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ABSTRACT

Strong-coupling polaron in a parabolic quantum dot is investigated by the Landau-Pekar variational treatment. The polaron binding energy and the average number of virtual phonons around the electron as a function of the effective confinement length of the quantum dot are obtained in Gaussian function approximation. It is shown that both the polaron binding energy and the average number of virtual phonons around the electron decrease by increasing the effective confinement length. The results indicate that the polaronic effects are more pronounced in quantum dots than those in two-dimensional and three-dimensional cases.

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1 Introdution

With recent advances in nanofabrication technology it has become possible to confine electrons in all three spatial dimensions in semiconductors called quantum dots [1-3]. These quantum dots are often referred to as artificial atoms in which the atomic potential is replaced by the artificially constructed dot potential. The novel effects of such systems have generated a great deal of interest. The interaction of the electrons with LO-phonons in such quantum dots has been investigated by several authors [4-12]. Recently, Roussignol et al.[4] have shown experimentally and explained theoretically that phonon broadening is quite important in very small semiconductor quantum dots. M.H.Degani and G.A.Farias [10] found that effects of the interface phonons are important and cannot be neglected in quantum dots. In a recent paper[11], we have investigated the polaron effects in a parabolic quantum dot by using the second order Rayleigh-Schrodinger perturbation theory. However, all of these studies are treated in the weak coupling regime. More recently, within the framework of the strong-coupling polaron theory ,T.Yildirim and A. Ercelebi[13] obtained the ground-state binding energy and the effective mass as a function of the effective dimensionality in a quantum well confinement. A.Chatterjee[14] utlized the Landau-Pekar variational theory to study the multidimensional free-optical-polaron problem in the strong-coupling regime. The general result is that the polaronic effects are more prounounced in lower dimensions. In the present paper, we use the same treatments used by Chatterjee to investigate zero-dimensional polarons in the strong-coupling limit. For the sake of simplity, the phonons are described by the corresponding bulk modes and the electron wave function is used by the Gaussian function approximation.

2 Theory

The electrons are much more strongly confined in one direction (taken as the z direction) than in other two directions. Therefore, we shall confine ourselves to consider only the motion of the electrons in the x-y plane. As an interesting theoretical model we assume that the confining potential in a single quantum dot is parabolic:[11],[12]

$$V(\rho) = \frac{1}{2}m^*\omega_o^2\rho^2, \tag{1}$$

where m^* is the bare band mass and ρ is the coordinate vector of a two-dimensional quantity. The Hamiltonian of electron-phonon system is given by

$$H = -(\hbar^2/2m^*)\nabla_\rho^2 + \frac{1}{2}m^*\omega_o^2\rho^2 + \sum_{\mathbf{q}}\hbar\omega_{LO}b_{\mathbf{q}}^+b_{\mathbf{q}} + \sum_{\mathbf{q}}(V_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}b_{\mathbf{q}} + V_{\mathbf{q}}^+e^{-i\mathbf{q}\cdot\mathbf{r}}b_{\mathbf{q}}^+), \tag{2}$$

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

$$V_q = i(\hbar\omega_{LO}/q)(\hbar/2m^*\omega_{LO})^{1/4}(4\pi\alpha/V)^{1/2}. \tag{3}$$

$$\alpha = (e^2/2\hbar\omega_{LO})(2m^*\omega_{LO}/\hbar)^{1/2}(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}). \tag{4}$$

where ϵ_∞ is the optical dielectric constant and ϵ_0 is the static dielectric constant.

The trial wave function for Hamiltonian (2) is chosen as[14]

$$|\psi>=|\phi(\rho)>|\xi(z)>exp[\sum_{\mathbf{q}}(f_{\mathbf{q}}b_{\mathbf{q}}^{+}+f_{\mathbf{q}}^{*}b_{\mathbf{q}})]|0_{\mathbf{q}}>, \tag{5}$$

where $f_{\mathbf{q}}$ will be treated as a variational function, $|0_{\mathbf{q}}>$ is the unperturbed zero phonon state which satisfies $b_{\mathbf{q}}|0_{\mathbf{q}}>=0$, and $\phi(\rho)$ is the electron wave function,

$$\phi(\rho)=(\lambda/\pi^{1/2})exp(-\lambda^{2}\rho^{2}/2), \tag{6}$$

where λ is a variational parameter, and $|<\xi(z)|\xi(z)>|^{2}=\delta(z)$ since the electrons are considered to be confined in an infinitesimally narrow layer. This is an idealization and, in reality, electron wave function will have some natural width[15]. We shall treat this effect in a forthcoming paper.

