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POLARON ENERGY SPECTRUM IN QUANTUM DOT

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Energy spectrum of a weak coupling polaron is considered in a disk-shaped quantum dot. An analitical expression for the polaron energy correction to the ground and the first excited state was calculated using a modified perturbation theory. Anticrossing of the polaron energy levels in the dependence on the quantum dot radius was obtained.

INTODUCTION

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. Most of these structures are made of polar materials. Therefore, the polaron phenomena can strongly influence the electron spectrum. There has been a great interest of the polaron phenomena in quantum well, quantum wire and quantum dot structures. It is known that the polaron effects are enhanced when going from 2D to 1D and then to 0D system. The normalized polaron energy shift of the ground state $\Delta E_0/\alpha h\omega_{LO}$, where α is the Frohlich coupling constant and $h\omega_{LO}$ is the energy of longitudinal optical (LO) phonon, equals to –1 and $-\pi/2$ in he case 0f 3D and 2D system respectively. In one-dimensional case $\Delta E_0/\alpha h\omega_{LO}$ is proportional to lnR when the radius of the cylindrical quantum wire is $R\to 0$ [1]. The most significant polaron effects are realized in quantum dots. Applying the Feyman variational principle the basic polaron parameters were obtained in the case of spherical quantum dot and it was shown that $\Delta E_0/\alpha h\omega_{LO}$ depends on the quantum dot radius more strongly than in 1D case [1].

On the other hand, one of the interesting experimental facts is absence of the expected LO-phonon bottleneck effect of photoexcited electrons in quantum dots. There is a number of papers proposed various reasons why the expected bottleneck effect may be bypassed [2-4]. In paricular, in the works [5,6] 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 case of the resonance where the distance between size-quantized levels equals to the LO-phonon energy.

Another interesting fact is that 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 ω_c is the cyclotron frequency, in bulk crystals in the presence of a magnetic field [7]. The anticrossing of energy levels was observed in absorption spectrum of quantum dots InAs/GaAs in magnetic field [8]. Appearance of the anticrossing in the dependence of polaron levels on the quantum dot radius theoretically was derived on the base of two-levels system [6]. More precisely, the disk-shaped InAs/GaAs quantum dot in the presence of a magnetic field by using the Davydov's canonical transformation was considered theoretically in the paper [9].

The goal of the present paper is to investigate polaron spectrum in the case of disk-shaped quantum dot. We shall use a modified perturbation theory taking into account the interaction between $E_1^{(0)}$ and $E_0^{(0)}+ h\omega_{LO}$, where $E_0^{(0)}$ and $E_1^{(0)}$ are the ground and the first excited energy level of the confined electron respectively. In spite of the fact that due to the electronic confinement in the low-dimensional structures, the strong-coupling regime can be realized even at the small value of the electron-phonon interaction constant α, we use the perturbation theory. As it will be shown below the weak-coupling regime still may be realized for small value α and quantum dot's size usually considered in experiments.

POLARON ENERGY

In the present paper we consider a disk-shaped quantum dot, i.e. a cylindrical quantum dot with the radius essentially exceeding its height. The same situation usually is realized in experiments. Usually the diameter of the disk 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 ω_z and in the plane of the disk with the frequency ω. According to the considered shape of the disk it is assumed that $\omega_z >> \omega$. 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:

$$[\partial^2 / \partial\rho^2 + (1/\rho)\, \partial / \partial\rho + (1/\rho^2)\, \partial^2 / \partial\varphi^2]\psi + \partial^2\psi / \partial z^2 + \\ + (2m_0 E^{(0)}/h^2 - m_0^2\omega^2\rho^2/h^2 - m_0^2\omega_z^2 z^2/h^2)\, \psi = 0, \tag{1}$$

where m_0 is the electron's effective mass in the quantum dot, ρ, φ, z are the cylindrical coordinates. The solution of the equation (1) is well known:

$$\psi_{nm} = (a a_z^{1/2} a_{nm}/\pi^{3/4})(a\rho)^{|m|} L_{(n-|m|)}^{|m|}(a^2\rho^2)\, \exp(-a^2\rho^2/2 - a_z^2 z^2/2 + im\varphi), \tag{2}$$

where $L_{(n-|m|)}^{|m|}(a^2\rho^2)$ are the associated Laguerre polinomials, $a^2 = m_0\omega/h$, $a_z^2 = m_0\omega_z/h$, $a_{nm}^2 = (n-|m|)!/(n+|m|)!$, $n=0,1,2,\ldots$, $m=0,\pm2,\pm4,\ldots,\pm n$ if n is even, $m=\pm1,\pm3,\ldots,\pm n$ if n is odd and m=0 for n=0. The energy spectrum is:

$$E_n^{(0)} = h\omega_z/2 + h\omega(n+1). \tag{3}$$

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

$$\varphi_q = (\Lambda/q)\, \exp(iq_\perp \rho\cos\varphi + iq_z z), \tag{4}$$

where $\Lambda = ih\omega_0(4\pi\alpha/\gamma_0 V)^{1/2}$, q is the phonon wave vector, $q_\perp$ and q_z are the components of the phonon wave vector laying in the plane of the disk and along z axes correspondingly, $q = (q_\perp^2 + q_z^2)^{1/2}$, $\gamma_0^2 = 2m_0\omega_0/h$, $h\omega_0$ is the energy of LO-phonon at q=0, V is the quantum dot's volume.

