distance is small enough. The interdot cou-

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pling due to the overlap of electron wave functions in those structures can be viewed as a creation of the artificial molecules. These molecules provide a base for quantum computing [3]. In spite of growing interest in this topic, most theoretical studies of these systems were only done on a 2D (lateral) geometry with 2D confinement potential models [3]. At the same time, the real 3D approach provides a new alternative to study and enhance the system tunability range comprehensively.

In this work, we compute the ground and induced energy levels of electrons confined in small 3D coupled quantum $\text{In}_x\text{Ga}_{1-x}\text{As}$ dots embedded in GaAs matrix. Based on the effective one electronic band Hamiltonian, the energy and position dependent electron effective mass approximation, a finite height hard-wall 3D confinement potential, and the Ben Daniel–Duke boundary conditions, this problem is formulated and solved numerically. The nonlinear 3D SE is solved with a nonlinear iterative algorithm to obtain the final self-consistent solutions [1,6,7]. In the iteration loops, the nonlinear SE is solved with the balanced and shifted QR method and the inverse iteration method.

Our result shows that one can modify the energy state of the 3D artificial molecule by changing $\text{In}_x\text{Ga}_{1-x}\text{As}$ dot parameters and the interdot distance. The paper is organized as follows. Section 2 describes the 3D model and simulation method. Section 3 shows the results. Section 4 is the conclusion.

2. 3D molecule model and method of calculation

We consider 3D structures in the one-band envelope-function formalism with the effective Hamiltonian being [8,9]

$$\hat{H} = -\frac{\hbar^2}{2} \nabla_{\mathbf{r}} \left(\frac{1}{m(E, \mathbf{r})} \right) \nabla_{\mathbf{r}} + V(\mathbf{r}), \quad (1)$$

where $\nabla_{\mathbf{r}}$ stands for the spatial gradient. The electron effective mass, $m(E, \mathbf{r})$, depending on energy and position is expressed as

$$\frac{1}{m(E, \mathbf{r})} = \frac{P^2}{\hbar^2} \left[\frac{2}{E + E_g(\mathbf{r}) - V(\mathbf{r})} + \frac{1}{E + E_g(\mathbf{r}) + \Delta(\mathbf{r}) - V(\mathbf{r})} \right], \quad (2)$$

where $V(\mathbf{r})$ is the confinement potential, $E_g(\mathbf{r})$ and $\Delta(\mathbf{r})$ stand for the position dependent band gap and the spin-orbit splitting in the valence band, respectively. The momentum matrix element is P .

For $\text{In}_x\text{Ga}_{1-x}\text{As}$ systems with a sharp discontinuity of the conduction band on the interface between the quantum dots (*material*₁ and *material*₂) and the crystal matrix (*material*₃), the hard-wall confinement potential can be written as $V(\mathbf{r}) = -V_{0x_1}$, when $\mathbf{r} \in \textit{material}_1$; $V(\mathbf{r}) = -V_{0x_2}$, when $\mathbf{r} \in \textit{material}_2$; and $V(\mathbf{r}) = 0$, when $\mathbf{r} \in \textit{material}_3$. The dot material parameters are computed with the following well-known rules [8,9]

$$\begin{aligned} V_{0x} &= 0.7(E_{g3} - E_{gx}), \\ E_{gx} &= x E_{g\text{InAs}} + (1-x) E_{g\text{GaAs}}, \\ \Delta_{gx} &= x \Delta_{g\text{InAs}} + (1-x) \Delta_{g\text{GaAs}}, \quad \text{and} \\ \frac{1}{m_x(0)} &= x \frac{1}{m_{\text{InAs}}(0)} + (1-x) \frac{1}{m_{\text{GaAs}}(0)}. \end{aligned} \quad (3)$$

For material parameters, we can use Eq. (3) for relatively small x . For large x a quadratic composition dependence should be deployed [8,9]. Strains in InGaAs/GaAs structures also can affect the result of calculations. But for electronic band of III–V semiconductor strains lead to relatively small changes in parameters (E_g , etc.) and strain effects can be adjusted by a proper selection of the parameters from literature. In this paper we concentrate on principal consequences of a 3D approach in modeling of electron states in artificial molecules. Further corrections will lead to a more accurate value of the electron energy states. At the same time, it should not affect the main tendencies and behaviors of the state in the structures.

