The Energy Levels of an Polaron in Parabolic potential well

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Abstract

On the basis of Buimistrov-Pekar method the polaron energy spectrum is studied in a spherical quantum dot of a polar semiconductor. The polaron correction for the ground and first excited states of the electron, depending on the size of the quantum dot is found. It is shown that refined approximation of the wave function of phonons leads to a more accurate estimation of energy polaron states and found energy levels better controlled quantum dot size than other approximations.

Keywords: *Polaron, Quantum Dot, Confining Potential, Buimistrov–Pekar Method, All Coupling Approximation*

I. INTRODUCTION

The development of semiconductor technology now makes it possible to obtain structures on the order of a few nanometers. Due to the spatial quantization of energy carriers, such as the structure of quantum dots (QDs) are an important target for a new generation of microelectronic devices [1-3].

Since the majority of QD structures made of polar semiconductors, we can expect that the interaction of carriers with polar optical phonons may significantly affect the energy levels of the carriers [4,5].

The ground state of the polaron is best estimated by Feynman path integral [6]. To calculate the number of lower levels, there are other approximate methods. Adiabatic Landau-Pekar method [7] is applicable, subject to strong localization, when the radius of the QD is much less than the radius of the polaron [8,9]. When this condition is violated, can apply the arbitrary coupling methods that allow calculate the energy levels of a wide range of relationships. One of them is the method LLPH (Lee-Low-Pines-Huybrechts) [10,11], in fact, it is the canonical transformations parameterized phonon coordinates [12]. Another method developed Buimistrov and Pekar (BP) [13] and developed by Gross [14]. Within a weak or strong ties LLPH methods and BP provide accurate results for energy polaron state, and in the intermediate region - approximately. As in QD electron wave function is usually localized, then the energy of the polaron state corresponding to the intermediate region is significantly improved.

In this paper, on the basis of BP method and parabolic potential model studied the ground and first excited state of the electron interacts with polarization oscillations of the medium. Refined approximation of the wave function of phonons leads to a more accurate assessment of energy polaron states, and these levels are better controlled by the size of QD compared with other approximations.

II. MODEL

The Hamiltonian of the electrons interacting with polarization fluctuations in the presence of the confining potential can be written as

$$H = -\frac{\hbar^2}{2m}\Delta + V(r) + \sum_{\mathbf{q}}[v_{\mathbf{q}}\, b_{\mathbf{q}} e^{i\mathbf{qr}} + v_{\mathbf{q}}^{*}\, b_{\mathbf{q}}^{+} e^{-i\mathbf{qr}}] + \sum_{\mathbf{q}}\hbar\omega_0\, b_{\mathbf{q}}^{+} b_{\mathbf{q}} \qquad (1)$$

where, m - band electron mass, $b_{\mathbf{q}}^{+}, b_{\mathbf{q}}$ - the creation and annihilation of phonons with momentum q, ω_0 - the frequency of optical phonons, $v_{\mathbf{q}}$ - form factor electron - phonon interaction, $V(r)$ - the potential localization

$$|v_{\mathbf{q}}|^2 = \frac{4\pi\alpha\, l_0(\hbar\omega_0)^2}{\Omega q^2}, \quad l_0 = \sqrt{\frac{\hbar}{2m\omega_0}}, \quad \sum_{\mathbf{q}}\ldots = \frac{\Omega}{(2\pi)^3}\int d\mathbf{q}\ldots, \quad V(r) = \frac{m\omega^2 r^2}{2} \qquad (2)$$

Averaging the Hamiltonian (1) in the basis

$$\Psi = \Phi_{ph}\,\varphi(r) = U|0\rangle\,\varphi(r),\quad U = \exp\left[\sum_{q}\left(F_q(r)\,b_q^{+} - F_q^{*}(r)\,b_q\right)\right],\quad U^{+}U = 1,\quad \langle 0|0\rangle = 1 \tag{3}$$

We get the functional

$$J\{F_q(r),\varphi(r)\} = E_0 + \sum_q \int d\mathbf{r}\varphi^2\left[\frac{\hbar^2}{2m}\left|\nabla F_q\right|^2 + \hbar\omega_0\left|F_q\right|^2 + v_q F_q e^{i\mathbf{qr}} + v_q^{*} F_q^{*} e^{-i\mathbf{qr}}\right] \tag{4}$$

$$E_0 = \frac{\hbar^2}{2m}\int d\mathbf{r}(\nabla\varphi)^2 + \int d\mathbf{r}V(r)\,\varphi^2\ . \tag{5}$$