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

$$M_{nm\to n'm'} = \int \Psi_{nm}\, e\, \varphi_q^* \Psi^*_{n'm'} dV, \tag{5}$$

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

$$M_{nm\to n'm'} = (2\Lambda a_{nm} a_{n'm'} (-i)^{m-m'}/q)\, \exp(-q_z^2/4a_z^2)\, I_{nm\to n'm'}(q_\perp/2a), \tag{6}$$

where

$$I_{nm\to n'm'}(y) = \int_0^\infty x^{|m|+|m'|+1} L_{(n-|m|)/2}^{|m|}(x^2)\, L_{(n'-|m'|)/2}^{|m'|}(x^2) \exp(-x^2) J_{m'-m}(2xy),$$

$J_{m'-m}(2xy)$ 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 sufficient number of quantum levels exists inside the quantum well. So, while calculating the polaron energy, we shall take into account the electron's transitions to the all levels. Far from the resonance the polaron correction to the energy in the second order of the perturbation theory is defined as follows:

$$\Delta E_n = \sum_{m,n',m',q} |M_{nm\to n'm'}|^2/(E_n^{(0)} - E_{n'}^{(0)} - h\omega_0). \qquad (7)$$

We shall substitute (3) and (6) into (7) and replace the summation over q with integration. For simplicity we shall consider the limit ω_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:

$$\int_{-\infty}^{\infty} \exp(-q_z^2/2a_z^2)/(q_\perp^2+q_z^2)dq_z = \pi/q_\perp.$$

As a result we shall obtain the following expression of the polaron energy shift normalized by $\alpha h\omega_0$:

$$\Delta E_n/\,\alpha h\omega_0 = -8(\Gamma/2)^{1/2} \sum_{m,n',m',q} a_{nm}^2\, a_{n'm'}^2 J_{nm\to n'm'}/[(n'-n)\,\Gamma+1] \qquad (8)$$

$J_{nm\to n'm'} = \int |I_{nm\to n'm'}|^2 dy$,

where $\Gamma=\omega/\omega_0$. From the kind of potential of the oscillator model it is obvious that Γ is proportional to 1/R, where R is the quantum dot radius. The case of $\Gamma\to\infty$ corresponds to the ultraquantum limit. On the other hand, the limit $\Gamma\to0$ corresponds to the two-dimensional case of a plane. The polaron energy shift of the ground state $\Delta E_0/\,\alpha h\omega_0$ calculated as a function of the parameter Γ is plotted in Fig.1. The quantity $\Delta E_0/\,\alpha h\omega_0$ trends to the well known value $-\pi/2$ for two-dimensional case in the limit $\Gamma\to0$. In the case of $\Gamma\to\infty$ the quantity of $\Delta E_0/\,\alpha h\omega_0$ diverges proportionally to $\Gamma^{1/2}$. It is known that the divergence is taken place also in the case of quantum wire if the wire radius tends to zero [1]. However, in one-dimensional case there is more weak logarithmic divergence.

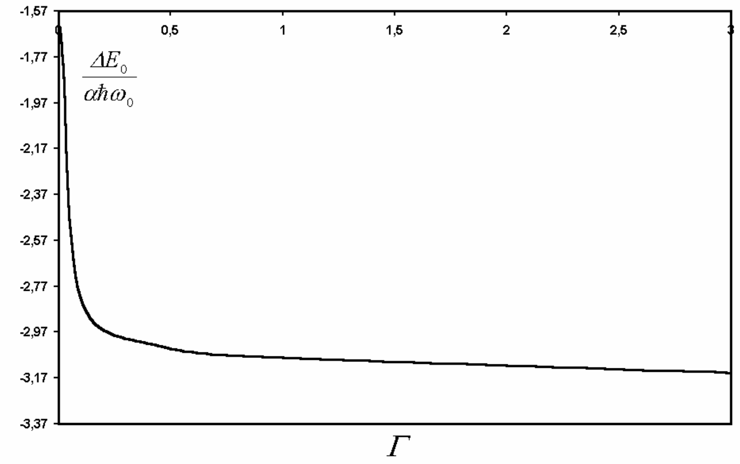

Fig.1.
Dependence of the polaron ground state shift $\Delta E_0/\,\alpha h\omega_0$ on Γ.

