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Temperature dependence of polarons in a harmonic quantum dot

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The temperature and the size dependences of the self-trapping energy of a polaron in a harmonic quantum dot are studied. It is found that the self-trapping energy of the polaron and the transition energy between the ground state and the low-lying excited state are a decreasing function of temperature, and the temperature effect becomes obvious in small quantum dots.

Recent developments in semiconductor fabrication enable the realization of a system in which free electrons are confined to zero dimension, called quantum dots [1–5]. These quantum dots are often referred to as artificial atoms with the atomic potential replaced by the artificially constructed dot potential. The novel physical effects and potential device applications for these zero-dimensional structures are a subject of growing experimental [1–5] and theoretical [6–10] interest.

The interaction of electrons with longitudinal-optical (LO) phonons in quantum dots has been investigated by various authors [4,5,7,9]. Recently, Roussignol et al. [4] have shown experimentally and explained theoretically that phonon broadening is quite important in very small semiconductor quantum dots. Degani and Farias [7] found that the polaron effects of the interface phonons are important and cannot be neglected in quantum wires and dots. In a recent paper, Zhu and Gu [11] have investigated the polaronic states in a harmonic quantum dot at zero absolute temperature.

In recent years there has been renewed interest in the temperature dependence of the properties of polarons [12–15]. Brummell et al. [12] have studied the temperature dependence of the effective mass of the polaron in $Ga_{1-x}Al_xAs/GaAs$ heterojunctions by cyclotron resonance measurements. Using Feynman's path-integral polaron theory, Wu et al. [13] evaluated the polaron mass for arbitrary temperature with the inclusion of full dynamical screening. Li and Gu [14] investigated the polarons in a polar crystal slab at finite temperature and find that both the effective mass and the self-energy decrease with increasing temperature. To our knowledge, there has been no investigation of the temperature dependence of a polaron in quantum dots until now. In the present paper, based on ref. [11], we shall investigate the temperature and the size dependences of the self-trapping energy of a polaron in a harmonic quantum dot. For the sake of analytic simplicity, we shall model the relevant vibrational modes by the corresponding bulk modes. This assumption has been used by Schmitt-Rink, Miller, and Chemla [16] and Bockelmann and Bastard [17] to treat the phonon broadening of optical spectra and the phonon scattering in quantum dots. Taking into account the effect of phonon confinement will certainly vary the results in comparison with those of the bulk-phonon model. We shall treat this effect in a forthcoming paper.

The electrons are much more strongly confined in one direction (taken as the z direction) than in the other

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two directions. Therefore, we shall confine ourselves to consider only the motion of the electrons in the x–y plane. Kumar et al. [8] have shown that the evolution of energy levels in a quantum dot with increasing magnetic field is similar to that for a harmonic potential. These results make the harmonic confining potential model very appealing. We shall use this harmonic confining potential model in the present work.

We assume that the confining potential in a single quantum dot is harmonic:

$$V(\rho)=\tfrac{1}{2}m^*\omega_0^2\rho^2\,, \tag{1}$$

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

$$H=H_0+H_1\,, \tag{2}$$

$$H_0=\frac{1}{2m^*}p^2+\tfrac{1}{2}m^*\omega_0^2\rho^2+\sum_q \hbar\omega_{\mathrm{LO}}b_q^+b_q\,, \tag{3}$$

$$H_1=\sum_q\left[V_q\exp(\mathrm{i}q\cdot r)b_q+V_q^+\exp(-\mathrm{i}q\cdot r)b_q^+\right]. \tag{4}$$

where b_q^+ creates a bulk LO phonon of wave vector q, $q=(q_\parallel, q_z)$ and $r=(\rho, z)$ is the coordinate of the electron,

$$V_q=\mathrm{i}(\hbar\omega_{\mathrm{LO}}/q)(\hbar/2m^*\omega_{\mathrm{LO}})^{1/4}(4\pi\alpha/V)^{1/2}\,. \tag{5}$$

At finite temperature, we choose $|n_q\rangle$ for the wave function to describe the phonon state, in which the n_q represent the number of LO phonons. When the temperature is lower than room temperature, even though the phonon frequencies will decrease with increasing temperature, we can still take them as a constant because of the small relative change of the frequencies (about 1%) [12]. On the other hand, the interaction energy between the electron and phonons is much smaller than the phonon energy, except in the strong-coupling case. As a consequence we assume that the eigenvalues of $b_q^+b_q$ in the phonon state are approximately equal to the thermal equilibrium values [4,14,15], that is

$$\langle n_q\rangle=[\exp(\hbar\omega_{\mathrm{LO}}/k_{\mathrm{B}}T)-1]^{-1}\,, \tag{6}$$

where k_{B} is the Boltzmann constant.

