Properties of the two- and three-dimensional quantum dot qubit*

Chen Shihua(陈时华)†

(College of Electrical Engineering, Huzhou Vocational Technology College, Huzhou 313000, China)

Abstract: On the condition of electric-longitudinal-optical (LO) phonon strong coupling in both two- and three-dimensional parabolic quantum dots (QDs), we obtain the eigenenergies of the ground state (GS) and the first excited state (ES), the eigenfunctions of the GS and the first ES by using a variational method of Pekar type. This system in QD may be employed as a quantum system–quantum bit (qubit). When the electron is in the superposition state of the GS and the first ES, we obtain the time evolution of the electron density. The relations of both the electron probability density and the period of oscillation with the electric-LO phonon coupling strength and confinement length are discussed.

Key words: quantum dot; qubit; strong coupling
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1. Introduction

Quantum computers (QCs) have attracted considerable attention in the information science field recently. A QC was introduced by Benioff[1] in 1980. In 1982, Feynman[2] pointed out that in order to simulate a quantum system, the computer has to operate quantum mechanically, i.e., one needs a QC. A proposal for the practical implementation of a QC was presented in 1993. The elementary unit of quantum information in a QC is the quantum bit (qubit). A single qubit can be envisaged as a two-state system such as a spin-half particle or a two-level atom. The potential power of a QC is based on the ability of quantum systems to be in a superposition of its basic states. In order to perform quantum computations, one should have the following basic conditions: (a) a two-level system $|0\rangle$ and $|1\rangle$ as a qubit; (b) the ability to prepare the qubit in a given state, say $|0\rangle$; (c) the capability of measuring each qubit; (d) the ability to perform basic gate operations such as a conditional logic gate (the control-not gate); and (e) a sufficiently long decoherence time. Several schemes have been proposed for realizing QCs in recent years[3−5]. In order to show the advantage of QCs over the most classical computers, QCs need to be composed of at least thousands of qubits to be feasible. Consequently, it is clear that a QC with a significant number of qubits would be more realizable in solid-state systems. However, self-assembled quantum dots (QDs) have attracted substantial attention due to their perfect crystal structures. Therefore, it is one of the most popular solid-state quantum information research fields that qubits can be realized by solid-state devices. Many schemes have been proposed for researching QD and have many kinds of contents, but they are in the initial research stage at present. The two-level QD system can be employed as a single qubit. For such a qubit, Li *et al.*[6, 7] presented a kind of parameter-phase diagram scheme and defined the parameter region for the use of InAs/GaAs as a two-level quantum system. Wang *et al.*[8, 9] recently studied the properties of a two-level qubit in two-dimensions (2D) parabolic QD. The phonon spontaneous emission causes the decoherence of the qubit. The relations between the decoherence time and the coupling strength and confinement length in both 2D and 3D parabolic QDs were discussed in our previous work[10]. In those works, however, the electron probability density and the period of oscillation for a qubit in both 2D and 3D QDs with parabolic confinement have never been studied.

In this article, the eigenenergies and their relevant eigenwavefunctions of the ground state (GS) and the first excited state (ES) of an electron have been obtained in both 2D and 3D QDs with parabolic confinement using the Pekar variational method in the electron–LO-phonon strong-coupling region. We have obtained the electron probability density oscillating with a period when the electron is in a superposition state of the GS and first ES. We discuss the relations of both the electron probability density and the period of oscillation with the electron–LO-phonon coupling strength and the confinement length in this paper. Our results should be meaningful for designing the solid-state implementation of quantum computing both theoretically and experimentally.