Integrating the SE with Hamiltonian (1) along the direction perpendicular to the interface, we obtain the Ben Daniel–Duke boundary conditions for wave function $\Psi(\mathbf{r})$

$$\Psi_A(\mathbf{r}_s) = \Psi_B(\mathbf{r}_s) \quad \text{and} \quad \frac{\hbar^2 \nabla_{\vec{n}} \Psi(\mathbf{r}_s)}{2m(E, \mathbf{r}_s)} = \text{const.}, \quad (4)$$

where \mathbf{r}_s denotes the position on the system interface of the region of *material*_{1–3} or *material*_{2–3}. Eqs. (1)–(4) can be used to calculate the electron energy levels in our system of two vertically coupled QDs with different material constants.

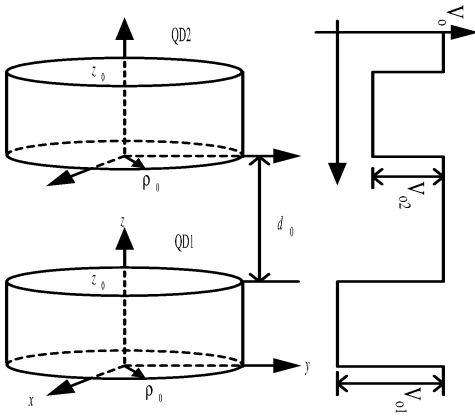


Fig. 1. The artificial molecule and potential schemes.

We consider specifically disk-shaped co-axial QDs with the same radius ρ_0 and thickness z_0 , and separated by the distance d_0 in the cylindrical coordinates (ρ, ϕ, z) , as shown in Fig. 1. The z -axis is chosen along the rotation axis. Since the system is cylindrically symmetric, the wave function can be represented as $\Psi(\mathbf{r}) = \Phi(\rho, z) \exp(il\phi)$, where $l = 0, \pm 1, \pm 2, \dots$ is the orbital quantum number. In the coordinates (ρ, z) , the problem remains

$$-\frac{\hbar^2}{2m_i(E)} \left(\frac{\partial^2}{\partial \rho^2} + \frac{\partial}{\rho \partial \rho} + \frac{\partial^2}{\partial z^2} - \frac{l^2}{\rho^2} \right) \Phi_i(\rho, z) + V(\rho, z) \Phi_i(\rho, z) = E \Phi_i(\rho, z), \quad (5)$$

and the boundary conditions (4) become

$$\begin{aligned} \Phi_j(\rho, z) &= \Phi_3(\rho, z), \quad z = f_{sj}(\rho), \\ \frac{1}{m_j(E)} \left\{ \frac{\partial \Phi_j(\rho, z)}{\partial \rho} + \frac{df_{sj}}{d\rho} \frac{\partial \Phi_j(\rho, z)}{\partial z} \right\} \Big|_{z=f_{sj}(\rho)} & \quad (6) \\ &= \frac{1}{m_3(E)} \left\{ \frac{\partial \Phi_3(\rho, z)}{\partial \rho} + \frac{dfs}{d\rho} \frac{\partial \Phi_2(\rho, z)}{\partial z} \right\} \Big|_{z=f_{sj}(\rho)}, \end{aligned}$$

where $i = 1, 2, 3$ and $z = f_{sj}(\rho)$ ($j = 1, 2$) presents a contour generator of the j th dot on the ρ and z plane. The composition parameter x is the key parameter. We use this model to investigate the electron energy states of the coupled dots when we can choose different x for different dots. The molecule parameters, e.g., E_{gj} , m_{0j} , Δ_j , and V_{0j} , are now tunable with the parameter x so that various molecule configurations can be obtained. Furthermore, there is an additional parameter, interdot distance d_0 , which will be modified in this study.

From Eq. (2), we know that the SE is a nonlinear equation in energy. To solve the final convergent solution of this model, we propose a nonlinear iteration scheme [1,6,7]. Its outline is:

- (i) set an initial energy E ,
- (ii) compute effective mass $m(E, r)$,
- (iii) solve the SE, and
- (iv) update the new energy and so back to step (ii).

If it converges, we stop the feedback iteration. In each iteration we discretize the nonlinear SE [10]. The discretized equation together with its boundary conditions (6) leads to a matrix eigenvalue problem: $A\mathbf{X} = \lambda\mathbf{X}$, where A is the matrix arising from the discretized SE and boundary conditions, and \mathbf{X} and λ are the corresponding eigenvectors (wave functions) and the eigenvalues (energy levels). We apply a balanced and shifted QR algorithm [11] to solve the above matrix eigenvalue problem, where we note that the matrix A is an energy dependent and large sparse matrix. When an eigenvalue is found, the inverse iteration method [11] is used for finding the corresponding eigenvector. In our calculation experience, the proposed solution algorithm is very stable and robust approach for quantum molecule simulation. Our iterative method converges monotonically to 10^{-9} eV (maximum norm error) by taking about 10–12 feedback iterations.

