European Journal of Molecular & Clinical Medicine
ISSN 2515-8260 Volume 7, Issue 2, 2020

THEORETICAL- METHODOLOGICAL ASPECTS OF QUANTUM PHYSICS SECTION IN THE CREDIT MODULE SYSTEM

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Abstract. In this work, the BP method was used and modeled on ICT in order to calculate the energy levels of electron in the KH for calculating polyaron effects , and the image of the compressive potential of the KH was considered parabolic. Because of the difficulty of solving the differential equation (6), its solution is sometimes used by linear combinations of specific solutions which are obtained in strong and weak interaction regimes. When this method is applied to the volumetric polar semiconductors, the interpolation estimation of the energy of polaron state is obtained. In this case the correction due to the polaron effect occurs in the regime of a strong interaction impact $\alpha > \alpha_c (\sim 6 \cdot \cdot 8)$ ***, in this condition the electron wave function is localized in the polarization field. In the field*** $\alpha < \alpha_c$ ***, the electron-wave function is in the extended state (delocalized), and the polaron state energy suits the Lee-Loue-Pains result, namely it is proportional to the*** α ***.***

Keywords BP method, ICT, KH for calculating, credit module system

Because the electron wave function in the *KH* is usually localized - the critical value α_c decreases and, as a result, the chosen approximation can adequately determine the solution of the differential equation.

We can write the normalized test functions for energy states 1s and 1p of the electron which is acting on the parabolic potential field.

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

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

Here δ is a variation parameter, it is determined by the minimum energy requirement. Full energy is defined separately for each energy cases 1s and 1p, thus the variation parameter δ is different δ_s and δ_p. It is difficult to calculate the unknown function $a_{\mathbf{q}}$ because the wave function of the excited state 1p links with θ angular. In order to simplify the calculations, we will almost find that it does not depend on the angle as the $a_{\mathbf{q}} = a_q$.

We put (1) and (2) test wave functions in functional and taking into account, do integration by the angle and find the following expression for energy of states 1s and (the energy expression is written in units of $\hbar\omega_0$):

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

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

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

In private case, if $a_x = a$ is given, functions (3) and (4) will be transferred to the results of LLPH [10]. In terms of functional meaning, (4) is full energy of the excited state 1p, the polarization potentials of expressions and are also calculated by (2) - state of the wave function 1p. This condition which consistent with the electronic configuration of the polarization of the environment (2), is called a relaxed excited state [7] (RES, relaxed excited state).

In particular, if $a_x = 0$ is given, in this case results of adiabatic strong linkage create from the functions (3) and (4) .

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

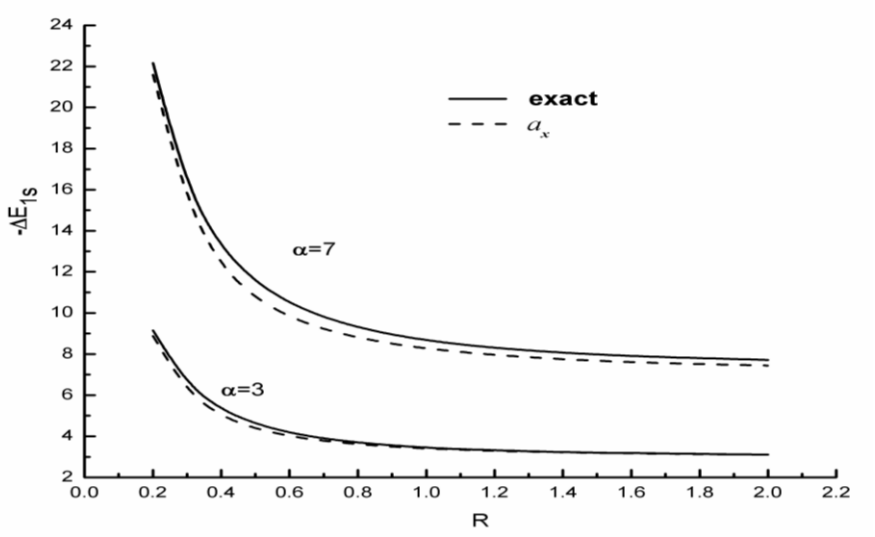
$$a_x = \frac{1+a_x^2 x^2}{1+a_x^2 x^2+2\mu^2} \approx \frac{1+\gamma x^2}{1+\gamma x^2+2\mu^2} \tag{5}$$