The energy of system is given by

$$E^{(0D)}(\lambda)=<\psi|H|\psi>=\hbar^{2}\lambda^{2}/2m^{*}+(\hbar^{2}/m^{*})/(2\lambda^{2}l_{0}^{4})-\frac{1}{2}(2\pi)^{1/2}(\hbar\omega_{LO})^{2}r_{0}\alpha\lambda, \tag{7}$$

where $l_0=(\hbar/m^{*}\omega_0)^{1/2}$ is the effective confinement length, $r_0=(\hbar/2m^{*}\omega_{LO})^{1/2}$ is the polaron radius. The energy levels are minimized numerically with respect to the variational parameter λ.

If the units have been chosen in usual polaron units ($\hbar=2m^{*}=\omega_{LO}=1$), then the ground state energy in a parabolic quantum dot is given by

$$E_{g}^{(0D)}/E_{g}^{(3D)}=3\pi\lambda_{0}^{2}/\alpha^{2}+3\pi/(2\lambda_{0}^{2}\alpha^{2}l_{0}^{4})-\frac{3}{2\alpha}\sqrt{2}\pi^{3/2}\lambda_{0}, \tag{8}$$

where $E_g^{(3D)}(=\alpha^2/3\pi)$ is the polaron binding energy in the three-dimensional case[14]. λ_0 can be obtained by minimizing Eq.(7).

The polaron binding energy, relative to the subband energy level, is given by

$$E_{b}^{(0D)}/E_{g}^{(3D)}=(3\pi/\alpha^{2}l_{0}^{2})-E_{g}^{(0D)}/E_{g}^{(3D)}. \tag{9}$$

We can also evaluate the average number of virtual phonons around the electron in the ground state which is given by,

$$N_{p}^{(0D)}=<\psi|\sum_{\mathbf{q}}b_{\mathbf{q}}^{+}b_{\mathbf{q}}|\psi>=\frac{1}{2}(2\pi)^{1/2}(\hbar\omega_{LO})^{2}r_{0}\alpha\lambda_{0}, \tag{10}$$

That is,

$$N_{p}^{(0D)}/N_{p}^{(3D)}=\frac{3\sqrt{2}}{4\alpha}\pi^{3/2}\lambda_{0}, \tag{11}$$

where $N_p^{(3D)}(=2\alpha^2/3\pi)$ is the average number of virtual phonons around the electron in the three-dimensional case.

3 Numerical Results and Discussions

The numerical results of the polaron binding energy and the average number of virtual phonons around electron in a parabolic quantum dot as a function of the effective confinement length of the quantum dot are presented in Fig.1 and Fig.2. Fig.1 displays the polaron binding energy with $\alpha=5$ as a function of the effective confinement length of the quantum dots. From the figure we can see that the polaron binding energy decreases with the enhancement of the effective confinement length and slowly approach that in the two-dimensional case as the effective confinement length trends to infinity.This result indicates that the binding becomes much deeper than in the two-dimensional case since now the polaron squeezed in all three directions, which agree with the results of T.Yildirim [13]. Fig.2 presents the average number of virtual phonons around the electron with $\alpha=5$ as a function of the effective confinement length of the quantum dots. It is shown that the average number of virtual phonons around the electron decreases rapidly with increasing the effective confinement length and approach those in two-dimensional case as the effective confinement length trends to infinity, which again show that the polaronic effects become stronger in quantum dots in the strong-coupling regime. Fig.3 and Fig.4 illustrate the polaron binding energy and the average number of virtual phonons around the electron as a function of electron-LO-phonon coupling constant(α) for $l_0=0.5$, respectively. With increasing the coupling constant, both the polaron binding energy and the average number of virtual phonons around the electron increase rapidly. This implies that the larger the coupling constant, the stronger the binding of polaron, which is similar with the result in three-dimensional case[14].