The energy levels of the unperturbed Hamiltonian H_0 are given by [18,19]

$$E_{nm}^{(0)}=(2n+|m|+1)\hbar\omega_0+\sum_q\langle n_q\rangle\hbar\omega_{\mathrm{LO}}\,, \tag{7}$$

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

$$|n, m, 0_q\rangle=\frac{1}{\sqrt{2\pi}}\exp(\mathrm{i}m\theta)\left(\frac{2m^*\omega_0 n!}{\hbar(n+|m|)!}\right)^{1/2}x^{|m|}L_n^{|m|}(x^2)\exp(-\tfrac{1}{2}x^2)|n_q\rangle\,, \tag{8}$$

where $x=\rho(m^*\omega_0/\hbar)^{1/2}$, $L_n^{|m|}$ are associated Laguerre polynomials.

Since the electron–phonon interaction is weak in $Ga_{1-x}Al_xAs/GaAs$ or similar systems, in the sense that the Frohlich coupling constant (α) is of the order of 0.1, we shall use the second-order Rayleigh–Schrödinger perturbation theory to obtain the electronic self-energy shift, δE_{nm}, given by

$$\delta E_{nm}=-\alpha(\hbar\omega_{\mathrm{LO}})^2\left(\frac{\hbar}{2m^*\omega_{\mathrm{LO}}}\right)^{1/2}\sum_{n'}\sum_{m'}\left(Q_{nmn'm'}(\langle n_q\rangle+1)\{[2(n'-n)+(|m'|-|m|)]\hbar\omega_0+\hbar\omega_{\mathrm{LO}}\}^{-1}\right.$$
$$\left.+Q_{nmn'm'}\langle n_q\rangle\{[2(n'-n)+(|m'|-|m|)]\hbar\omega_0-\hbar\omega_{\mathrm{LO}}\}^{-1}\right)\,, \tag{9}$$

where

$$Q_{nmn'm'} = \int_0^\infty \mathrm{d}q_\parallel \, [V_{nmn'm'}(q_\parallel)]^2 , \tag{10}$$

$$V_{nmn'm'}(q_\parallel) = 2\left(\frac{n'!n!}{(n'+|m'|)!(n+|m|)!}\right)^{1/2} \int_0^\infty \mathrm{d}x \, x^{|m'|+|m|+1} L_{n'}^{|m'|}(x^2) L_n^{|m|}(x^2) J_{m-m'}(-q_\parallel l_0 x) , \tag{11}$$

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

In eq. (9), the first term corresponds to the emission of a virtual phonon during the electron–phonon interactions, and the second term represents the absorption of a virtual phonon in the process of electron–phonon interaction [15]. The numerical results will show that the two processes must be considered at finite temperatures.

We put $n=0$ and $m=0$ and the ground-state energy correction is given by

$$\delta E_{00} = -\alpha\hbar\omega_{\mathrm{LO}}\left(\frac{\hbar}{2m^*\omega_{\mathrm{LO}}}\right)^{1/2} \sum_{n'}\sum_{m'}\left[Q_{00n'm'}(\langle n_q\rangle+1)\left((2n'+|m'|)\frac{\omega_0}{\omega_{\mathrm{LO}}}+1\right)^{-1}\right.$$

$$\left. + Q_{00n'm'}\langle n_q\rangle\left((2n'+|m'|)\frac{\omega_0}{\omega_{\mathrm{LO}}}-1\right)^{-1}\right]. \tag{12}$$

