Polaron Energy Spectrum in Quantum Dots

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Abstract.

Energy spectrum of a weak coupling polaron is considered in a cylindrical quantum dot. An analytical expression for the polaron energy shift is obtained using a modified perturbation theory.

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1. Introduction

Investigation of electron spectrum in quantum dots has been attracted much attention in the last decade as it has been technologically possible to produce well characterized quasi-zero-dimensional structures. The energy spectrum depends on the physical parameters of the quantum dot’s material, its shape and size. Also, the important factor influences on the electron spectrum in polar semiconductor is interaction between electrons and longitudinal optical LO phonons. In low-dimensional structures the importance of polaron effects increases. So, the knowledge of the polaron energy spectrum is important for understanding the infrared properties of quantum dots. One of the interesting experimental facts is the absence of the LO phonon bottleneck effect of photoexcited electrons. There is a number of papers proposed various reasons why the expected bottleneck effect may be bypassed [1-3]. In particular, in the works [4,5] the energy relaxation of the excited electrons in quantum dots was discussed in connection with polaron effects. So, it is interesting to investigate polaron spectrum in quantum dots in the region where the distance between size-quantized levels equals to the LO-phonon energy.

In magneto-optical experiments in bulk crystals the electron-LO-phonon interaction leads to anticrossing of the energy levels. Larsen was the first to point out the level repulsion at \( \omega_c = \omega_{LO} \), where \( \omega_c \) is the cyclotron frequency and \( \omega_{LO} \) is the frequency of LO-phonon [6]. The anticrossing of energy levels was observed in absorption spectrum of quantum dots \( InAs/GaAs \) in magnetic field in the work [7]. Appearance of the
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In the dependence of polaron levels on the quantum dot radius theoretically was derived on the base of two-levels system [5]. However, in order to obtain more correct expressions for the polaron energy shift it is necessary to take into account the influence of the all size-quantized levels. In present paper we consider an optical weak-coupling polaron at low temperature in a cylindrical quantum dot. An analytical expression for the polaron energy shift is obtained using a modified perturbation theory.

2. Polaron energy

In the present paper we consider a disc shape quantum dot, i.e. a cylindrical quantum dot with the radius essentially exceeding the height. The same situation usually is realized in experiments. Usually the diameter of the disc exceeds its height by the order. Besides, we use the oscillator model of the potential confining electron’s movement along the cylindrical axis $z$ with the frequency $\omega_z$ and in the plane of the disk with the frequency $\omega$. According to the cosidered shape of the disc it is assumed that $\omega_z \gg \omega$. It is considered that the levels connected with confinement along $z$ are situated too over the ground state and their influence can be neglected. It is suggested that the coupling constant of a polar crystal in a quantum dot is too little (for GaAs $\alpha \approx 0.07$). In this connection we use the perturbation theory for polaron energy shift. The suggested model of the quantum dot is related to the following Schrödinger equation for electron noninteracting with phonons

$$\left( \frac{\partial}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} \right) \Psi + \frac{\partial^2 \Psi}{\partial z^2} + \left( \frac{2m_0 E^{(0)}}{\hbar^2} - \frac{m_0^2 \omega^2 \rho^2}{\hbar^2} - \frac{m_0^2 \omega_z^2 z^2}{2} \right) \Psi = 0, \quad (1)$$

where $m_0$ is electron’s effective mass in the quantum dot, $\rho$, $\varphi$, $z$ are the cylindrical coordinates. The solution of the equation (1) is well known

$$\Psi_{nm} = \frac{aa_{\pi}^m}{\pi^\frac{1}{4}} (a\rho)^{|m|} L_{\frac{|m|}{2}} \left( a^2 \rho^2 \right) \exp \left( -\frac{a^2 \rho^2}{2} - \frac{a^2 z^2}{2} + im\varphi \right), \quad (2)$$

where $L_n^\lambda(x)$ are the associated Laguerre polynomials, $a^2 = \frac{m_0 \omega}{\hbar}$; $a_z^2 = \frac{m_0 \omega_z}{\hbar}$; $a_{nm}^2 = \frac{(n+|m|)}{(n-|m|)}$; $(n = 0, 1, 2, ..., m = 0, \pm 2, \pm 4, ..., \pm n$ if $n$ is even, $m = \pm 1, \pm 3, ..., \pm n$ if $n$ is odd and $m = 0$ for $n = 0$). The energy spectrum is:

