The optical phonon effect of quantum rod qubits*

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(Received 9 August 2011; revised manuscript received 12 November 2011)

The Hamiltonian of a quantum rod with an ellipsoidal boundary is given by using a coordinate transformation in which the ellipsoidal boundary is changed into a spherical one. Under the condition of strong electron–longitudinal optical phonon coupling in the rod, we obtain both the electron eigenfunctions and the eigenenergies of the ground and first-excited state by using the Pekar-type variational method. This quantum rod system may be used as a two-level qubit. When the electron is in the superposition state of the ground and first-excited states, the probability density of the electron oscillates in the rod with a certain period. It is found that the oscillation period is an increasing function of the ellipsoid aspect ratio and the transverse and longitudinal effective confinement lengths of the quantum rod, whereas it is a decreasing function of the electron–phonon coupling strength.

Keywords: quantum rod, qubit, probability density, oscillation period

PACS: 71.38.–k, 63.20.kd, 63.22.–m **DOI:** 10.1088/1674-1056/21/5/057108

1. Introduction

In recent years, quantum computing has been extensively researched. At present, it is still a very popular field of study. The key point is to utilize a two-state quantum system to store information and realize quantum computing based on the principle of quantum mechanics. In recent years, there has been a large amount of experimental work[1−3] on the quantum computer (QC). Meanwhile, a number of investigators have studied its properties in many aspects using a variety of theoretical methods.[4−7] Several schemes have been proposed to realize the QC in recent years.[8,9] In order to show the advantages of the QC over the classical computer, the QC needs to be composed of at least thousands of qubits. It is clear that a QC with a large number of qubits is more realizable in solids,[10] especially when invoking semiconductor nanostructures or quantum dots (QDs).[11] The semiconductor QD has been extensively studied because of its novel physical properties and potential applications in optoelectronics.[12] The two-level quantum system can be viewed as a single qubit in the QD. For such a single electron QD qubit, Li *et al.*[8,13] proposed 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 and Xiao[14] and Yin *et al.*[15] recently studied the properties of a two-level parabolic linear bound potential QD qubit and the influence of electric field on the parabolic QD qubit using a linear-combination operator method. We studied the ground state energy of the strong-coupling polaron in a quantum rod (QR).[16] However, the optical phonon effect of the electron QR qubit has not yet been investigated.

In the present article, we study the eigenenergies and the eigenfunctions of the ground and first-excited states of an electron which is strongly coupled to the longitudinal-optical (LO) phonon in a QR. We use a variational method of Pekar type. This system in the QR may be used as a two-level qubit. We obtain the probability density of the electron in the QR that oscillates with a certain period when the electron is in a superposition state of the ground and the first-excited states. The effects of the ellipsoid aspect ratio, the transverse and the longitudinal effective confinement lengths of the QR, and the electron–phonon coupling strength on the oscillation period, are discussed.

2. Theoretical model

The electron under consideration moves in a polar crystal QR with a three-dimensional anisotropic harmonic potential, and interacts with bulk LO phonons. The Hamiltonian of this electron–phonon interaction

*Project supported by the National Natural Science Foundation of China (Grant No. 10964005).
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system can be written as

$$H = \frac{p_\parallel^2}{2m} + \frac{p_z^2}{2m} + \sum_{\boldsymbol{q}} \hbar\omega_{\rm LO} a_{\boldsymbol{q}}^+ a_{\boldsymbol{q}} + \frac{1}{2}m\omega_\parallel^2\rho^2 + \frac{1}{2}m\omega_z^2 z^2 + \sum_{\boldsymbol{q}} \left[V_q a_{\boldsymbol{q}} \exp\left(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}\right) + \text{h.c.}\right], \quad (1)$$

where m is the band mass, $\omega_\parallel$ and ω_z are the measures of the transverse and the longitudinal confinement strengths of the three-dimensional anisotropic harmonic potential in the radius and the length directions of the rod, respectively, $a_{\boldsymbol{q}}^+$ ($a_{\boldsymbol{q}}$) denotes the creation (annihilation) operator of the bulk LO phonon with wave vector $\boldsymbol{q}(\boldsymbol{q}_{||}, q_z)$, $\boldsymbol{p} = (\boldsymbol{p}_\parallel, p_z)$ and $\boldsymbol{r} = (\boldsymbol{\rho}, z)$ are the momentum vector and the position vector of the electron, respectively. V_q and α are

