

METHODS OF ATOMIC PHYSICS CLASSES ORGANIZATION BASED ON E-LEARNING TECHNOLOGIES

Jalolova Phokiza Muzapharovna

Candidate of pedagogical sciences, PhD, docent

Tashkent university of information technologies named after Muhammad al-Kharezmi, UZBEKISTAN
Karshi branch

E-mail: pokiza-namdu@mail.ru

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INTRODUCTION, LITERATURE REVIEW AND DISCUSSION

The energetic spectrum of the polaron is studied by the method of Buymistrov-Pekar in a spherical quantum dot which consists of polarizing (polar) semiconductors. The connection of the correction of polaron effect to the size of the quantum dot was found for the primary and the first excited state energy of the electron. It has been shown that the determined expression of the wave function of the phonons can be more accurately estimated by the energy of polar state, and these found energy surfaces are more strongly connected to the size of quantum dot than the result of other methods.

Setting the issue

Nowadays, it is possible to obtain structures which consist of several nanometers in size, due to the development of modern semiconductor materials technology. Due to the spatial quantization of current energy transmitters - structures such as quantum dots (KH) serve an important object in creating new types of microelectronic devices [1-3].

The most semiconductor materials have polar properties, the electrons in KH which are prepared them, or strong interaction of pores with polar-optical phonons can give a significant correction to their energy surfaces [4,5].

The main state energy of the polaron is most accurately calculated in Feynman's trajectory integration method [6]. There are other approximate methods for calculating the energy of several sub-states. The *adiabatic method* of Landau-Pekar [7] can be used when conditions of electron polarization strongly localized - that is, when the KH radius is much smaller than the polaronic radius $R \ll l_0$ [8,9]. If this condition does not do, then an *optional strong linkage method* can be used, this method allows to calculate the energetic surfaces of the polarized state in the optimal values of l_0 / R .

One of such methods is LLPH (Lee-Low-Pines-Huybrechts) method [10,11], according to its meaning it is based on the parameterized exchange of phonon coordinates [12]. Another method [13] was created by Buymistrov and Pekar (BP), was developed by Gross [14]. In the strong and weak electron-phonon interaction regime, LLPH and BP methods give a clear value for the polaronic energy states and give approximate results in the intermediate regime. Due to the electron-wave function is usually localized within the KH, it is possible to obtain a more clear result for the polarized state energy which is suitable for the intermediate regime.

Below, the main 1s and first excited state 1p energies of electrons which interact with polar-optical phonons, are calculated in the BP method and the parabolic potential model. The exact wave function expression of the phonons are found, it is defined that polaron state energy can be more accurately estimated, and it is shown that these found energy surfaces more strongly connected to the quantum dot size than the result of other methods.

Model

The Hamilton operator of electron which interacts with polar-optical phonons and moves in the parabolic potential field of KH can be written in the following:

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

Here, m is the mass of the electron in the transmission zone of the electrons, $b_{\mathbf{q}}^+, b_{\mathbf{q}}$ - the operators which produce and lose phonons which have \mathbf{q} impulse, ω_0 - the frequency of the optical phonons, $v_{\mathbf{q}}$ - the electron-phonon interaction form factor, $V(\mathbf{r})$ - the potential field of the KH

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

(1) The following base (test variation function) can be used to give the a diagonal view of Hamiltonian (1):

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

In this case, the average amount of the Hamiltonian (1) gives the following functionality

$$J\{F_{\mathbf{q}}(\mathbf{r}), \varphi(\mathbf{r})\} = E_0 + \sum_{\mathbf{q}} \int d\mathbf{r} \varphi^2 \left[\frac{\hbar^2}{2m} |\nabla F_{\mathbf{q}}|^2 + \hbar \omega_0 |F_{\mathbf{q}}|^2 + v_{\mathbf{q}} F_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} + v_{\mathbf{q}}^* F_{\mathbf{q}}^* e^{-i\mathbf{q}\mathbf{r}} \right] \quad (4)$$

Here

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

An unknown function $F_{\mathbf{q}}$ can be defined. To do this, we find the following non-homogeneous differential equation, when we equalize the variation of the function (4) to zero by $F_{\mathbf{q}}$:

$$-\frac{\hbar^2}{2m} \nabla^2 F_{\mathbf{q}}(\mathbf{r}) - 2 \frac{\hbar^2}{2m} \frac{\nabla \varphi}{\varphi} \nabla F_{\mathbf{q}}(\mathbf{r}) + \hbar \omega_0 F_{\mathbf{q}}(\mathbf{r}) + v_{\mathbf{q}}^* e^{-i\mathbf{q}\mathbf{r}} = 0. \quad (6)$$