$$E^{(0)}_n = \frac{\hbar \omega_z}{2} + \hbar \omega (n + 1). \quad (3)$$

The electrons are assumed to be coupled to dispersionless LO-phonons of the bulk crystal. The potential yielded by one LO-phonon is

$$\varphi_q = \frac{\Lambda}{q} e^{iq_\perp \rho \cos \varphi + iq_\parallel z}, \quad (4)$$

where $\Lambda = i\hbar \omega_0 (4\pi\alpha/\gamma_0 V)$, $q$ is the phonon wavevector, $q_\perp$ and $q_\parallel$ are the components of the phonon wavevector laying in the plane of the disc and along $z$ axes correspondingly,
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\[ q = \sqrt{q_{\perp}^2 + q_z^2}, \quad \gamma_0^2 = \frac{2n_0\omega_0}{\hbar}, \quad \hbar\omega_0 \text{ is the energy of LO phonon at } q = 0, \quad V \text{ is the quantum dot's volume.} \]

The matrix element corresponding to the emission of the LO phonon is

\[ M_{nm \to n'm'} = \int \Psi_{nm}\varphi_q^*\Psi_{n'm'}^*dV, \quad (5) \]

where \( e \) is the electron charge. Using the expressions (2), (4) and (5) we obtain

\[ M_{nm \to n'm'} = \frac{2\Lambda a_{nm}a_{n'm'}(-i)^{m'-m}}{q}\varepsilon - \frac{q^2}{4a^2}I_{nm \to n'm'} \left( \frac{q_{\perp}}{2a} \right), \quad (6) \]

where

\[ I_{nm \to n'm'}(y) = \int_0^\infty x^{m|+m'|+1} L_{n-m|}^{[m']} \left( x^2 \right) L_{n-m|}^{[m']} \left( x^2 \right) e^{-x^2} J_{m'-m}(2xy), \]

\( J_{m'-m}(2xy) \) is the Bessel function.

It is assumed that the difference between conductivity bands of the material of quantum dot and surroundings is quite large and a sufficient number of the quantum levels can exist inside the quantum well. Therefore, while calculating the polaron energy, we shall take into account the electron’s transitions to all levels. Far from the resonance \( \left( E_n^{(0)} - E_{n'}^{(0)} \right) = \hbar\omega_0 \), the polaron correction to the energy in the second order of the perturbation theory is defined as follows:

\[ \Delta E_n = \sum_{m,n',m',q} \frac{|M_{nm \to n'm'}|^2}{E_n^{(0)} - E_{n'}^{(0)} - \hbar\omega_0}. \quad (7) \]

The expression (7) differs from the one, usually being used for calculation of a correction to the ground state, by the additional sum over degenerate states of the level \( E_n^{(0)} \) (summation over \( m \)). We shall substitute (3) and (6) in (7) and replace the summation over \( \frac{q_{\perp}}{2a} \) with integration. For simplicity we shall consider the limit \( \omega_z, a_z \to \infty \) related to the case of zero height cylinder. According to this limit the integral over \( q_z \) is equal to:

\[ \int_{-\infty}^{\infty} \exp \left( -\frac{q_z^2}{2a_z^2} \right) dq_z \bigg|_{q_z\to\infty} = \frac{\pi}{q_{\perp}}. \]

As a result we shall obtain the following expression of the polaron energy shift normalized by \( \alpha\hbar\omega_0 \):

\[ \frac{\Delta E_n}{\alpha\hbar\omega_0} = -8 \left( \Gamma \right)^{\frac{3}{2}} \sum_{m,n,m'} \frac{a_{nm}a_{n'm'}}{(n' - n)\Gamma + 1} J_{nm \to n'm'}, \quad (8) \]

\[ J_{nm \to n'm'} = \int_0^\infty |I_{nm \to n'm'}|^2 dy, \]