3. Results and discussion

The artificial molecule is a more complicated object than a single QD and it gives us a wider range of opportunities to manipulate the energy states of the system. A very interesting example of this manipulation can be demonstrated if we first perform two completely separated QDs ($d_0 \rightarrow \infty$) and QD₁ has only one bounded electron state and QD₂ does not have any bounded state. Then, the decrease in d_0 can lead to an induction of an “additional” weak bounded electron energy state in the system.

We use the following parameters for the vertically aligned artificial cylindrical molecule calculation. Both of the dots have $\rho_0 = 7.5$ nm and $z_0 = 1.5$ nm. For QD₁ we choose $x = 0$ (a complete InAs QD) and $E_{g1} = E_{\text{InAs}} = 0.42$ eV, $m_{01} = m_{0\text{InAs}} =$

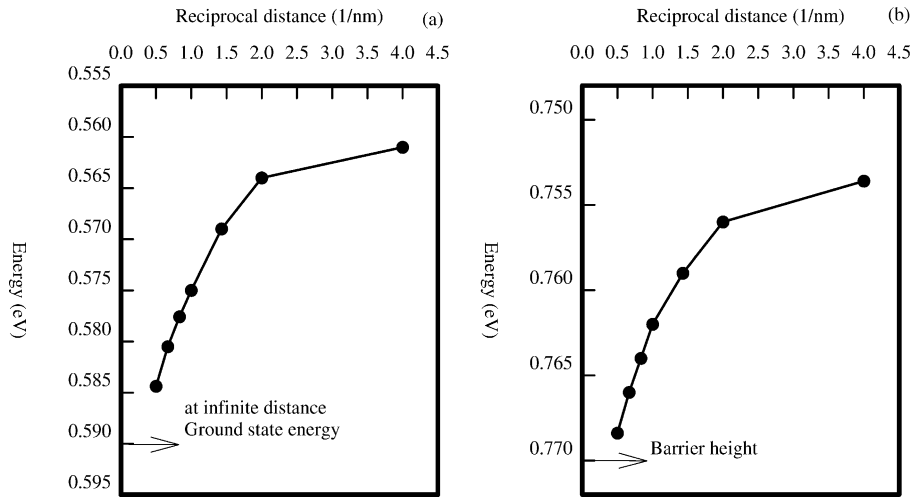


Fig. 2. (a) The ground state energy versus the reciprocal distance. (b) The induced energy state.

$0.024 \times m_0$, $\Delta_1 = \Delta_{1\text{InAs}} = 0.38$ eV, $V_{01} = 0.77$ eV [9] (m_0 is the free electron effective mass). For QD₂ (to assure that there is no bounded state) $x = 0.2$ and all parameters can be calculated by using Eq. (3), where $E_{g2} = 1.30$ eV, $m_{02} = 0.031 \times m_0$, $\Delta_2 = 0.33$ eV, $V_{02} = 0.15$ eV.

Fig. 2(a) shows the calculated (in the first dot) energy that depends on the interdot reciprocal distance d_0^{-1} . The energy state behavior is a result of the increasing electron wave function penetration into the second dot region when the distance becomes small. It presents a relatively strong influence of the second dot potential well on the ground energy state for $d_0 \lesssim 5.0$ nm that can be verified by photoluminescence experiments [12].

In Fig. 2(b), a new energy state which is induced only by decreasing the interdot distance is presented. This state never exists for a system with completely separated dots. For our system parameters the state arises when the distance between two dots is less than 2.0 nm. The state playing the role of an excited state in the molecule gives a possibility to form different electronic configurations [3]. It is worth to doing further study with the multielectronic theory.

4. Conclusion

The coupling between the electron energy states of two small cylindrical hard-wall QDs has been studied

theoretically. Our calculation results demonstrate that one can perform and modify the energy state system of the 3D artificial molecule by changing $\text{In}_x\text{Ga}_{1-x}\text{As}$ dot constants and interdot distance. In the case when the two dots have a big difference in the x parameter we can consider a situation where one of the separated dots has at most one bounded state and the other does not have any bounded state. Then, the decrease in distance will lead to an induction of an “additional” weak bounded electron energy state. The predictable phenomenon can be verified and investigated experimentally. This work is a starting point to estimate the energy states in semiconductor artificial molecules. The model with the self-consistent potential and the multi-band approach should also be considered for more proper studies.

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