Varying the functional (4) of F_q an inhomogeneous differential equation

$$-\frac{\hbar^2}{2m}\nabla^2 F_q(r) - 2\frac{\hbar^2}{2m}\frac{\nabla\varphi}{\varphi}\nabla F_q(r) + \hbar\omega_0 F_q(r) + v_q^{*} e^{-i\mathbf{qr}} = 0\ . \tag{6}$$

The extreme value of the functional (4) now takes the form

$$J\{\varphi(r)\} = E_0 + \sum_q v_q \int d\mathbf{r}\,\varphi^2(r) F_q(r) e^{i\mathbf{qr}} \tag{7}$$

To calculate the polaron energy use variational methods, where the test function of the electron is selected some localized function. If the ground state of the electron is described by a Gaussian function $\varphi(r) \sim \exp(-\delta^2 r^2)$ of the equation (6) can be solved exactly [14, 15]. To calculate the energy of the excited states of the solution of this equation is difficult. However, the approximate form of the function $F_q(r)$ can also be determined by a variational method by selecting it in the form

$$F_q(r) = g_q \exp(-i\ a_q \mathbf{qr}) \tag{8}$$

and determining the parameters a_q and g_q of the extreme (4). Using approximation (8) in principle can be defined as ground, and the excited state of the electron for any potential location. Substituting (8) to (4), and determining the condition extremality (4), we find

$$J\{a_q,\varphi(r)\} = E_0 - \frac{4\pi\alpha\,\hbar\omega_0 l_0}{\Omega}\sum_q \frac{1}{q^2}\frac{|e_q|^2}{1 + a_q^2 l_0^2 q^2} \tag{9}$$

where

$$e_q = \langle\varphi(r)|\exp\left[(1-a_q)i\mathbf{qr}\right]|\varphi(r)\rangle\ . \tag{10}$$

III. ENERGY LEVELS

The normalized trial function of electrons for $1s$ и $1p$ states in parabolic potential, we choice respectively

$$\varphi_{1s}(r) = \frac{\delta^{3/2}}{\pi^{3/4}}\exp\left(-\frac{\delta^2 r^2}{2}\right) \tag{11}$$

$$\varphi_{1p}(r) = \frac{\sqrt{2}\delta^{5/2}}{\pi^{3/4}} z \exp\left(-\frac{\delta^2 r^2}{2}\right), \qquad z = r\cos\theta \tag{12}$$

Since the wave function of the excited state has an angular dependence, the function a_q definition is much more complicated. For simplicity, assume that it is independent of the angle $a_q = a_q$. Substituting (11) and (12) in the functional (9), taking into account (5) and (10) by performing integration, we obtain an expression for the energy, and states (per unit $\hbar\omega_0$)

$$\varepsilon_{1s} = \frac{3\mu^2}{2} + \frac{3}{8\mu^2 R^4} - \frac{2\alpha}{\pi}\int_0^\infty dx \frac{exp\left[(1-a_x)^2 x^2/(2\mu^2)\right]}{1+a_x^2 x^2} \tag{13}$$

$$\varepsilon_{1p} = \frac{5\mu^2}{2} + \frac{5}{8\mu^2 R^4} - \frac{2\alpha}{\pi}\int_0^\infty dx \frac{exp\left[(1-a_x)^2 x^2/(2\mu^2)\right]}{1+a_x^2 x^2}\left[1 - \frac{(1-a_x)^2 x^2}{3\mu^2} + \frac{(1-a_x)^4 x^4}{20\mu^4}\right] \tag{14}$$

where $\mu = \delta l_0$, $R = \sqrt{\hbar/2m\omega}/l_0$ - dimensionless parameters introduced. In particular, if we assume $a_x = a$ that (13) and (14) obtained in the functional approach LLPH [10, 11]. The functional (14) is the total energy of the excited state system where the polarization potential (9) and (10) as described by the wave function (12). The state of the system in which the polarization of the medium is adapted to the electronic configuration (12) is relaxed excited state [7] (RES, relaxed excited state).