where \( \Gamma = \omega/\omega_0 \). As the parameter \( \Gamma \) is proportional to \( 1/R \), where \( R \) is the quantum dot radius, the limit \( \Gamma \to \infty \) corresponds to the ultraquantum limit. On the other
hand, the limit $\Gamma \to 0$ corresponds to the two-dimensional case of a plane. The polaron energy shift of the ground state $\Delta E_0/\alpha \hbar \omega_0$ calculated as a function of the parameter $\Gamma$ is plotted in Fig.1. The quantity of $\Delta E_0/\alpha \hbar \omega_0$ trends to the well known value $-\pi/2$ for two-dimensional case in the limit $\Gamma \to 0$. In the case of $\Gamma \to \infty$ the quantity of $\Delta E_0/\alpha \hbar \omega_0$ diverges proportionally to $\Gamma^{1/2}$. It is known that the divergence is taken place also in the case of a quantum wire if the wire radius tends to zero [8]. However, in one-dimensional case there is more weak logarithmic divergence. Now we shall calculate the polaron energy shift of the level $E^{(0)}_1$ for any value of $\Gamma$ including the resonance region.

As it is seen from the expression (9) for $n = 1$, the term corresponding to $n' = 0$ diverges in the limit $\Gamma \to 1$. The formula (9) is not applicable near the resonance $\Gamma = 1$. In order to calculate the energy shift of the level $E^{(0)}_1$ in this area we shall exclude from (9) the term corresponding to the transition from the state $n = 1$ to $n' = 0$ and shall take into account this contribution using the perturbation theory applicable in the case of degeneracy of two levels $E^{(0)}_1$ and $E^{(0)}_0 + \hbar \omega_0$. We shall consider the system consisted from an electron, which has the state $n = 0, m = 0$ of the level $E^{(0)}_0$ and two degenerate states $n = 1, m = \pm 1$ of the level $E^{(0)}_1$, and a phonon which will have the occupation number $n_q = 0$ if the electron is on the level $E^{(0)}_0$ and $n_q = 1$ if the electron is on the level $E^{(0)}_1$. So, the united noninteracting electron-phonon system may exist on the level $E^{(0)}_1$ with two degenerate states $|n = 1, m = \pm 1, n_q = 0\rangle$ and on the level $E^{(0)}_0 + \hbar \omega_0$ with the state $|n = 0, m = 0, n_q = 1\rangle$. Then including the Fröhlich coupling one can easy obtain
the following expression for the energy of the two-level system:

$$E = \frac{E_1^{(0)} + E_0^{(0)}}{2} \pm \sqrt{\frac{1}{4} \left( E_1^{(0)} - E_0^{(0)} - \hbar \omega_0 \right)^2 + |V_{01}|^2}, \quad (9)$$

where $E_0^{(0)} = \hbar \omega$, $E_1^{(0)} = 2 \hbar \omega$, $|V_{01}|^2 = \sum_{\delta} (|M_{0,0\rightarrow 1,1}|^2 + |M_{0,0\rightarrow 1,-1}|^2)$.

From (9) we can define $\Delta E_1 = E - E_1^{(0)}$ in the following form:

$$\frac{\Delta E_1}{\alpha \hbar \omega_0} = \frac{1 - \Gamma}{2\alpha} \pm \frac{1}{\alpha} \sqrt{\left( \frac{1 - \Gamma}{2} \right)^2 + \frac{|V_{01}|^2}{(\hbar \omega_0)^2}}, \quad (10)$$

where $\frac{|V_{01}|^2}{(\hbar \omega_0)^2} = 16 \left( \frac{\Gamma}{2} \right)^{\frac{1}{2}} \alpha J_{1,1\rightarrow 0,0}$.

The sign plus corresponds to the region $\Gamma \gtrsim 1$, the sign minus to the region $\Gamma \ll 1$. The contribution into the energy shift $\Delta (E_0 + \hbar \omega_0) = E - E_0^{(0)} - \hbar \omega_0$ corresponding to the same transition is defined by the formula (11), but with the sign plus in the region $\Gamma \ll 1$ and with the sign minus in the region $\Gamma \gtrsim 1$.

$$\frac{\Delta (E_0 + \hbar \omega_0)}{\alpha \hbar \omega_0} = -\frac{1 - \Gamma}{2\alpha} \pm \frac{1}{\alpha} \sqrt{\left( \frac{1 - \Gamma}{2} \right)^2 + \frac{|V_{01}|^2}{(\hbar \omega_0)^2}}, \quad (11)$$

The value of the integral $J_{1,1\rightarrow 0,0}$ is 0.039.