Now we shall calculate the polaron energy shift of the level $E_1^{(0)}$ for any value of Γ including the resonance region. As it is seen from the expression (8) for n=1, the term corresponding to n'=0, diverges in the limit $\Gamma\to1$. The formula (8) is not applicable near the resonance $\Gamma=1$. In order to calculate the energy shift of the level $E_1^{(0)}$ in this area we shall exclude from (8) 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 $E_1^{(0)}$ and $E_0^{(0)}+h\omega_0$. 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=±1 of the level $E_1^{(0)}$, 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 $E_1^{(0)}$. So, the united noninteracting electron-phonon system may exist on the level $E_1^{(0)}$ with two degenerate states $|n=1,m=\pm1, n_q=0\rangle$ and on the level $E_0^{(0)}+h\omega_0$ with the state $|n=1,m=0,n_q=1\rangle$. Then including the Fröhlich coupling one can easy obtain the following expression for the energy of the two-level system:

$$E=(E_1^{(0)}+E_0^{(0)}+h\omega_0)/2\pm[(E_1^{(0)}+E_0^{(0)}+h\omega_0)^2/4+|V_{01}|^2]^{1/2}, \qquad (9)$$

where $E_0^{(0)}= h\omega$, $E_1^{(0)}=2\ h\omega$, $|V_{01}|^2 = \sum_Q (|M_{0,0\to 1,1}|^2+|M_{0,0\to 1,-1}|^2)$.

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

$$\Delta E_1/\ \alpha h\omega_0=(1-\Gamma)/2\alpha\pm[(1-\Gamma)^2/4+|V_{01}|^2/(h\omega_0)^2]^{1/2}/\alpha, \tag{10}$$

where $|V_{01}|^2/(h\omega_0)^2=16(\Gamma/2)^{1/2}\alpha J_{1,1\to 0,0}$. The sign plus corresponds to the region $\Gamma\geq 1$, the sign minus to the region $\Gamma\leq 1$. The contribution into the energy shift $\Delta(E_0+h\omega_0)=E- E_0^{(0)}-h\omega_0$ corresponding to the same transition is defined by the formula (11), but with the sign plus in the region $\Gamma\leq 1$ and with the sign minus in the region $\Gamma\geq 1$

$$\Delta(E_0+h\omega_0)/\alpha h\omega_0=-(1-\Gamma)/2\alpha\pm[(1-\Gamma)^2/4+|V_{01}|^2/(h\omega_0)^2]^{1/2}/\alpha. \tag{11}$$

The value of the integral $J_{1,1\to 0,0}$ is 0.039. The total shift $\Delta E_1/\ \alpha h\omega_0$ and $\Delta(E_0+h\omega_0)/\ \alpha h\omega_0$ is calculated excluding from (8) the term related to the transition $n=1,m=\pm 1\to n=0,m=0$ and adding the contribution defined by (10) and (11) respectively. The shifts $\Delta E_1/\ \alpha h\omega_0$ and $\Delta(E_0+h\omega_0)/\ \alpha h\omega_0$ as the functions of Γ are plotted in Fig.2 and Fig.3 respectively for $\alpha\approx 0.07$. The picture of the levels $E_1/\ \alpha h\omega_0$ and $(E_0+h\omega_0)/\ \alpha h\omega_0$ is represent in Fig.4, where $E_1^{(0)}/\ h\omega_0=2\Gamma$ and $(E_0^{(0)}+h\omega_0)/\ h\omega_0= \Gamma+1$ are represented by dashed lines. In the resonance area the energy levels correspond to the wave function represented as a superposition of the states $|n=1,m=\pm 1, n_q=0>$ and $|n=1,m=0, n_q=1>$.

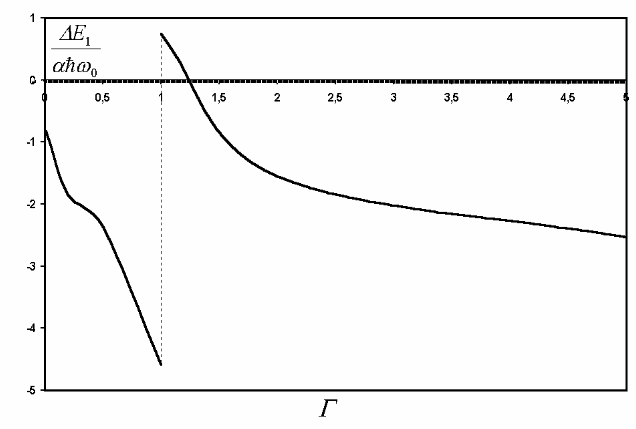

Fig.2.
Dependence of the
polaron energy shift $\Delta E_1/\alpha h\omega_0$ on Γ.