In the case $a_x = 0$ from (13) and (14) we obtain the results of adiabatic strong coupling. From the condition extremality of functional (13) and (14) we obtain the equation against the third and seventh degrees, respectively. However, to perform numerical integration is convenient to introduce a simpler work function, which can be determined from the following iterative scheme solutions. For an equation of the third degree (i.e., in the case of $1s$ states) can be written as

$$a_x = \frac{1+a_x^2 x^2}{1+a_x^2 x^2 + 2\mu^2} \approx \frac{1+\gamma x^2}{1+\gamma x^2 + 2\mu^2} \tag{15}$$

where γ - a new variational parameter $0 < \gamma < 1$. As the tests conducted, the approximate function (15) fairly well approximates the exact solution of the equation (6) obtained in [15]. Furthermore, it significantly refines the energy of the excited state (14) in comparison with the methods LLPH [10,11].

IV. DISCUSSION

Excluding the polarization of the medium, the exact $1s$ and $1p$ energy levels for spherical oscillator are $(3/2)\hbar\omega$ and $(5/2)\hbar\omega$ [16]. Then polaron corrections for these levels is defined as (per unit $\hbar\omega_0$)

$$\Delta E_{1s} = \varepsilon_{1s} - \frac{3}{2R^2}, \; \Delta E_{1p} = \varepsilon_{1p} - \frac{5}{2R^2} \tag{16}$$

Figure 1 shows the R dependence of the polaron shift of $1s$ - electron energy level obtained from (13) using the approximation (15) for the values of the coupling constant $\alpha = 3$ and $\alpha = 7$ (dashed line). The same figure also represented polaron shift obtained from the exact solution of the equation (6) by Green-function method [15] (solid line). It is evident that the used approximation gives satisfactory results; there is only a slight deviation at large α.

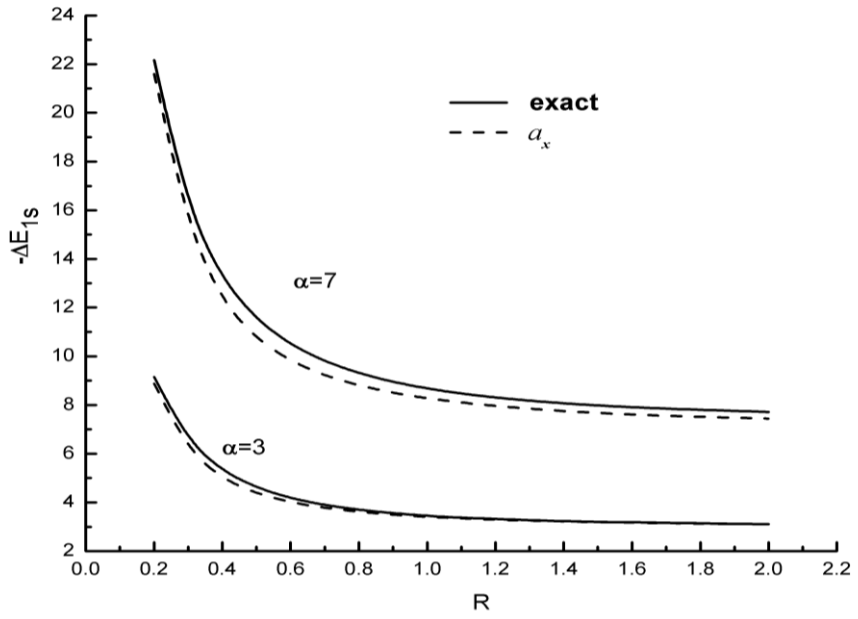

Fig.1. 1S **- polaron shift with reduced QD radius** R **obtained by the approximation (15) (dashed line) and obtained by Green-function method [15] (solid line) for** $\alpha = 3$ **and** $\alpha = 7$ **.**

Figures 2 and 3 shows the dependence of the polaron shift's of $1s$ and $1p$ energy levels of an electron from the reduced QD radius using the approximation (15) for the values of the coupling constant $\alpha = 1,3,7$ (solid line), in the approach LLPH: $a_x = a$ (dashed line) and in the strong coupling approximation $a_x = 0$ (dash dotted line).