4 Conclusions

In conclusion, we have investigated the strong coupling polaron in a parabolic quantum dot. We find that both the polaron binding energy and the average number of virtual phonons around the electron decrease with increasing the effective confinement length. These results indicate that the polaronic effects are more pronounced in quantum dots than those in two-dimensional and three-dimensional cases. It should be emphasized that the treatment used here fails to reflect the characterizations of the problem since the electron-phonon coupling is rather weak in actual materials of interest. We hope that this paper will stimulate more experimental work which will be helpful in a better understanding of the role of electron-LO-phonon interaction in quantum dots.

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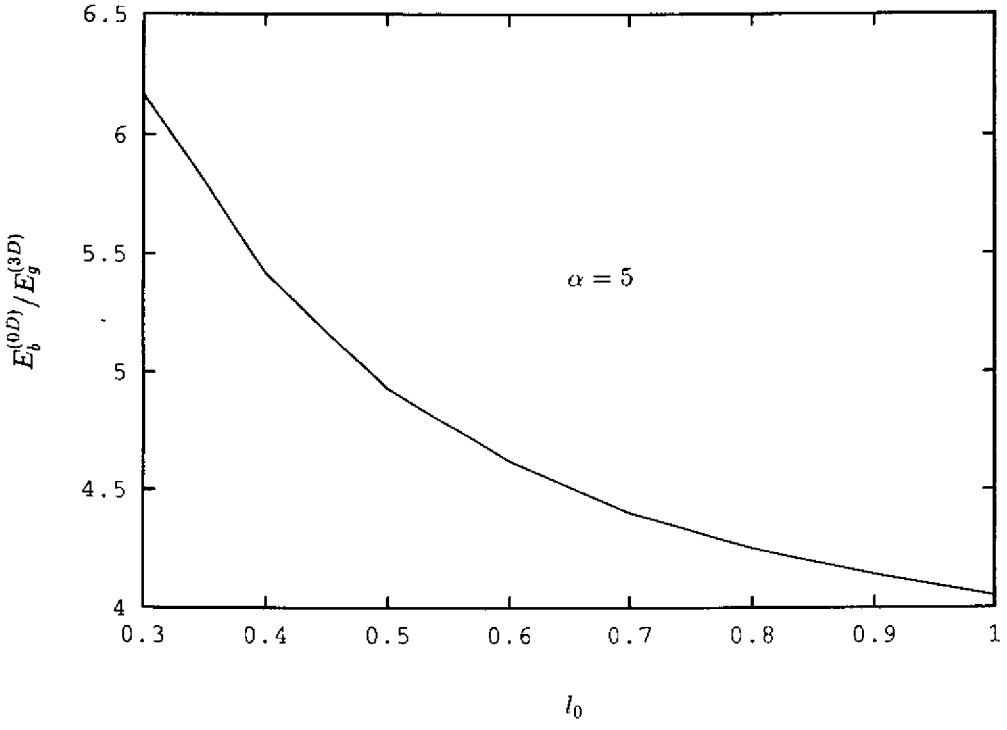
FIGURE CAPTIONS

Fig.1 The polaron binding energy $E_b^{(0D)}$ of parabolic quantum dots($\alpha = 5$) in units $E_g^{(3D)}(=\alpha^2/3\pi)$ as a function of the effective confinement length of the quantum dot(l_0).

Fig.2 The average number $N_p^{(0D)}$ of virtual phonons around the electron in the ground-state of parabolic quantum dots($\alpha = 5$) in units $N_p^{(3D)}(=2\alpha^2/3\pi)$ as a function of the effective confinement length of the quantum dot(l_0).

Fig.3 The polaron binding energy as a function of electron-LO-phonon coupling constant(α) for $l_0 = 0.5$.