2. Theoretical model

The system under study consists of an electron interacting with the longitudinal optical (LO) phonons of an N-dimensional (ND) polar semiconductor QD. Theoretically one can simulate the ND QD geometry approximately by considering the electron's motion in an ND box. This model is, however, not very realistic since the force experienced by the electron within the dot is not really zero. The Hamiltonian for an electron moving in an ND parabolic QD and interacting with LO phonons of the system can be written as

$$H = -\frac{1}{2}\nabla_{\boldsymbol{r}}^2 + \frac{1}{2}\omega^2\boldsymbol{r}^2 + \sum_{\boldsymbol{q}} b_{\boldsymbol{q}}^{+} b_{\boldsymbol{q}} + \sum_{\boldsymbol{q}} (\xi_{\boldsymbol{q}}\, \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} b_{\boldsymbol{q}} + H.c.), \tag{1}$$

where all vectors are ND and the units have been chosen such that $\hbar = m = \omega_{\mathrm{LO}} = 1$ (Feynman units), m being the Bloch

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† Corresponding author. Email: shihuachen@yahoo.com.cn
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effective mass of the electron, and $\omega_{\rm LO}$ is the LO-phonon frequency which is assumed to be dispersionless. In Eq. (1), $\boldsymbol{r}$ refers to the position vector of the electron, $b_{\boldsymbol{q}}^{+}(b_{\boldsymbol{q}})$ is the creation (annihilation) operator for an LO-phonon of wave vector $\boldsymbol{q}$ and $\xi_{\boldsymbol{q}}$ is given by[11]

$$\left|\xi_{\boldsymbol{q}}\right|^2 = \frac{\Gamma[(N-1)/2]2^{N-3/2}\pi^{(N-1)/2}}{V_{\rm N}q^{N-1}}\alpha, \tag{2}$$

where $V_{\rm N}$ is the volume of the ND dot and α is the electron–phonon coupling constant.

By using the well-known Lee–Low–Pines (LLP) transformation

$$U = \exp\left[\sum_{\boldsymbol{q}}\left(f_q b_{\boldsymbol{q}}^{+} - f_q^{*} b_{\boldsymbol{q}}\right)\right], \tag{3}$$

where $f_q(f_q^{*})$ is the variational function, we obtain

$$H' = U^{-1}HU. \tag{4}$$

The variational energy is now written as

$$E = \left\langle\phi\left|\left\langle 0\left|H'\right|0\right\rangle\right|\phi\right\rangle, \tag{5}$$

where $\phi(r)$ is the electronic function to be chosen variationally and $|0\rangle$ is the unperturbed zero phonon state. The variational energy then simplifies to

$$E = -\frac{1}{2}\left\langle\phi\left|\nabla_r^2\right|\phi\right\rangle + \frac{1}{2}\omega^2\left\langle\phi\left|r^2\right|\phi\right\rangle + \sum_{\boldsymbol{q}}\left|f_q\right|^2 + \sum_{\boldsymbol{q}}\left(\xi_{\boldsymbol{q}} f_q^{*}\rho_q^{*} + H.c.\right), \tag{6}$$

where

$$\rho_q = \left\langle\phi\left|\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\right|\phi\right\rangle. \tag{7}$$

Minimizing E with respect to f_q^{*} now yields

$$f_q = -\xi_q\rho_q^{*}, \tag{8}$$

and thus Equation (6) reduces to

$$E = -\frac{1}{2}\left\langle\phi\left|\nabla_r^2\right|\phi\right\rangle + \frac{1}{2}\omega^2\left\langle\phi\left|r^2\right|\phi\right\rangle - \sum_q\left|\xi_q\right|^2\left|\rho_q\right|^2. \tag{9}$$

2.1. Ground state

For the GS we may choose the electronic wavefunction as

$$\phi_0(r) = \frac{\lambda^{N/2}}{\pi^{N/4}}\mathrm{e}^{-\lambda^2 r^2/2}, \tag{10}$$

with a variational parameter λ. Hence the GS energy becomes

$$E_{\rm GS} = \frac{N}{4}\lambda^2 + \frac{N}{4\lambda^2 l^4} - \frac{\Gamma[(N-1)/2]}{2\Gamma(N/2)}\lambda\alpha, \tag{11}$$

where l is the dimensionless confinement length given by $l = \frac{1}{\sqrt{\omega}}$; variation of Eq. (11) with respect to λ gives

$$\frac{N}{2}\lambda^4 - \frac{\alpha\Gamma[(N-1)/2]}{2\Gamma(N/2)}\lambda^3 - \frac{N}{2l^4} = 0. \tag{12}$$