$$V_q = \mathrm{i}\left(\frac{\hbar\omega_{\rm LO}}{q}\right)\left(\frac{\hbar}{2m\omega_{\rm LO}}\right)^{1/4}\left(\frac{4\pi\alpha}{v}\right)^{1/2},$$
$$\alpha = \left(\frac{e^2}{2\hbar\omega_{\rm LO}}\right)\left(\frac{2m\omega_{\rm LO}}{\hbar}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right). \quad (2)$$

We introduce a coordinate transformation,[17] $x' = x$, $y' = y$, $z' = z/e'$, where e' is the ellipsoid aspect ratio, and (x', y', z') is the transformed coordinate. With the above transformation, the ellipsoidal boundary is converted into a spherical one. The Hamiltonian of the electron–phonon system in the new coordinate is changed into H'. By employing the well-known Lee–Low–Pines (LLP) transformation

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

where f_q (f_q^*) is the variational function, and we obtain

$$H'' = U^{-1}H'U. \quad (4)$$

For convenience, we use spherical coordinates, and then the ground state wave function is a Gaussian. Following the Pekar variational method, we may choose the trial ground state wavefunction of the electron–phonon system to be

$$|\phi_0\rangle = |0\rangle|0_{\rm ph}\rangle = \pi^{-3/4}\lambda_0^{3/2}\exp\left(-\frac{\lambda_0^2 r^2}{2}\right)|0_{\rm ph}\rangle, \quad (5)$$

where λ_0 is the variational parameter, $|0_{\rm ph}\rangle$ is the unperturbed zero-phonon state, which satisfies $a|0_{\rm ph}\rangle = 0$, and $|0\rangle$ is the trial ground state wavefunction of the electron. Similarly, the trial wave function of the electron–phonon system in the first-excited state may be chosen as

$$|\phi_1\rangle = |1\rangle|0_{\rm ph}\rangle = \left(\frac{\pi^3}{4}\right)^{-1/4}\lambda_1^{5/2} r\cos\theta \times \exp\left(-\frac{\lambda_1^2 r^2}{2}\right)|0_{\rm ph}\rangle, \quad (6)$$

where λ_1 is the variational parameter, and $|1\rangle$ is the first-excited state trial wavefunction of the electron with $\langle 0|0\rangle = 1$, $\langle 1|1\rangle = 1$, $\langle 1|0\rangle = 0$. The above equation satisfies the following normalized relation:

$$\langle\phi_0|\phi_0\rangle = 1, \quad \langle\phi_0|\phi_1\rangle = 0, \quad \langle\phi_1|\phi_1\rangle = 1. \quad (7)$$

By minimizing the expectation value of the Hamiltonian, we then obtain the electron ground state energy $E_0 = \langle\phi_0|H''|\phi_0\rangle$ and the first-excited state energy $E_1 = \langle\phi_1|H''|\phi_1\rangle$. The ground state energy of the electron in the QR can be written as

$$E_0(\lambda_0) = \left(1 + \frac{e'^2}{2}\right)\lambda_0^2 + \frac{1}{\lambda_0^2 l_{\rm p}^4} + \frac{1}{2\lambda_0^2 e'^2 l_{\rm v}^4} - \frac{\sqrt{2}}{\sqrt{\pi}}\alpha\lambda_0 A(e'), \quad (8)$$

where $l_{\rm p} = \sqrt{\hbar/m\omega_\parallel'}$ and $l_{\rm v} = \sqrt{\hbar/m\omega_z'}$ are the transverse and the longitudinal effective confinement lengths, respectively, and

$$A(e') = \begin{cases} \dfrac{\arcsin\sqrt{1-e'^2}}{\sqrt{1-e'^2}}, & e' < 1, \\ 1, & e' = 1, \\ \dfrac{1}{2\sqrt{e'^2-1}}\ln\dfrac{e'+\sqrt{e'^2-1}}{e'-\sqrt{e'^2-1}}, & e' > 1. \end{cases} \quad (9)$$