Fig.4 The average number of virtual phonons around the electron as a function of electron-LO-phonon coupling constant(α) for $l_0 = 0.5$.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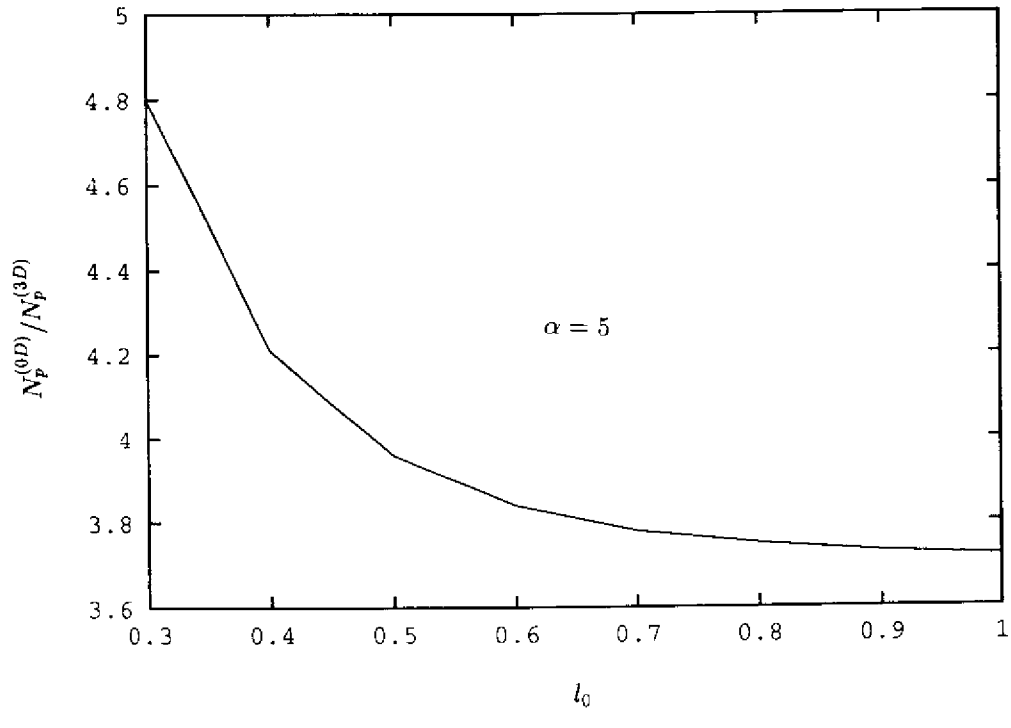
6
5.5
5
4.5
4
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
$\alpha = 5$
$E_b^{(0D)} / E_g^{(3D)}$
l_0

Fig.1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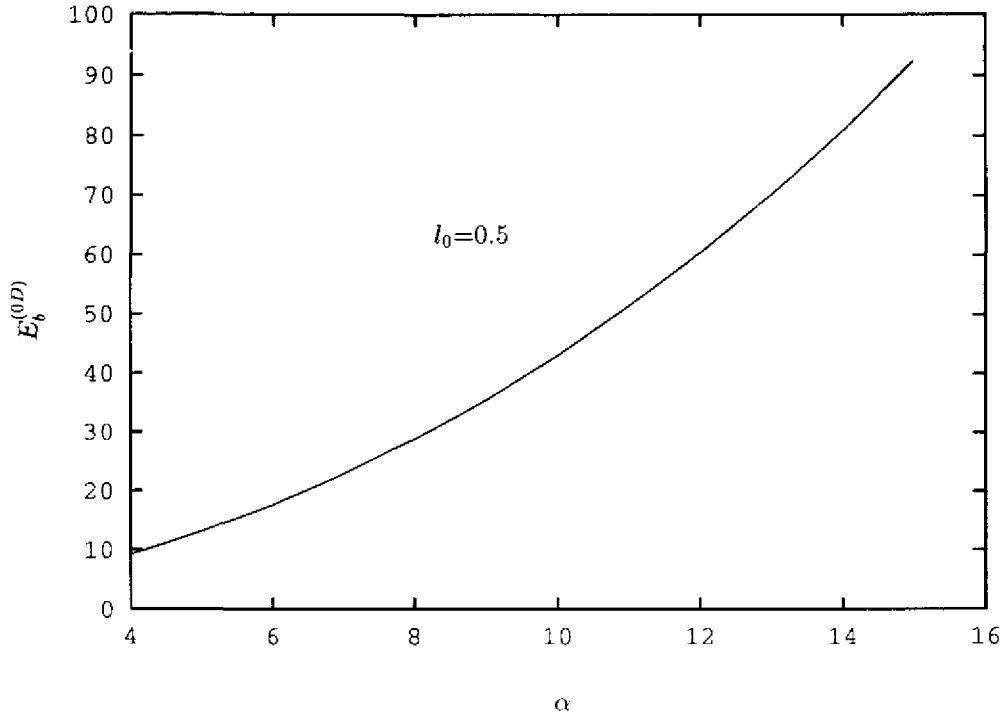
4.6
4.4
4.2
4
3.8
3.6
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
$\alpha = 5$
$N_p^{(0D)} / N_p^{(3D)}$
l_0