2.2. First excited state

Assuming the electron is excited in the z-direction (θ is the angle of the electron coordinate vector and z-direction), and then according to the standard quantum transition theory, the first ES trial wavefunction of the system is given by

$$\phi_1(r) = \left(\frac{2\lambda^{N+2}}{\pi^{N/2}}\right)^{1/2} r\mathrm{e}^{-\lambda^2 r^2/2}\cos\theta, \tag{13}$$

which satisfies the following orthonormal relations.

$$\langle\phi_0|\phi_1\rangle = 0, \tag{14}$$

$$\langle\phi_1|\phi_1\rangle = 1. \tag{15}$$

Hence the first ES energy becomes

$$E_{\rm ES} = \frac{N+2}{4}\lambda^2 + \frac{N+2}{4\lambda^2 l^4} - \frac{(2N+1)^2\Gamma[(N-1)/2]}{16(N+2)\Gamma[(N/2)+1]}\lambda\alpha. \tag{16}$$

Variation of Eq.(16) with respect to λ gives

$$\frac{N+2}{2}\lambda^4 - \frac{(2N+1)^2\Gamma[(N-1)/2]}{16(N+2)\Gamma[(N/2)+1]}\alpha\lambda^3 - \frac{N+2}{2l^4} = 0. \tag{17}$$

Then we can get the eigen level and the eigen wavefunction. Then, we obtain the two-level system needed by a single qubit. The superposition state of the electron can be expressed as

$$|\phi_{01}\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \tag{18}$$

where $|0\rangle = \phi_0$ and $|1\rangle = \phi_1$. The time evolution of the quantum state of the electron can be written as

$$\phi_{01}(t,r,\theta) = \frac{1}{\sqrt{2}}\phi_0\exp\left(-\frac{\mathrm{i}E_0 t}{\hbar}\right) + \frac{1}{\sqrt{2}}\phi_1\exp\left(-\frac{\mathrm{i}E_1 t}{\hbar}\right). \tag{19}$$

The probability density is in the following form,

$$\begin{aligned} Q(r,t) &= |\phi_{01}(t,r,\theta)|^2 \\ &= \frac{1}{2}\left[|\phi_0(r)|^2 + |\phi_1(r)|^2 + \phi_0^{*}(r)\phi_1(r)\exp(\mathrm{i}\omega_{01}t) + \phi_1^{*}(r)\phi_0(r)\exp(-\mathrm{i}\omega_{01}t)\right], \end{aligned} \tag{20}$$

where

$$\omega_{01} = \frac{E_1 - E_0}{\hbar}. \tag{21}$$

3. Results and discussions

To prevent the transition of the electron from higher energy, the discussions in the following are carried out at a temperature of near 0 K, and Feynman units are adopted in this section. The numerical results of the electron probability density and the period of oscillation versus the electron–phonon coupling strength and confinement length in a symmetric QD with parabolic confinement in both 2D and 3D are presented in Figs. 1–3.