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 $(0, 1)$ [20,21]. Consequently, the correction δE_{01} to the excited level $(0, 1)$ is given by

$$\delta E_{01} = -\alpha\hbar\omega_{\mathrm{LO}}\left(\frac{\hbar}{2m^*\omega_{\mathrm{LO}}}\right)^{1/2} \sum_{n'}\sum_{m'}\left[Q_{01n'm'}(\langle n_q\rangle+1)\left((2n'+|m'|-1)\frac{\omega_0}{\omega_{\mathrm{LO}}}+1\right)^{-1}\right.$$

$$\left. + Q_{01n'm'}\langle n_q\rangle\left((2n'+|m'|-1)\frac{\omega_0}{\omega_{\mathrm{LO}}}-1\right)^{-1}\right]. \tag{13}$$

and the correction $\delta E_{0,-1}$ to the excited level $(0, -1)$ is given by

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

$$\left. + Q_{0,-1n'm'}\langle n_q\rangle\left((2n'+|m'|-1)\frac{\omega_0}{\omega_{\mathrm{LO}}}-1\right)^{-1}\right]. \tag{14}$$

The relevant transition energy for the $(0, 0)\rightarrow(0, 1)$ transition is given by

$$\Delta E_{01} = (E_{01}+\delta E_{01}) - (E_{00}+\delta E_{00}) . \tag{15}$$

The relevant transition energy for the $(0, 0)\rightarrow(0, -1)$ transition is given by

$$\Delta E_{0,-1} = (E_{0,-1}+\delta E_{0,-1}) - (E_{00}+\delta E_{00}) . \tag{16}$$

The numerical results of the temperature and the size dependences on the ground-state energy correction and the transition energy between the ground state and the low-lying excited state in GaAs harmonic quantum dots are presented in figs. 1–4. Figure 1 shows the absolute values of the ground-state energy correction in GaAs harmonic quantum dots as a function of temperature for three effective confinement lengths of the quantum dots ($l_0 = 1.7r_0$, $2.0r_0$ and $2.5r_0$, where r_0 is the polaron radius and $\theta_{\mathrm{D}} = 426$ K is the Debye temperature). From fig. 1 we can see that the absolute values of the ground-state energy correction decrease with increasing temperature. That is to say, the self-trapping of the polaron will be weakened with enhancement of temperature.

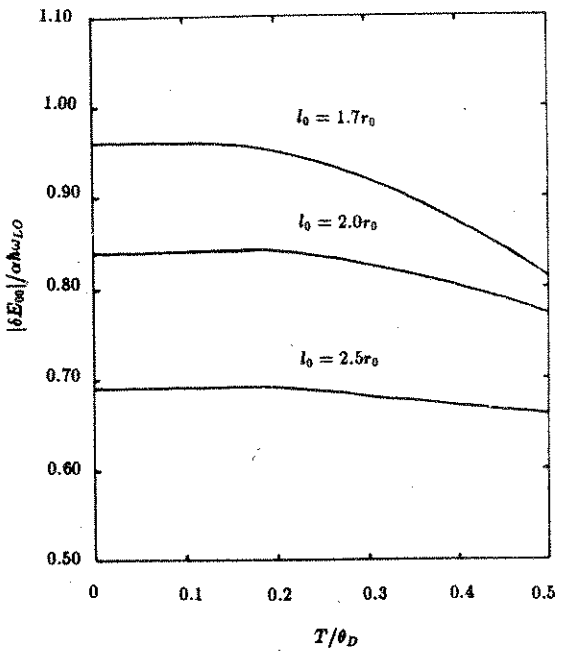

Fig. 1. The ground-state energy correction (in units of $\alpha\hbar\omega_{LO}$) in GaAs harmonic quantum dots as a function of temperature for three effective confinement lengths of the quantum dots. ($r_0=(\hbar/2m^*\omega_{LO})^{1/2}$ is the polaron radius, $\theta_D=426$ K is the Debye temperature.)