Now, the extremal value of the function (4) is equal to the following:

$$J\{\varphi(r)\} = E_0 + \sum_q v_q \int d\mathbf{r} \varphi^2(r) F_q(r) e^{i\mathbf{q}\cdot\mathbf{r}} \quad (7)$$

Variation methods are often used for the calculation of polar energy, where a localized function is chosen as an electronic test function $\varphi(r)$. If the Gauss function is chosen as a test function in the estimation of the main state energy, in this case the differential equation (6) can be exactly solved [14, 15].

It is difficult to solve the differential equation for excited states (6). However, we are looking for the approximate solution of $F_q(r)$ function in the variational method. In order to do this, let's choose the view of it as follows

$$F_q(r) = g_q \exp(-i a_q \mathbf{q}\cdot\mathbf{r}) \quad (8)$$

In this case, the unknown a_q and g_q functions are defined by the minimum functional (4) condition. In general, using the approximation (8) can be calculated the energy of the main and excited state of the electron which moves in the optional potential field.

We set the expression (8) to functional (4) and determine g_q from the minimum condition of (4) and we find

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

here

$$e_q = \langle \varphi(r) | \exp[(1-a_q)i\mathbf{q}\cdot\mathbf{r}] | \varphi(r) \rangle \quad (10)$$

Calculation of energy surfaces

We write the normalized test functions for energy states 1s and 1p of electron which acts on the parabolic potential field as follows:

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

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

Here δ is a variation parameter, it is determined by the minimum energy condition. Full energy is defined separately for each energy cases 1s and 1p, thus it means that the variation parameter δ is different δ_s and δ_p . It is difficult to calculate the unknown function a_q due to the excited state 1p is dependent on the angle function θ . In order to simplify the calculations, we almost find that it does not depend on the angle, namely, $a_q = a_q$.

We put (11) and (12) test wave functions into functional (9), consider (5) and (10), and do integral by angel and find the following expression for energy of states 1s and 1p (energy expression is written in $\hbar\omega_0$ units):

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

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

Here, a new dimensionless variation parameter $\mu = \delta l_0$ has been replaced instead of δ , and also the designation $R = \sqrt{\hbar/2m\omega} / l_0$ can be considered as a dimensionless radius of KH.

In particular, if $a_x = a$ is given, functionals (13) and (14) will be transferred to the results of LLPH [10,11]. According to the meaning of functional (14), it is full energy of the state of excited 1p, in this case the polarization potentials of expressions (9) and (10) are also calculated by (12) 1p - state of the wave function. This condition which is corresponding to the electron configuration of the environment polarization (12), is called a relaxed excited state [7] (RES, relaxed excited state).

In particular, if $a_x = 0$ is given, then adiabatic strong linkage results will be derived from functionals (13) and (14).

In general cases, the unknown function a_x is found for states 1s and 1p using the minimum condition for functionals (13) and (14). As a consequence, it is possible to obtain algebraic equations of 3- and 7-degree equations for a_x accordingly 1s and 1p states. However, in order to simplify calculations, it is advisable to choose a simpler approximate function for a_x . To do this, we use iterative solution of 3 degree algebraic equation

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

Here, γ - is a new variation parameter, $0 < \gamma < 1$. The test results show that the approximate function (15) gives very close result to the exact solution [15] of the differential equation (6). In addition, the approximate function (15) also gives a more accurate result for the excited state energy (14), these results are more exact than the other LLPH methods [10,11].

Discussion of obtained results

If the environment polarization is not considered, the problem under consideration will be the spherical oscillator problem, its 1s and 1p state energies are equal to $(3/2)\hbar\omega$ and $(5/2)\hbar\omega$ [16]. So the correction for the polaron effect on these surfaces should be equal to the following (energies are written in $\hbar\omega_0$ units)

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

In figure 1 the connection of the polaron shift of the surface 1s to the radius R of KH is illustrated using (15) for the Fryolix constant values $\alpha = 3$ and $\alpha = 7$ (dashed line).