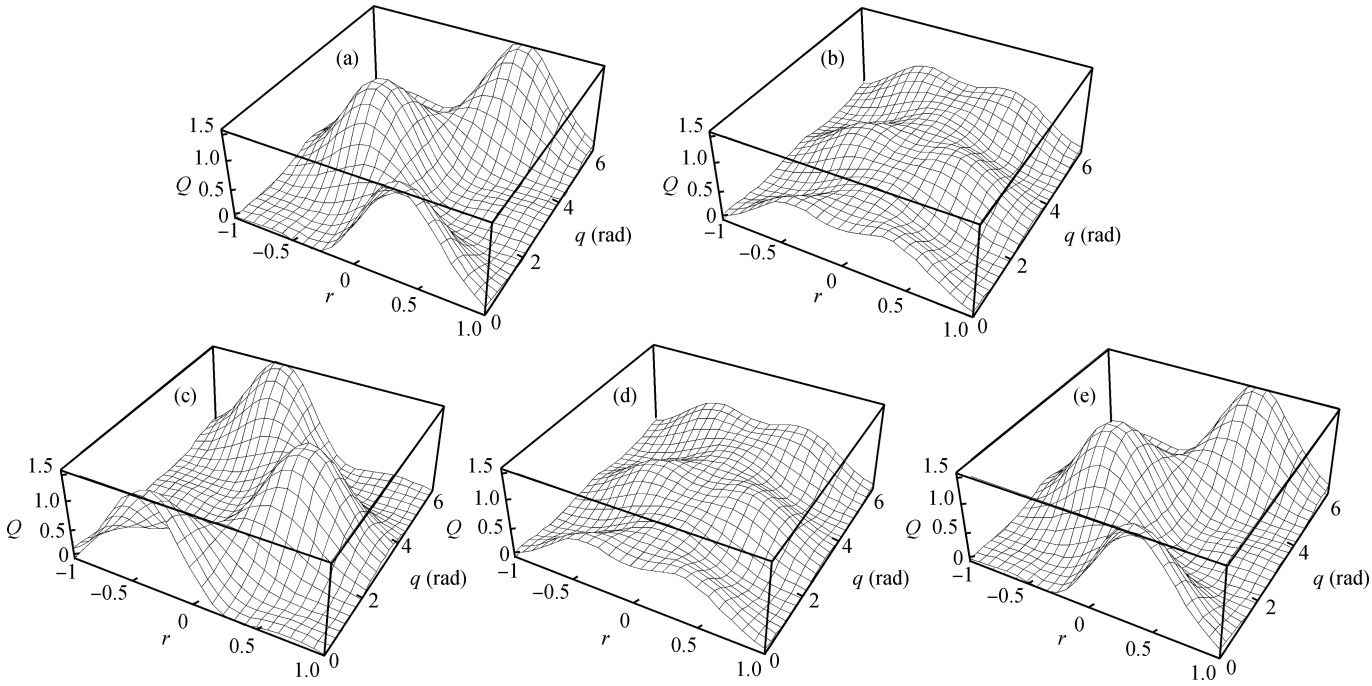

Fig. 1. Time evolution of the electron probability density in superposition of $|0\rangle$ and $|1\rangle$ in 2D QD. (a) $t = 0$. (b) $t = 0.25\ T_0$. (c) $t = 0.5\ T_0$. (d) $t = 0.75\ T_0$. (e) $t = T_0$.