The first-excited state energy of the electron in the QR is given by

$$E_1(\lambda_1) = \left(1 + \frac{e'^2}{2}\right)\lambda_1^2 + \frac{1}{\lambda_1^2 l_{\rm p}^4} + \frac{3}{2\lambda_1^2 e'^2 l_{\rm v}^4} - \frac{7\sqrt{2}\alpha}{8\sqrt{\pi}}\lambda_1 A(e'). \quad (10)$$

We can obtain λ_0 and λ_1 by using the variational method and thus acquire the eigen levels and the eigen wave functions. So a two-level system as a single qubit has been built up. The superposition state of the electron in the QR can be expressed as

$$|\psi_{01}\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right), \quad (11)$$

where

$$|0\rangle = \psi_0(r) = \pi^{-3/4}\lambda^{3/2}\exp\left(-\frac{\lambda^2 r^2}{2}\right), \quad (12)$$
$$|1\rangle = \psi_1(r)$$

$$= \left(\frac{\pi^3}{4}\right)^{-1/4} \lambda^{5/2} r\cos\theta \exp\left(-\frac{\lambda^2 r^2}{2}\right). \quad (13)$$

The time evolution of the quantum state of the electron in the QR can be written as

$$\psi_{01}(r,t) = \frac{1}{\sqrt{2}}\psi_0(r)\exp\left(-\frac{\mathrm{i}E_0 t}{\hbar}\right) + \frac{1}{\sqrt{2}}\psi_1(r)\exp\left(-\frac{\mathrm{i}E_1 t}{\hbar}\right). \quad (14)$$

The probability density of the electron in the QR is given by

$$\begin{aligned} Q(r,t) &= \left|\psi_{01}(r,t)\right|^2 \\ &= \frac{1}{2}\left[\left|\psi_0(r)\right|^2 + \left|\psi_1(r)\right|^2 \right. \\ &\quad + \psi_0^*(r)\psi_1(r)\exp(\mathrm{i}\omega_{01}t) \\ &\quad \left. + \psi_0(r)\psi_1^*(r)\exp(-\mathrm{i}\omega_{01}t)\right], \end{aligned} \quad (15)$$

where $\omega_{01} = (E_1 - E_0)/\hbar$ is the transition frequency between the first-excited state and the ground state. The oscillation period of the probability density of the electron in the QR is

$$T_0 = \frac{h}{E_1 - E_0}. \quad (16)$$

3. Results and discussion

We use the usual polaron units ($\hbar = 2m = \omega_{\mathrm{LO}} = 1$). The numerical results of electron probability density $Q(r,t)$ are presented in Fig. 1. The results of the oscillation period T_0 versus ellipsoid aspect ratio e' and electron–phonon coupling strength α and versus the transverse and the longitudinal effective confinement lengths of the QR l_{p} and l_{v} are presented in Figs. 2 and 3, respectively.

Figure 1 shows the time evolution of the probability density $\left|\psi_{01}(\rho,z,t)\right|^2$ when the electron is in the superposition state of $\left(1/\sqrt{2}\right)(|0\rangle + |1\rangle)$ with electron–phonon coupling strength $\alpha = 6.0$. The transverse and the longitudinal effective confinement lengths are $l_{\mathrm{p}} = 2.0$ and $l_{\mathrm{v}} = 3.0$, the phase difference has $\cos\theta = 1$, and the ellipsoid aspect ratio is $e' = 1.4$. We find that the electron oscillates in the QR with an oscillation period of $T_0 = h/(E_1 - E_0)$. The values of time t in Figs. 1(a)–1(e) are $0T_0$, $0.25T_0$, $0.5T_0$, $0.75T_0$, and $1T_0$, respectively. From Figs. 1(a)–1(e), we find that the electron probability density varies periodically with ρ and z. Moreover, due to the presence of the three-dimensional anisotropic harmonic potential in the radius and the length directions of the QR, the electron probability density shows a double-peak configuration, whereas there is only one peak if the confinement is a two-dimensional symmetric one in the x- and the y-directions of the QR. This result is similar to that of the QD case in Refs. [14] and [15].