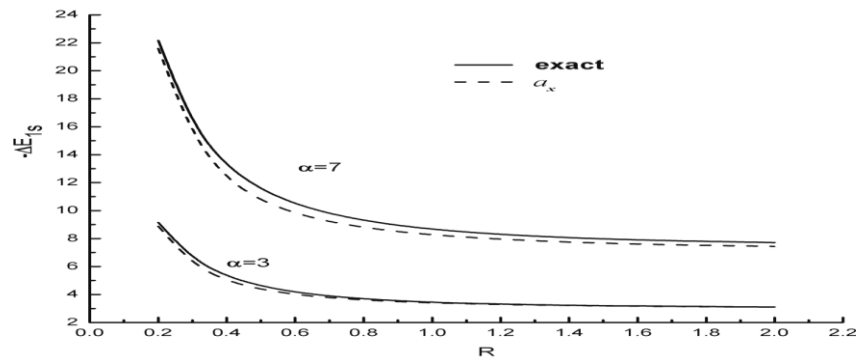


Figure 1. The graph of connection of the polaron shift of the surface of electron 1s to dimensionless radius R of KH in the values of the Fryolix constant $\alpha = 3$ and $\alpha = 7$: dashed line is given on the basis of the function (15), continuous line is given on the basis of the exact solution [15].

This figure also presents the results of polaron shift based on the exact solution [15] of the equation (6) (continuous line). As can be seen from the figure, the use of approximation (15) can give satisfactory results for all surfaces of energy.

In the figures 2 and 3 is illustrated the connection of the polaron shift of the surface of electron 1s and 1p to radius R of KH: in this case, the connection obtained by approximation (15) is shown in the continuous line, the connection obtained by the LLPH method is in the dashed line, and the connection obtained by the adiabatic strong connection is the bar-dashed line.

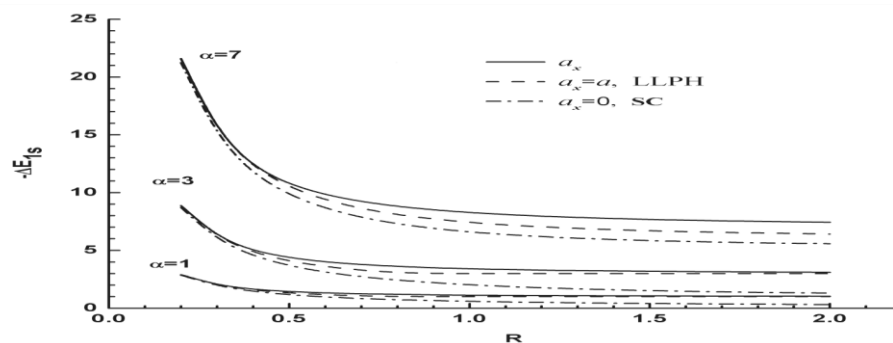


Figure 2. The graph of connection of the polaron shift of the surface of electron 1s to dimensionless radius R of KH in the values of the Fryolix constant $\alpha = 1, 3, 7$ the connection obtained by approximation (15) is shown in the continuous line, the connection obtained by the LLPH method is in the dashed line, and the connection obtained by the adiabatic strong connection is the bar-dashed line.

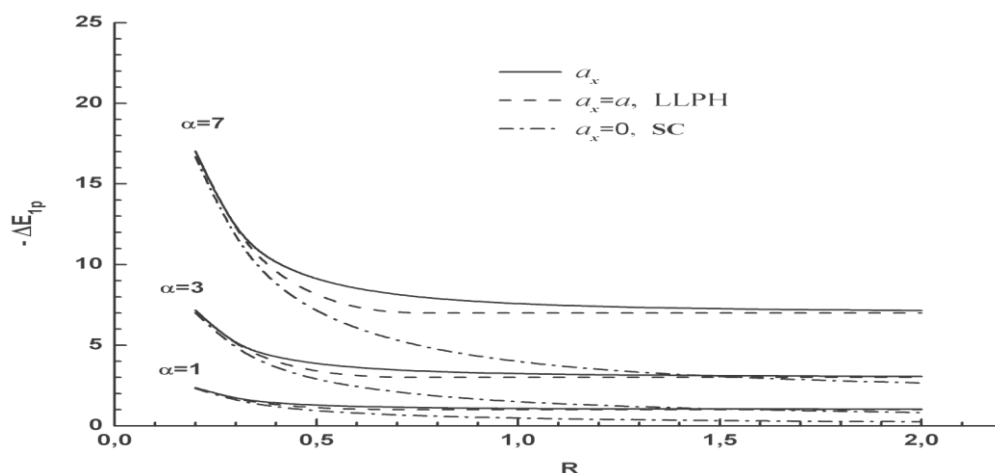


Figure 3. The graph of connection of the polaron shift of the 1p surface of electron to dimensionless radius R of KH in the values of the Fryolix constant $\alpha = 1, 3, 7$ the connection obtained by approximation (15) is shown in the continuous line, the connection obtained by the LLPH method is in the dashed line, and the connection obtained by the adiabatic strong connection is the bar-dashed line .