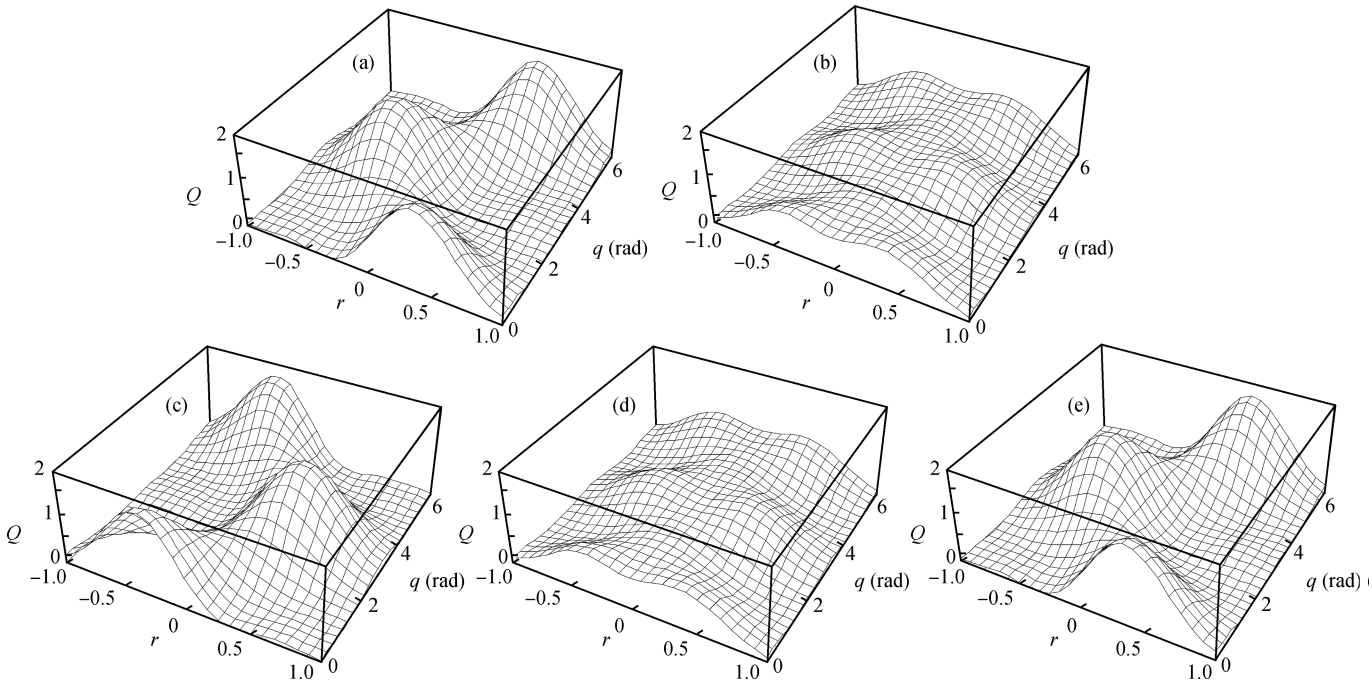

Fig. 2. Time evolution of the electron probability density in superposition of $|0\rangle$ and $|1\rangle$ in 3D QD. (a) $t = 0$. (b) $t = 0.25\ T_0$. (c) $t = 0.5\ T_0$. (d) $t = 0.75\ T_0$. (e) $t = T_0$.

Figures 1 and 2 show the time evolution of the electron probability density when the electron is in the superposition state of $(1/\sqrt{2})(|0\rangle + |1\rangle)$ for electron–LO-phonon coupling constant $\alpha = 6$, the confinement length $l = 0.5$ in a symmetric QD with parabolic confinement in both 2D (Fig. 1) and 3D (Fig. 2). We find that the electron probability density oscillates with the period of oscillation $T_0 = h/(E_1 - E_0)$ for the above material and shape parameters in both 2D and 3D parabolic QD. The time t in Figs. 1(a), 1(b), 1(c), 1(d), and 1(e) is 0, 0.25 T_0, 0.5 T_0, 0.75 T_0, and 1 T_0, respectively. The time t in Figs. 2(a), 2(b), 2(c), 2(d), and 2(e) is also 0, 0.25 T_0, 0.5 T_0, 0.75 T_0, and 1 T_0, respectively. Because of the use of Feynman units, the normalized result of the electron probability density cannot be obtained directly. But it can be seen that the quantum coherence of the system is obvious. When the electron is excited in the direction of $\theta = 0$, the maximum value of the

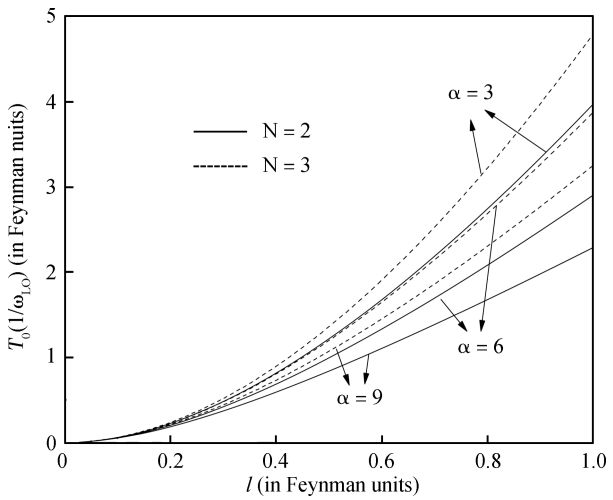

Fig. 3. Period of oscillation as a function of the confinement length l (in Feynman units) with three coupling strengths. The solid line and the dashed line represent the 2D and 3D, respectively.

probability density mainly appears in the direction of $\theta = 0$ or π and oscillates periodically. At the same time, as the value of the probability density is not equal to 0, the quantum tunneling probability exists. Certainly, we can adopt a deep energy potential barrier to prevent the occurrence of the tunneling possibility. Figures 1 and 2 also show that the electron probability density is larger in a 3D dot than in a 2D dot, which can be easily understood since one of the dimensions is strongly confined in the 2D QD.