Here, γ is a new variation parameter, $0<\gamma<1$. According to the conducted test calculations the approximate function (5) gives very close results to the exact solution [5] of the differential equation. In addition, the approximate function (5) also yields a more accurate result for the excited state energy (4), these results are more accurate than other LLPH methods [1,2].

Discussion of the obtained results

If environment polarization is not taken a consideration, the problem under consideration is the spherical oscillator issue, its state energy 1s and 1p are equal to $(3/2)\hbar\omega$ and $(5/2)\hbar\omega$ [1]. So the correction for the polyaron effect on these levels should be equal to the followings (energies are written in units of $\hbar\omega_0$)

$$\Delta E_{1s} = \varepsilon_{1s} - \frac{3}{2R^2}, \quad \Delta E_{1p} = \varepsilon_{1p} - \frac{5}{2R^2} \tag{6}$$



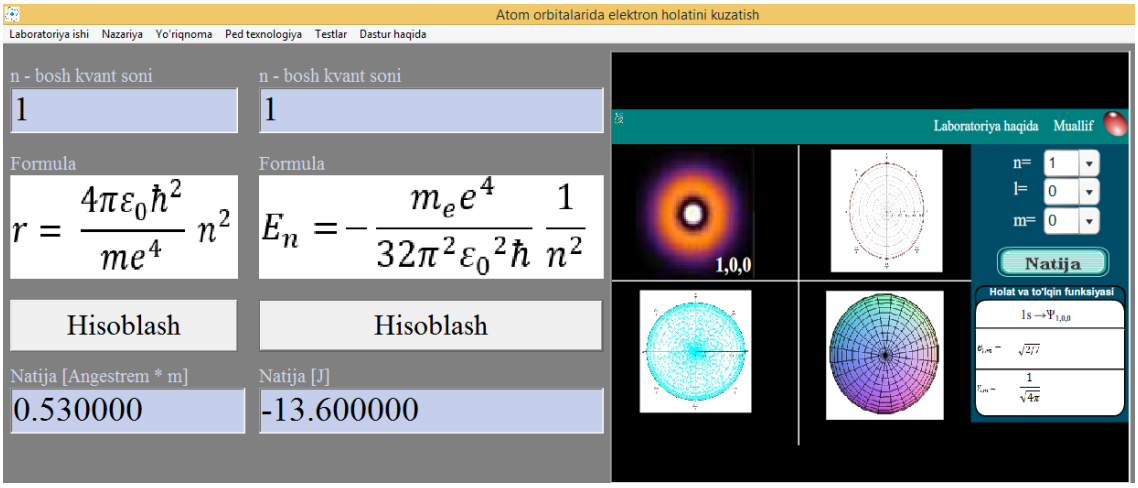


Figure 1. Graph of linkage the polaron shift of 1s level of the electron in the values $\alpha = 3$ and $\alpha = 7$ of Fryolix constant to the R dimensionless radius of KN: a dashed line - is given on the basis of the function (5), a continuous line - is given on the basis of the exact solution [5], and is given 3D model in the means of ICT.

In the figure 1 is illustrated the linkage of the polaron shift of 1s level of the electron for the values of the Fryolix constant $\alpha = 3$ and $\alpha = 7$ to the KN radius (dashed line) R using (5), and is given the 3D model on the basis of ICT.

In this figure is also given the results (continuous line) of the polaron shift based on the exact solution of [5] of the of (6) equation . As can be seen from the figure, using approximation (5) can yield satisfactory results for all levels of energy.

