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The Polaron Self-Energy in a Parabolic Quantum Dot

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Abstract

Polaronic states in a parabolic quantum dot are investigated by using the second order Rayleigh-Schrödinger perturbation theory. It is shown that the absolute values of the ground state energy correction and the excited state energy correction as well as the relevant transition energies increase with decreasing the size of the quantum dot. The results also indicate that the polaron effects in small quantum dots are stronger than those in the corresponding bulk materials.

I. Introduction

With recent advances in nanofabrication technology it is possible to confine electrons in all three spatial dimensions in semiconductors called quantum dots[1-3]. They are typically a few hundred nanometers long or wide and a few nanometers thick. The electron energy spectrum of such quantum dots is fully quantized. These quantum dots are often referred to as artificial atoms which the atomic potential is in place of the artificially constructed dot potential. Because of the potential device applications and a lot of new physical effects in such structures, understanding the electronic properties of these systems is particularly important.

The interaction of the electrons with longitudinal-optical (LO) phonons in quantum dots has been investigated by various authors[4-8]. Recently, Roussignol *et al.*[4] have shown experimentally and explained theoretically that phonon broadening is quite important in very small semiconductor quantum dots. M.C. Klein *et al.*[6] studied the size dependence of electron-phonon coupling in semiconductor nanospheres, and derived the expression of the vibrational LO and SO eigenfunctions for a sphere in the continuum approximation. Zhu and Gu[9] have shown that the polaron effects play a prominent role in thin quantum wires. In a recent paper, M.H. Degani and G.A. Farias[10] also investigated the polaron effects in quantum wires and dots and found that the effects of the interface phonons are important and cannot be neglected in quantum wires and quantum dots. We will further investigate the polaronic states in a parabolic quantum dot in this paper. For the sake of analyticity, we will model the relevant vibrational modes by the corresponding bulk modes, i.e., we will neglect any size quantization of the phonons. This assumption has been used by Schmitt-Rink, Miller and Chemla[7] and Bockelmann and Bastard[8] to treat the phonon broadening of optical spectra and the phonon scattering in quantum dots. Taking into account the effect of phonon confinement, one would certainly vary the results in comparison with those of the bulk-phonon model. We will treat this effect in a forthcoming paper.

II. Theory

Since the electrons are much more strongly confined in one direction (taken as the z direction) than in other two directions, we will confine ourselves to consider only the motion

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of the electrons in the $x-y$ plane. Kumar *et al.*[11] have shown that even if the defining cap layer is square shaped, the confining potential seen by electrons in a quantum dot has nearly circular symmetry. The energy levels are found to be insensitive to the charge in the dot at a fixed gate voltage, and the evolution of energy levels with increasing magnetic field is similar to that for a parabolic potential. Recently, it was pointed out by F.M. Peeters[12] that this is a consequence of the generalized Kohn's theorem which is valid for a quadratic confinement potential. These results make the parabolic confining potential model very appealing. We will use this parabolic confining potential model in the present work.

We assume that the confining potential in a single quantum dot is parabolic $V(\rho) = m^*\omega_0^2\rho^2/2$, where m^* is the bare band mass and ρ is the coordinate vector of a two-dimensional quantity. The Hamiltonian of electron-phonon systems is given by

$$H = H_0 + H_1\,, \tag{1}$$

$$H_0 = \frac{1}{2m^*}p^2 + \frac{1}{2}m^*\omega_0^2\rho^2 + \sum_{\mathbf{q}}\hbar\omega_{\mathrm{LO}}b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}\,, \tag{2}$$

$$H_1 = \sum_{\mathbf{q}}(V_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}b_q + V_{\mathbf{q}}^{+}e^{-i\mathbf{q}\cdot\mathbf{r}}b_{\mathbf{q}}^{\dagger})\,, \tag{3}$$

where $b_{\mathbf{q}}^{\dagger}$ creates a bulk LO-phonon of wave vector $\vec{\mathbf{q}}$, $\vec{\mathbf{q}} = (\vec{q}_{\parallel}, q_z)$ and $\vec{r} = (\vec{\rho}, z)$ is the coordinate of the electron,

$$V_{\mathbf{q}} = i\frac{\hbar\omega_{\mathrm{LO}}}{q}\Big(\frac{\hbar}{2m^*\omega_{\mathrm{LO}}}\Big)^{1/4}\Big(\frac{4\pi\alpha}{V}\Big)^{1/2}. \tag{4}$$