Figure 3 presents the period of oscillation as a function of the confinement length with the different coupling strengths ($\alpha = 3, 6, 9$) in 2D (solid line) and 3D (dashed line) parabolic QDs. It is shown that the period of oscillation increases with increasing confinement length in both 2D and 3D QDs. The reason for this is that the energy spacing between the GS and the first ES decreases with increasing confinement length in both 2D and 3D QDs. Figure 3 also shows that the confinement length effect is stronger in a 3D dot than in a 2D dot. The reason for this is that the energy difference ($E_1 - E_0$) is larger in a 2D dot than in a 3D dot, which can also be easily understood since one of the dimensions is strongly confined in 2D. From Fig. 3 we can also find that the period of oscillation decreases with increasing electron–phonon coupling strength because the coupling strength of the electron–phonon interaction is weaker in the first ES than that in the GS; the energy spacing increases with increasing coupling strength. The increase in energy spacing causes a decrease in the period of oscillation. A qubit cannot be independent of the environment and must interact with the heat bath. As a result, the interaction destroys the superposition state of a qubit, which is decoherence[12]. The period of oscillation T_0 decreases, that is, the life time of a qubit reduces, so the process of decoherence is sped up. It is very harmful to store information which makes the QD its elementary unit. But, in principle, this effect can be minimized by a more precise fabrication technology, by cooling the crystal and by choosing the state and the physical parameters properly[13].

4. Summary

The eigenenergies and the relevant eigenwavefunctions of the GS and the first ES of electron have been obtained in both 2D and 3D QD with parabolic confinement using the Pekar type variational method in the electron–LO-phonon strong-coupling region. The single qubit can be envisaged as this kind of two-level quantum system in a QD. The electron probability density oscillates with a period when the electron is in the superposition state of the GS and the first ES. The results also indicate that this effect becomes much more pronounced with decreasing dimensionality.

References

[1] Benioff P. The computer as a physical system: a microscopic quantum mechanical Hamiltonian model of computers as represented by Turing machines. Journal of Statistical Physics, 1980, 22: 563
[2] Feyneman R. Simulating physics with computers. International Journal of Theoretical Physics, 1982, 21: 467
[3] Li S S, Wu X G, Zheng H Z. Recent progress in solid-state quantum computing. Physics, 2004, 33: 404 (in Chinese)
[4] Angelakis D G, Santos M F, Yannopapas V, et al. A proposal for the implementation of quantum gates with photonic-crystal waveguides. Phys Lett A, 2007, 362: 377
[5] Hao Xiang, Zhu Shiqun. Swap action in a solid-state controllable anisotropic Heisenberg model. Phys Lett A, 2008, 372: 1119
[6] Li S S, Xia J B, Liu J L, et al. InAs/GaAs single-electron quantum dot qubit. J Appl Phys, 2001, 90: 6151
[7] Li S S, Long G L, Bai F S, et al. Quantum computing. Proceedings of the National Academy of Sciences USA, 2001, 98: 11847
[8] Wang Z W, Li W P, Yin J W, et al. Properties of parabolic linear bound potential and coulomb bound potential quantum dot qubit. Commun Theor Phys, 2008, 49: 331
[9] Wang Z W, Xiao J L. Parabolic linear bound potential quantum dot qubit and its optical phonon effect. Acta Phys Sinica, 2007, 56: 0678
[10] Chen S H. The decoherence of the two- and three-dimensional parabolic quantum dot qubit. Physica B, 2010, 405: 843
[11] Peeters F M, Wu X, Devreese J T. Ground-state energy of a polaron in n-dimensions. Phys Rev B, 1986, 33(6): 3926
[12] Li C Z, Huang M Q, Chen P X. Quantum communication and quantum computing. Changsha: National University of Defense Technology Press, 2000 (in Chinese)
[13] Berenco A, Deutsch D, Ekert A, et al. Conditional quantum dynamics and logic gates. Phys Rev Lett, 1995, 74(19): 4083