Fig.2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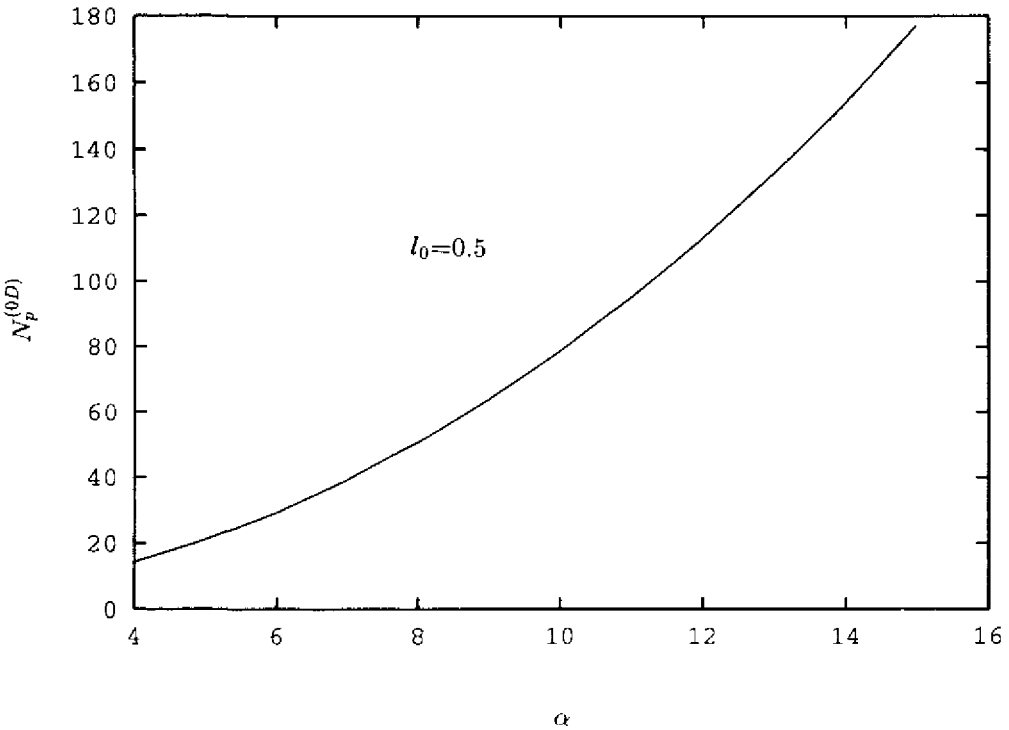
80
70
60
50
40
30
20
10
0
4
6
8
10
12
14
16
l_0=0.5
$E_b^{(0D)}$
α

Fig.3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100
80
60
40
20
0
4
6
8
10
12
14
16
l_0=0.5
$N_p^{(0D)}$
α

Fig.4