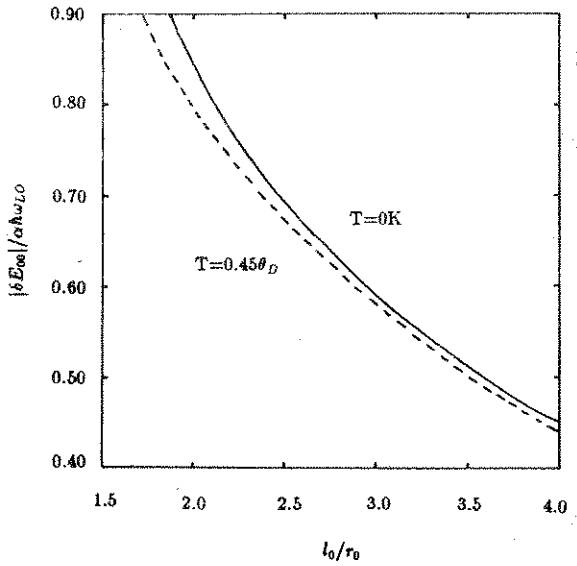

Fig. 2. The ground-state energy correction (in units of $\alpha\hbar\omega_{LO}$) in GaAs harmonic quantum dots as a function of the effective confinement length of the quantum dot for two temperatures. ($r_0=(\hbar/2m^*\omega_{LO})^{1/2}$ is the polaron radius, $\theta_D=426$ K is the Debye temperature.)

The figure also shows that as the size of the quantum dots becomes small, the change in the ground-state energy correction with temperature will be obvious. This result indicates that the temperature effect is quite significant in small quantum dots. Figure 2 illustrates the absolute values of the ground-state energy correction as a function of the effective confinement length of the quantum dot for two temperature values ($T=0$ K and $0.45\theta_D$). It is shown that the ground-state energy correction increases with decreasing effective confinement length of the quantum dot. The result indicates that the polaron effect is also quite important in small quantum dots at finite temperature. The figures also show that the self-energy at $T=0.45\theta_D$ is smaller than that at $T=0$ K, especially for small quantum dots. Figures 3 and 4 present the relevant transition energy for $(0, 0)\rightarrow(0, 1)$ and $(0, 0)\rightarrow(0, -1)$ as a function of temperature for four effective confinement lengths of the quantum dot. We can see that the transition energies shrink slowly with enhancement of temperature. With decreasing the size of the quantum dot, the temperature effects on the transition energies become more obvious. From figs. 3 and 4, it is noted that the transition energy for $(0, 0)\rightarrow(0, 1)$ and the transition energy for $(0, 0)\rightarrow(0, -1)$ are nearly identical, but slightly different, since $Q_{01n'm'}$ is not equal to $Q_{0,-1n'm'}$ (see eqs. (10), (11)).

In conclusion, we have investigated the temperature and the size dependence of the self-trapping energy of a polaron in GaAs harmonic quantum dots. It is found that the absolute values of the ground-state energy correction and the transition energy between the ground state and the low-lying excited state in GaAs harmonic quantum dots decrease with increasing temperature and increase with decreasing the effective confinement length of the quantum dot at finite temperatures. The results also indicate that the temperature effects become obvious in small quantum dots. In addition, in the present paper we also show from the numerical results that the virtual-phonon absorption process and the emission process must be considered at the same time for finite temperature. The absorption process will weaken the self-trapping of a polaron, while the emission process will

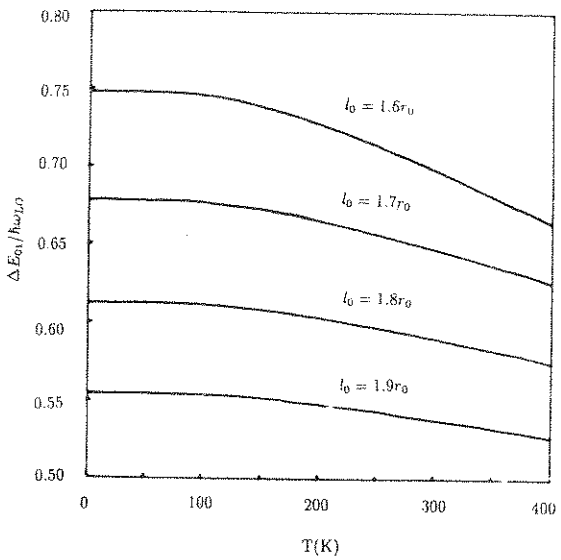

Fig. 3. The transition energy for $(0, 0) \rightarrow (0, 1)$ (in units of $\hbar\omega_{LO}$) in GaAs harmonic quantum dots as a function of temperature for four effective confinement lengths of the quantum dots. ($r_0 = (\hbar/2m^*\omega_{LO})^{1/2}$ is the polaron radius.)