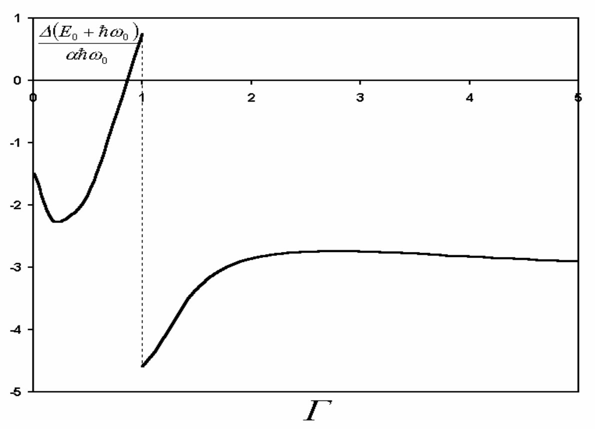

Fig.3.
Dependence of the
$\Delta(E_0+h\omega_0)/\alpha h\omega_0$ on Γ.

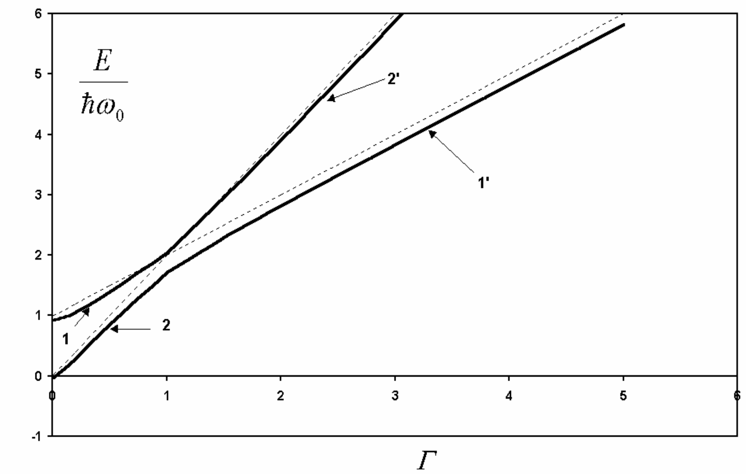

Fig.4
Anticrossing of the levels $E_1/h\omega_0$ and $(E_0+ h\omega_0)/h\omega_0$ on Γ. The levels $E_1^{(0)}/h\omega_0$ and $(E_0^{(0)}+h\omega_0)/h\omega_0$ are plotted by dashed lines.
1- $(E_0+h\omega_0)/h\omega_0$ in $\Gamma\leq 1$ region;
1'-$(E_0+h\omega_0)/h\omega_0$ in $\Gamma\geq 1$ region;
2- $E_1/h\omega_0$ in $\Gamma\leq 1$ region;
2'- $E_1/h\omega_0$ in $\Gamma\geq 1$ region.

As it is shown in the Fig.4 the polaron spectrum (solid line) is situated sufficiently close to the unperturbed electron spectrum (dashed lines). So, use of the perturbation theory for little value of α in the considered range of the parameter Γ is quite correct.

CONCLUSION

Using the perturbation theory the polaron energy shift was obtained. The polaron shift of the 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 $E_0+h\omega_0$ was obtained near the resonance region.

Far from the resonance the level $E_0+h\omega_0$ 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. Apart from the allowed transition $E_0 \to E_1$, the transition $E_0 \to E_0+h\omega_0$ may also take place because the wave functions of these levels are mixed in the anticrossing region.

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DİSK FORMALI KVANT NÖQTƏSİNDƏ POLYARONUN ENERJİ SPEKTRİ

O.Z. ƏLƏKBƏROV, N.M. HÜSEYNOV

Disk formalı kvant nöqtəsində zəif əlaqəli polyaronun enerji spektrinə baxılıb. Genişləndirilmiş həyəcanlanma nəzeriyyəsindən istifadə edilərək, polyaronun əsas və birinci enerji səviyyələri üçün analitic ifadə alınmışdır. Enerji səviyyələrinin qarşılıqlı dəf olunma qiymətinin kvant nöqtəsinin radiusundan asılılığı alınmışdır.

ЭНЕРГЕТИЧЕСКИЙ СПЕКТР ПОЛЯРОНА В ДИСКООБРАЗНОЙ КВАНТОВОЙ ТОЧКЕ

О.З.АЛЕКПЕРОВ, Н.М.ГУСЕЙНОВ

Рассматривается энергетический спектр слабо связанного полярона в квантовой точке в форме диска. Используя модифицированную теорию возмущений, получены аналитические выражения к поправкам основного и первого возбужденного состояний полярона. Получена величина анти-кроссинга энергетических уровней в зависимости от радиуса квантовой точки.

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