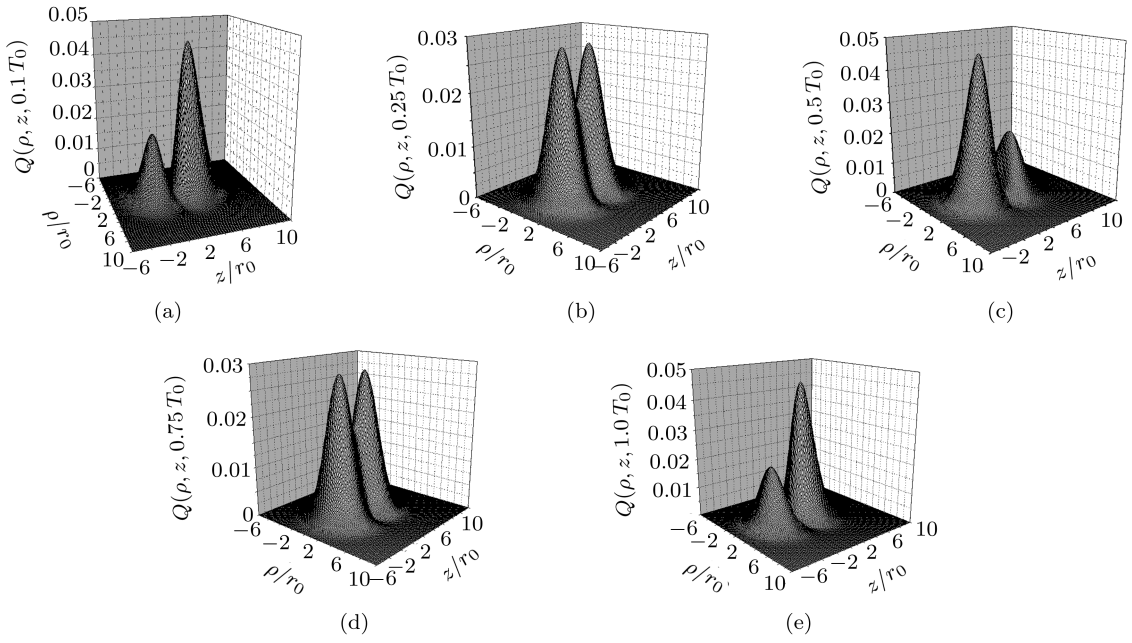


Fig. 1. Time evolution of probability density $\left|\psi_{01}(\rho,z,t)\right|^2$ of the electron in the superposition state of $|0\rangle$ and $|1\rangle$ at the time of (a) $0\,T_0$, (b) $0.25\,T_0$, (c) $0.5\,T_0$, (d) $0.75\,T_0$, and (e) $1\,T_0$.

Figure 2 shows the oscillation period T_0 as a function of ellipsoid aspect ratio e' and electron–phonon coupling strength α for $l_{\rm p} = 2.0$ and $l_{\rm v} = 3.0$. From Fig. 2, we find that the oscillation period T_0 increases with the increase in ellipsoid aspect ratio e', because the influence of the ellipsoid aspect ratio is weaker in the first-excited state than that in the ground state, and its increase in the first-excited state is smaller than that in the ground state with decreasing ellipsoid aspect ratio. For this reason, the energy spacing between the first-excited state and the ground state increases with the decrease in ellipsoid aspect ratio, and the oscillation period decreases. The results of our investigation[18] indicate that when the aspect ratio is quite small, the shape of the rod approaches that of a two-dimensional quantum well. In the extreme case of the aspect ratio being 1, the rod becomes a zero-dimensional QD. If the aspect ratio is large enough, the rod resembles a one-dimensional quantum wire. In other words, QRs constitute a bridge between two-dimensional quantum wells, zero-dimensional QDs, and one-dimensional quantum wires. Investigations of the transition regimes from quantum wells to QDs and to quantum wires are of particular interest in the case of colloidal semiconductor QRs, and the size and shape control enable the synthesis of QRs with precise lengths and diameters. Therefore, by tuning the aspect ratio of the ellipsoid, we can follow the transition from two- to zero- and to one-dimensional systems. This opens a new way to tune the oscillation period of the electron probability density by changing the ellipsoid aspect ratio of the rod, thus changing the life time of the qubit, which suggests a new way to suppress the decoherence. From Fig. 2, we can also see that the oscillation period decreases with the increase in electron–phonon coupling strength. Because the coupling strength of the electron–phonon interaction in the QR is weaker in the first-excited state than that in the ground state, and the increase in the first-excited state is smaller than that in the ground state with the increasing coupling strength, the energy spacing between the first-excited state and the ground state increases with the increase in coupling strength. The increase in the energy spacing causes a reduction in the oscillation period.