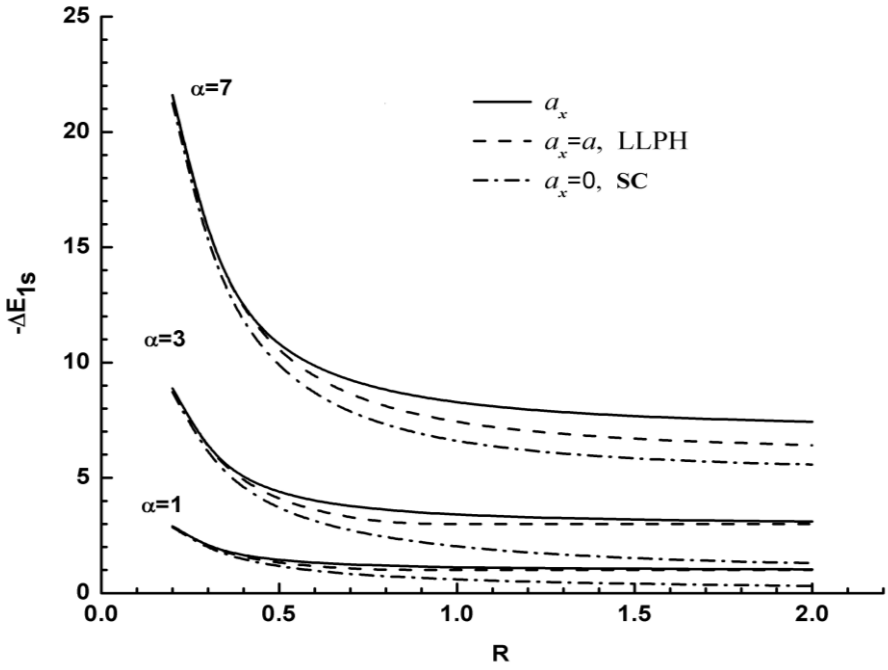

Fig.2. 1S **- polaron shift with reduced QD radius** R **obtained by the approximation (15) (solid line), in the approach LLPH:** $a_x = a$ **(dashed line) and in the strong coupling approximation** $a_x = 0$ **(dash dotted line) for the values** $\alpha = 1,3,7$ **.**