The energy levels of the unperturbed Hamiltonian H_0 are given by[13,14]

$$E_{nm}^{(0)} = (2n + |m| + 1)\hbar\omega_0\,, \tag{5}$$

where m is the angular quantum number, $m = 0, \pm1, \pm2, \cdots$, and n is the radial quantum number, $n = 0, 1, 2, \cdots$. The corresponding wave functions are given by

$$|n, m, 0_{\mathbf{q}}\rangle = \frac{1}{\sqrt{2\pi}}e^{im\theta}\Big[\frac{2m^*\omega_0 n!}{\hbar(n+|m|)!}\Big]^{1/2}x^{|m|}L_n^{|m|}(x^2)e^{-x^2/2}|0_{\mathbf{q}}\rangle\,, \tag{6}$$

where $x = \rho(m^*\omega_0/\hbar)^{1/2}$, L_n^m are associated Laguerre polynomials, and $|0_{\mathbf{q}}\rangle$ is a vacuum state of the phonon, which satisfies $b_{\mathbf{q}}|0_{\mathbf{q}}\rangle = 0$.

Since the electron-phonon interaction is weak in these systems (e.g., Al_xGa_{1-x} As/GaAs), in the sense that the Frohlich coupling constant (α) is of the order of 0.1, we will use the second order Rayleigh-Schrödinger perturbation theory to obtain the electronic self-energy shift δE_{nm}, which is given by

$$\delta E_{nm} = -\alpha(\hbar\omega_{\mathrm{LO}})^2\Big(\frac{\hbar}{2m^*\omega_{\mathrm{LO}}}\Big)^{1/2}\sum_{n'm'}Q_{nmn'm'}\{[2(n'-n) + (|m'|-|m|)]\hbar\omega_0 + \hbar\omega_{\mathrm{LO}}\}^{-1}\,, \tag{7}$$

where

$$Q_{nmn'm'} = \int_0^{\infty}dq_{\parallel}[V_{nmn'm'}(q_{\parallel})]^2\,, \tag{8}$$

$$\begin{aligned}V_{nmn'm'}(q_{\parallel}) = 2\Big[\frac{n'!n!}{(n'+|m'|)!(n+|m|)!}\Big]^{1/2}&\int_0^{\infty}dx x^{|m'|+|m|+1}L_{n'}^{|m'|}(x^2)\\ &\times L_n^{|m|}(x^2)J_{m-m'}(-q_{\parallel}l_0x)\,,\end{aligned} \tag{9}$$

where $l_0 = (\hbar/m^*\omega_0)^{1/2}$, and J_n is the first kind of Bessel functions.

Putting $n = 0$ and $m = 0$, then the ground state energy correction is given by

$$\delta E_{00} = -\alpha\hbar\omega_{\mathrm{LO}}\Big(\frac{\hbar}{2m^*\omega_{\mathrm{LO}}}\Big)^{1/2}\sum_{n'm'}Q_{00n'm'}\Big[(2n'+|m'|)\frac{\omega_0}{\omega_{\mathrm{LO}}} + 1\Big]^{-1}. \tag{10}$$

When only the lowest energy level is occupied, the selection rules allow only two excitations, from the state (0, 0) to (0, −1), and from (0, 0) to (0, 1)[15,16]. Consequently, the correction δE_{01} to the excited level (0, 1) is given by

$$\delta E_{01} = -\alpha\hbar\omega_{LO}\left(\frac{\hbar}{2m^*\omega_{LO}}\right)^{1/2}\sum_{n'm'} Q_{01n'm'}\left[(2n'+|m'|-1)\frac{\omega_0}{\omega_{LO}}+1\right]^{-1}, \tag{11}$$

and the correction δE_{0-1} to the excited level (0, −1) is given by

$$\delta E_{0-1} = -\alpha\hbar\omega_{LO}\left(\frac{\hbar}{2m^*\omega_{LO}}\right)^{1/2}\sum_{n'm'} Q_{0-1n'm'}\left[(2n'+|m'|-1)\frac{\omega_0}{\omega_{LO}}+1\right]^{-1}. \tag{12}$$

The relevant transition energy for (0, 0) → (0, 1) transition is given by $\Delta E_{01} = (E_{01} + \delta E_{01}) - (E_{00} + \delta E_{00})$. The relevant transition energy for (0, 0) → (0, −1) transition is given by $\Delta E_{0-1} = (E_{0-1} + \delta E_{0-1}) - (E_{00} + \delta E_{00})$.

III. Numerical Results

The numerical results of the ground state energy correction and the excited state energy correction in GaAs parabolic quantum dots are presented in Fig. 1 and Fig. 2. From Fig. 1 we can see that the absolute values of the ground state energy correction increase with decreasing the effective confinement length of the quantum dot. Especially, when the effective confinement length is less than $1.5r_0$ (r_0 is the polaron radius), the ground state energy correction is larger than $\alpha\hbar\omega_{LO}$ which is the ground state energy correction of the three-dimensional case. That is, the polaron effects in small quantum dots are stronger than those in three-dimensional case. Figure 2 illustrates that the absolute values of the excited state energy correction also increase with decreasing the effective confinement length of the quantum dot. The figures also show that δE_{01} is nearly the same as δE_{0-1}.