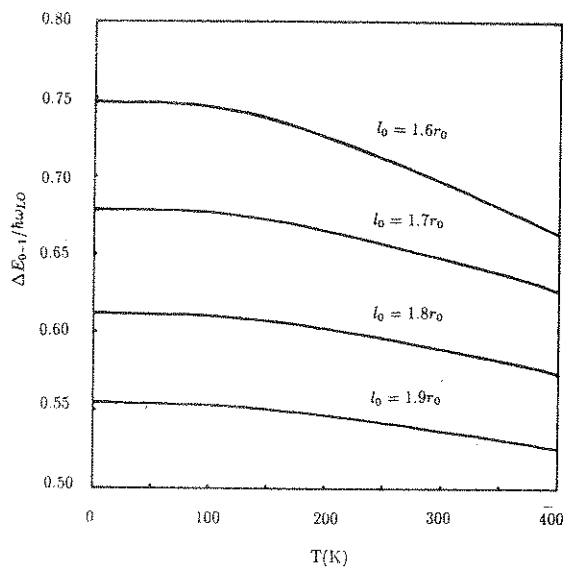

Fig. 4. The transition energy for $(0, 0) \rightarrow (0, -1)$ (in units of $\hbar\omega_{LO}$) in GaAs harmonic quantum dots as a function of temperature for four effective confinement lengths of the quantum dots. ($r_0 = (\hbar/2m^*\omega_{LO})^{1/2}$ is the polaron radius.)

always strengthen the self-trapping of a polaron, which agrees with the results obtained in ref. [15]. It should be emphasized that the use of the 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 the z direction into the above formalism is straightforward and will reduce the effective electron–phonon interaction [22]. But the qualitative features in this paper are independent of this approximation.

References

[1] C. Sikorski and U. Merkt, Phys. Rev. Lett. 62 (1989) 2164.
[2] T. Demel, D. Heitmann, P. Grmbow and K. Ploog, Phys. Rev. Lett. 64 (1990) 788.
[3] A. Lorke, J.P. Kotthaus and K. Ploog, Phys. Rev. Lett. 64 (1990) 2559.
[4] P. Roussignol, D. Ricard and C. Flytzanis, Phys. Rev. Lett. 62 (1989) 312.
[5] M.G. Bawendi, W.L. Wilson, L. Rothberg, P.J. Carrol, T.M. Jedju, M.L. Steigerwald and L.E. Brus, Phys. Rev. Lett. 65 (1990) 1623.
[6] F.M. Peeters, Phys. Rev. B 42 (1990) 1486.
[7] M.H. Degani and G.A. Farias, Phys. Rev. B 42 (1990) 11950.
[8] A. Kumar, S.E. Laux and F. Stern, Phys. Rev. B 42 (1990) 5166.
[9] M.C. Klein, F. Hache, D. Ricard and C. Flytzanis, Phys. Rev. B 42 (1990) 11123.
[10] N.F. Johnson and M.C. Payne, Phys. Rev. Lett. 67 (1991) 1157.
[11] K.D. Zhu and S.W. Gu, Phys. Lett. A 163 (1992) 435.
[12] M.A. Brummell, R.J. Nicholas, M.A. Hopkins, J.J. Harris and C.T. Foxon, Phys. Rev. Lett. 58 (1987) 77.
[13] X. Wu, F.M. Peeters and J.T. Devreese, Phys. Rev. B 36 (1987) 9765.
[14] Y.C. Li and S.W. Gu, J. Phys. Condens. Matter 1 (1989) 3201.
[15] B.H. Wei and S.W. Gu, Phys. Rev. B 43 (1991) 9190.
[16] S. Schmitt-Rink, D.A.B. Miller and D.S. Chemla, Phys. Rev. B 35 (1987) 8113.
[17] U. Bockelmann and G. Bastard, Phys. Rev. B 42 (1990) 8947.

[18] V. Fock, Z. Phys. 47 (1928) 446.
[19] C.G. Darwin, Proc. Cambridge Philos. Soc. 27 (1930) 86.
[20] W. Que, G. Kirczenow and E. Castano, Phys. Rev. B 43 (1991) 14079.
[21] T. Chakraborty, V. Halonen and P. Pietilainen, Phys. Rev. B 43 (1991) 14289.
[22] S.D. Sarma, Phys. Rev. Lett. 52 (1984) 859.