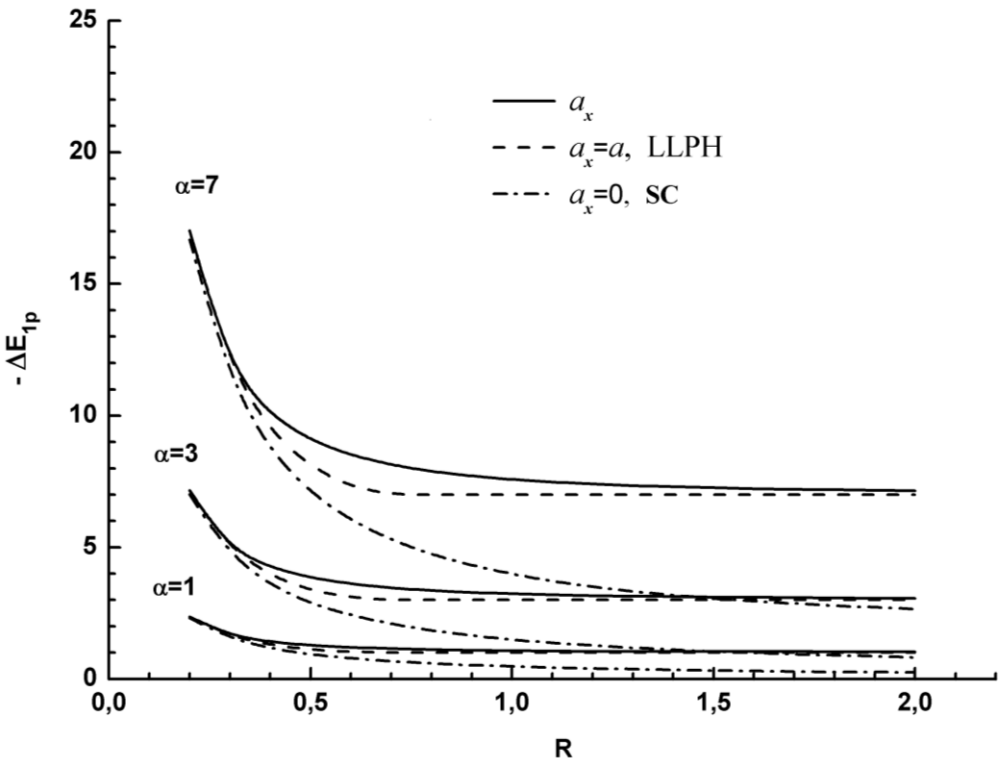

Fig.3. 1p **-polaron shift with reduced QD radius** R **obtained by the approximation (15) (solid line), in the approach LLPH:** $a_x = a$ **(dashed line) and in the strong coupling approximation** $a_x = 0$ **(dash dotted line) for the values** $\alpha = 1,3,7$.

It can be seen that the strong polaron confinement effects is observed if the QD radius is much less than the polaron radius $R / l_0 << 0.5$. This limit corresponds to the strong-coupling polaron. In the intermediate coupling polaron mode: additional polaron correction due to the electron-phonon correlations. In BP theory these correlations into account the dependence of the phonon wave functions of the electron coordinates (3). As can be seen from Figures 2 and 3, despite a simplified approximation (15), the amendment of this correlation significantly clarifies the polaron shift depending on the size of the electron energy QD compared with other approximations.

Approximate methods LLPH, ($a_x = a$) is shown by the fact that even at QD values of the radius of the electron levels have a constant shift of the order α characteristic of Lee-Low-Pines and practically does not depend on the QD size (see. Figure 3).

Figure 4 shows the dependence of the $1s$ and 1p electron levels by R using the approximation (15) for a value α, which is characteristic of the semiconductor CuCl.

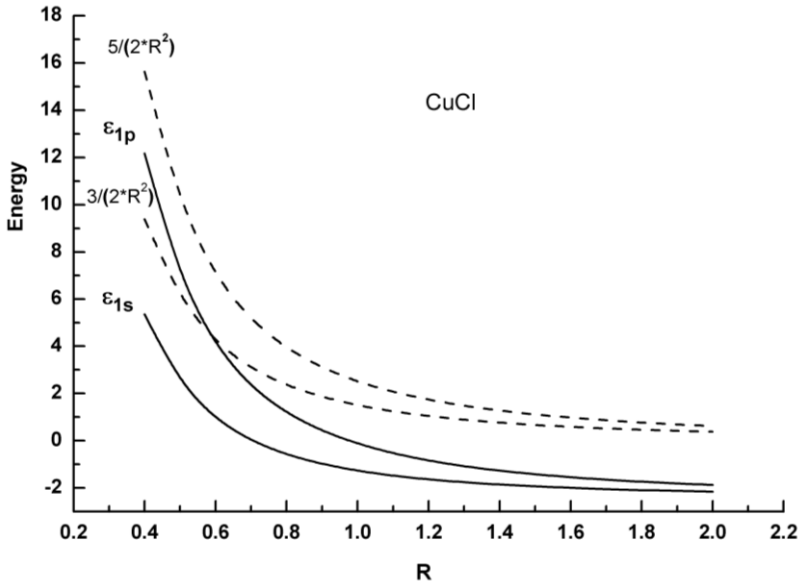

Fig.4. 1s **- and** 1p **- energy levels taking into account (solid line) and without the polaron shift (dashed line) for a semiconductor CuCl (** $\alpha = 2.45$**).**

V. CONCLUSION

In this paper, the theory of BP applied to the electron in the QD due parabolic potential model. Due to the mathematical difficulties, the solution of equation (6) is often approximated by a linear combination of expressions limit corresponding to the cases of weak and strong ties. The massive polar semiconductors viewed interpolation techniques allow evaluation of energy polaron states. The corrections come from the strong coupling $\alpha > \alpha_c (\sim 6 \cdot \cdot 8)$, where the electron wave is localized in the polarization well. At $\alpha < \alpha_c$ the electron wave delocalized, and the polaron energy corresponds to the result of Lee-Low-Pines is proportional α. As in QD electron wave function is usually localized, the critical point α_c is suppressed and the use of the approximation (8) significantly clarifies the solution of the equation (6).

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