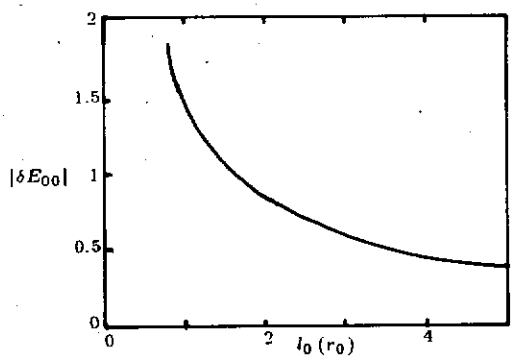

Fig. 1. The ground state energy correction (in unit of $\alpha\hbar\omega_{LO}$) in GaAs parabolic quantum dots as a function of the confinement length of the quantum dot.

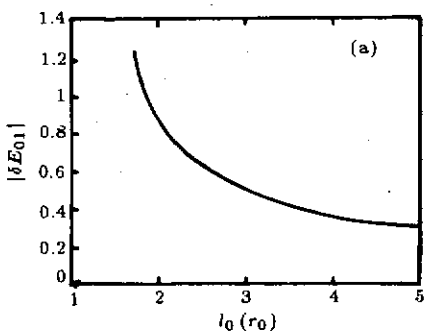

Fig. 2a. The same as Fig. 1 but for the excited state energy correction for the level (0, 1).

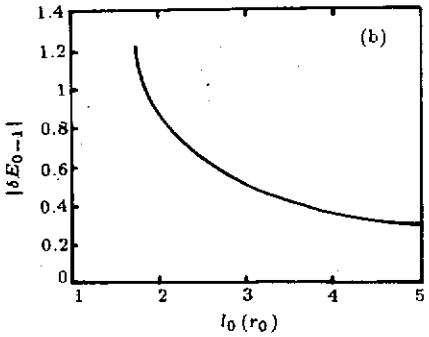

Fig. 2b. The same as Fig. 1 but for the excited state energy correction for the level (0, −1).

Figure 3 presents the relevant transition energy for $(0, 0) \rightarrow (0, 1)$ and $(0, 0) \rightarrow (0, -1)$ as a function of the effective confinement length of the quantum dot. It is shown that the relevant transition energies are enhanced as the effective confinement length of the quantum dot is reduced.

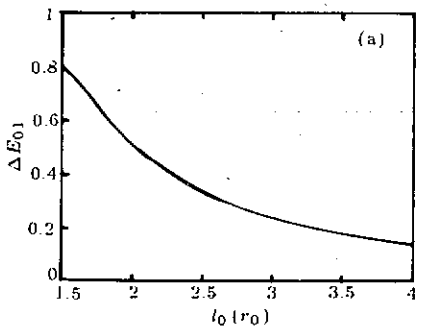

Fig. 3a. The transition energy for $(0, 0) \rightarrow (0, 1)$ (in unit of $\hbar\omega_{LO}$).

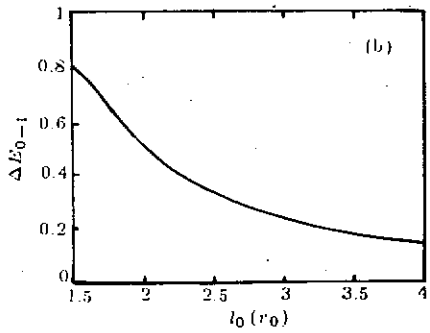

Fig. 3b. The transition energy for $(0, 0) \rightarrow (0, -1)$ (in unit of $\hbar\omega_{LO}$).

IV. Conclusions

In conclusion, we have investigated the polaron effects in GaAs parabolic quantum dots. We find that the absolute values of the ground state energy correction and the excited state energy correction increase with decreasing the effective confinement length of the quantum dot, and the relevant transition energy is also enhanced as the effective confinement length of the quantum dot is reduced. The results also indicate that the polaron effects in small quantum dots are stronger than those in the corresponding bulk materials. It should be emphasized that the use of 2D disk approximation for the electronic wave function is not an essential restriction of this paper, it has been done only for the sake of analytic convenience. Introduction of the finite width of the electronic wave function in z direction into the above formalism is straightforward and it will reduce the effective electron-phonon interaction[17]. But, the qualitative features in this paper are independent of this approximation.

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