**Figure 2.** Dependence of the polaron energy shift $\Delta E_1/\alpha \hbar \omega_0$ on $\Gamma$.

The total shift $\Delta E_1/\alpha \hbar \omega_0$ and $\Delta (E_0 + \hbar \omega_0)/\alpha \hbar \omega_0$ is calculated excluding from (9) the term related to the transition $n = 1, m = \pm 1 \rightarrow n = 0, m = 0$ and adding
the contribution defined by (11) and (12) respectively. The shifts $\Delta E_1/\alpha \hbar \omega_0$ and $\Delta (E_0 + \hbar \omega_0)/\alpha \hbar \omega_0$ as the functions of $\Gamma$ are plotted in fig.2 and fig.3 respectively for $\alpha \approx 0.07$. It is seen from fig.2 and fig.3 that $\Delta E_1|_{\Gamma \to \Gamma_0} = \Delta (E_0 + \hbar \omega_0)|_{\Gamma \to \Gamma_0}$. The picture of the levels $E_1/\hbar \omega_0$ and $(E_0 + \hbar \omega_0)/\hbar \omega_0$ is represented in fig.4, where $E_1^{(0)}/\hbar \omega_0 = 2\Gamma$ and $(E_0^{(0)} + \hbar \omega_0)/\hbar \omega_0 = \Gamma + 1$ are represented by the dashed lines. In the resonance area of the energy levels the corresponding wave function are represented as a superposition of the states $|n = 1, m = \pm 1, n_q = 0\rangle$ and $|n = 0, m = 0, n_q = 1\rangle$.

3. Conclusion

Using the perturbation theory the polaron energy shift was obtained. The polaron shift of ground state tends to the well known value $-\pi/2$ for two-dimensional system in the case of $\Gamma \to 0$. In the limit of $\Gamma \to \infty$ the polaron shift diverges more sharp than in the case of quantum wire, when its radius tends to zero.

Using the modified perturbation theory the anticrossing of the polaron levels $E_1$ and $E_0 + \hbar \omega_0$ was obtained near the resonance region.

The picture like the one plotted in fig.4 was obtained in experimental dependence of polaron spectrum on the magnetic field directed along axes $z$ of the cylindrical quantum dots [7]. In the presence of magnetic field the derived formulas are the same with substitution of $\omega$ by $(\omega^2 + \omega_c^2/4)^{1/2}$. The role of the parameter $\Gamma$ will play the magnitude $(\omega^2 + \omega_c^2/4)^{1/2}/\omega_0$. 

Figure 3. Dependence of the $\Delta (E_0 + \hbar \omega_0)/\alpha \hbar \omega_0$ on $\Gamma$. 
Figure 4. Dependence of the levels $E_1/\hbar\omega_0$ and $(E_0 + \hbar\omega_0)/\hbar\omega_0$ on $\Gamma$. The levels $E_1^{(0)}/\hbar\omega_0$ and $(E_0^{(0)} + \hbar\omega_0)/\hbar\omega_0$ are plotted by dashed lines. Here 1 - $(E_0 + \hbar\omega_0)/\hbar\omega_0$ in $\Gamma \leq 1$ region; 1’ - $(E_0 + \hbar\omega_0)/\hbar\omega_0$ in $\Gamma \geq 1$ region; 2 - $E_1/\hbar\omega_0$ in $\Gamma \leq 1$ region; 2’ - $E_1/\hbar\omega_0$ in $\Gamma \geq 1$ region.

Note that the splitting of the levels $E_1$ and $E_0 + \hbar\omega_0$ in light absorption experiment will be observed also in the absence of magnetic field if $\omega \approx \omega_0$. Besides the allowed transition $E_0 \rightarrow E_1$, the transition $E_0 \rightarrow E_0 + \hbar\omega_0$ may also take place because the wave functions of these levels are mixed in the anticrossing region. Far from the resonance the level $E_0 + \hbar\omega_0$ has not the particular physical meaning, however, the states corresponding to this level in the resonance region may be realized in experiments on light absorption.

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