In the figures 2 and 3 are illustrated the linkage of the polaron shift of 1s and 1p the energy level of electron to the given radius of KN R: here (15) the linkage is obtained by approximation is shown in the continuous line, the linkage which is obtained on the basis of LLPH method is shown in the dashed line, and the linkage which is obtained on the basis of adiabatic strong linkage method is shown in the *bar-dashed* line.

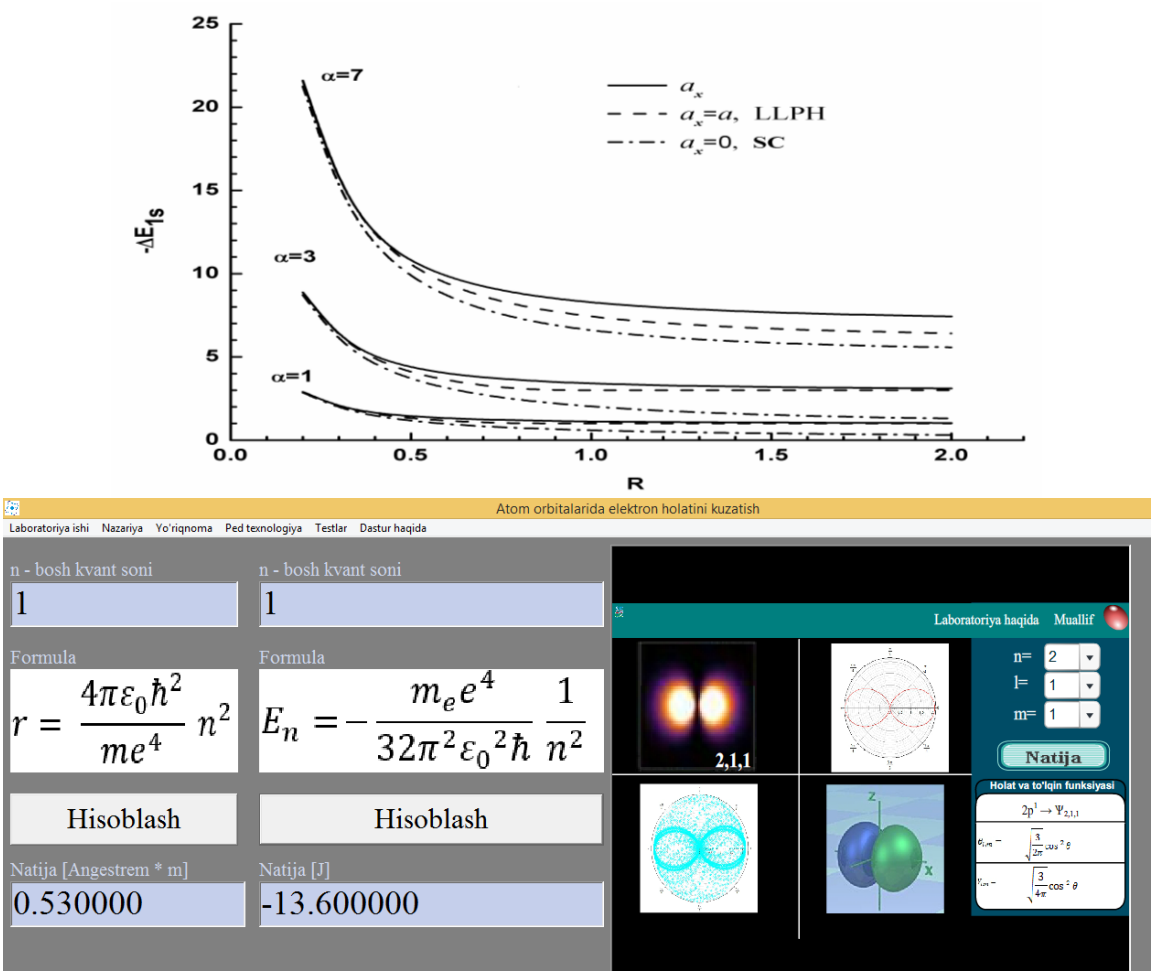
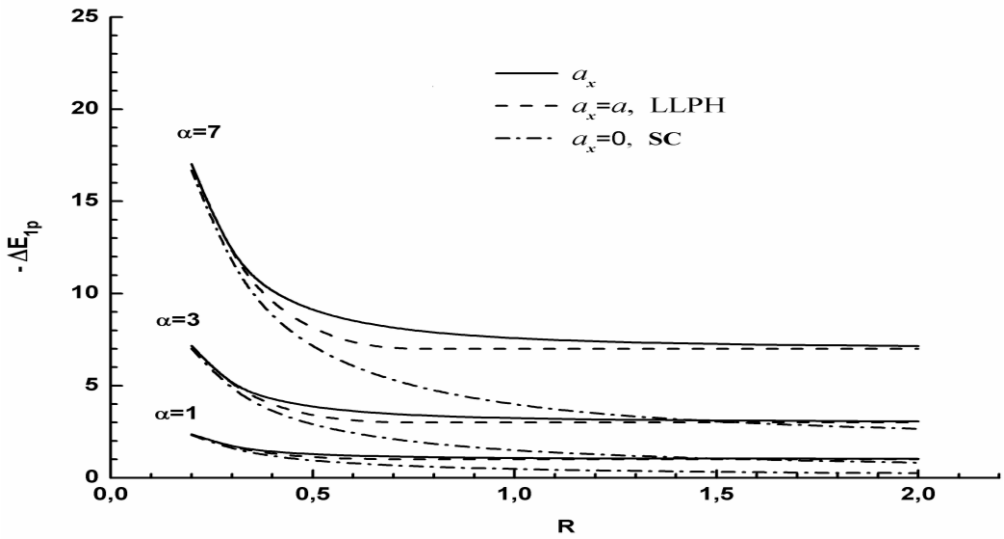