Figure 3 shows the period of oscillation T_0 as a function of the transverse and the longitudinal effective confinement lengths $l_{\rm p}$ and $l_{\rm v}$ of the QR for $\alpha = 6.0$ and $e' = 1.4$. It can be seen that the period of oscillation T_0 increases with the increases in $l_{\rm p}$ and $l_{\rm v}$. This is because the electron energy and the interaction energy of the electron–phonon, which takes the phonon as a medium, are enhanced when the particle motion range becomes smaller due to the decreasing confinement length. The energy spacing between the first-excited state and the ground state decreases with the increases in the effective confinement lengths of the QR, and the oscillation period increases. These phenomena can be attributed to the interesting quantum confinement effect.

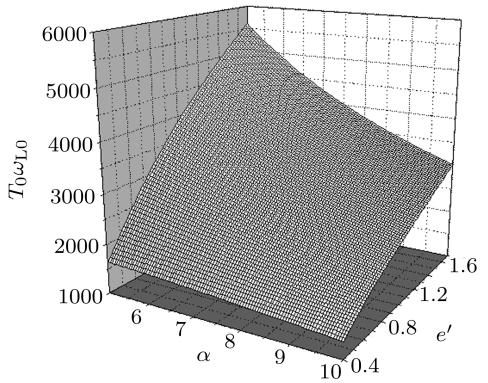


Fig. 2. The period of oscillation, T_0, in the QR as a function of ellipsoid aspect ratio, e', and electron–phonon coupling strength, α.

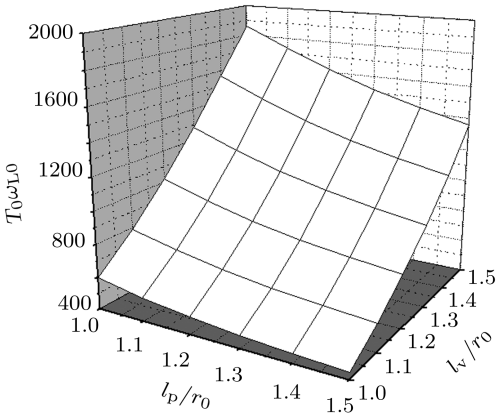


Fig. 3. The period of oscillation, T_0, in the QR as a function of the transverse and the longitudinal effective confinement lengths, $l_{\rm p}$ and $l_{\rm v}$, of the QR.

To use the ground and the first-excited states as a qubit, their energy difference must be smaller than that between the first- and the second-excited states. Theoretically, this can be realized by choosing appropriate trial eigenfunctions of the ground and the first-excited states, as well as the second-excited state, with the help of the Pekar-type variational method. From an experimental point of view, the energy levels in

the rod can be well controlled by tuning the rod size, the aspect ratio of the rod, or the material of the rod (electron–phonon coupling strength α). In addition, by introducing an external electric or magnetic field or impurities (Coulomb interaction), the energy difference between the ground and the first-excited states can also be set to be smaller than that between the first- and the second-excited states.

The above results indicate that to increase the lifetime of the qubit, the oscillation period of the electron density must be enlarged, which can be fulfilled by using (i) weak-coupling materials for the rod, (ii) a larger vertical radius and longitudinal length, and (iii) a larger ellipsoid aspect ratio. In all the above methods, the decoherence process can be suppressed.

4. Conclusion

Based on the Pekar-type variational method, we study the eigenenergies and eigenfunctions of the ground and first-excited states of an electron strongly coupled to the LO phonons in a QR. This quantum rod system may be used as a two-level qubit. When the electron is in a superposition state of the ground and the first-excited states, the probability density of the electron oscillates in the QR with a certain period. It is found that the oscillation period is an increasing function of the ellipsoid aspect ratio and the effective confinement length, whereas it is a decreasing one of the coupling strength.

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