It can be seen that the correction of the polaron effect to the energy surfaces increases under the strong localization conditions $R/l_0 \ll 0.5$, when the radius of the KH is much smaller than the polaron radius. This regime corresponds to the polaron which has adiabatic strong connection: the rate of movement of an electron in polarization field are greater than the rate of movement of ions and ions cannot be synchronized to the electron.

The case $R/l_0 > 0.5$ corresponds to the intermediate connected polarone regime, in this case the additive polaron correlation in surfaces appears due to electron-phonon correlation. In Buymistrov-Pekar's theory, this correlation is accounted for by the connection of the phonon wave function (3) to the electron's coordinate.

As can be seen from Figures 2 and 3, the approximate function (15) allows to more accurately calculate connection of the polar shift of the energy surfaces to the KH radius compared to other approximate methods.

The approximation of the LLPH, ($a_x = a$) method shows that, when the value of the KH radius is $R/l_0 > 0.5$, the polar shift of the surfaces remains constant in the order α as the Li-Lou-Pains theory - namely, it is almost not independent of the radius of the KH (see the Figure 3).

In Figure 4 the connection of energy surfaces 1s and 1p of electron which is calculated on the basis of (15) approximation to the KH radius R is given. The Fryolix constant $\alpha = 2.45$ is obtained, this value roughly corresponds to the CuCl semiconductor.

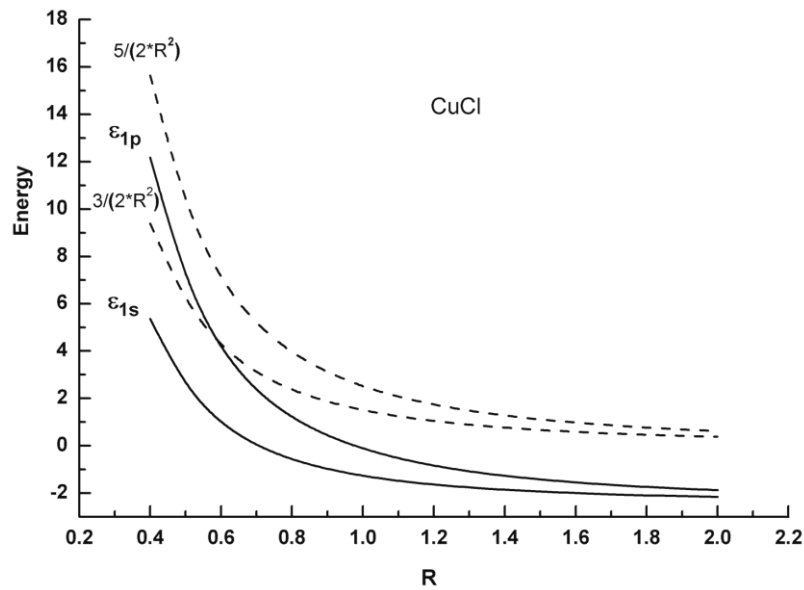


Figure 4. The connection of energy surfaces 1s and 1p of electron which is prepared CuCl ($\alpha = 2.45$) semiconductor in KH to the KH radius R : continuous line - polaronic effects are included, the dashed line - polaronic effects are excluded.

CONCLUSIONS

In this work, we used the BP method to determine the electron energy surfaces in the KH in calculating the polaron effects, and the view of the compressive potential of the KH is considered as parabolic. Due to the difficulty of solving the differential equation (6), the linear combination of exact solutions which are obtained in strong and weak interaction regimes, are sometimes used. When this method is applied to the quantitative polar semiconductors, the interpolation estimation of the polar state energy will be obtained. The correction occurs in a strong interaction regime $\alpha > \alpha_c (\sim 6 \cdot 8)$ due to the polaron effect, in this case the electron wave function is localized in the polarization field $\alpha < \alpha_c$. In the field, the electron-wave function is in delocalized position, and the polar state energy is proportional to the Li-Lou-Pains result, namely to α .

Due to the electron wave function in the KH is usually localized - the critical value α_c decreases and, as a result, the chosen (8) approximation can adequately determine the solution of the differential equation (6).