Figure 2. Graph of linkage polaron shift of the 1s level of electron in the values of Fryolix constant $\alpha = 1,3,7$ to the dimensionless radius of KN R: *continuous* line - the linkage which is obtained by approximation 15), the linkage which is obtained on the basis of LLPH method is shown in *dashed line* and the linkage which is obtained on the basis of the adiabatic strong linkage method is shown in the *bar-dashed* line.



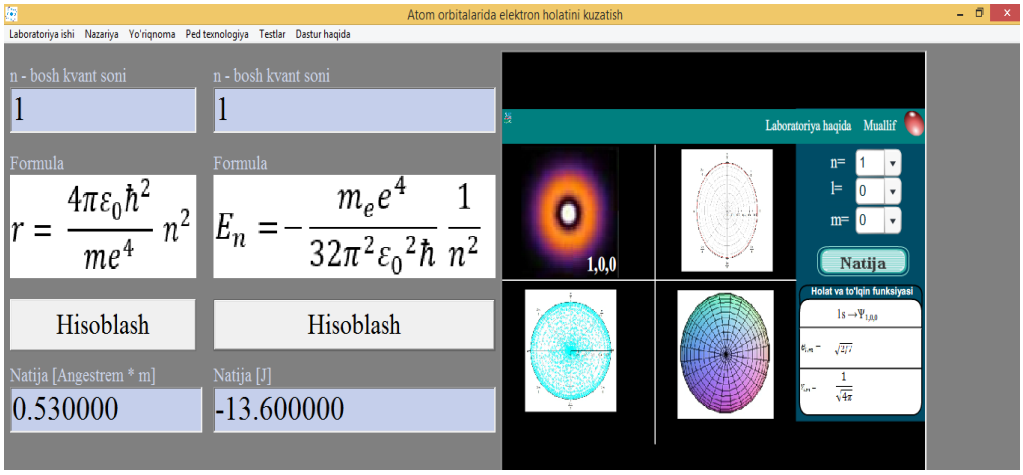


Figure 3. Graph of linkage polaron shift of the $1p$ level of electron in the values of Fryolix constant $\alpha = 1,3,7$ to the dimensionless radius of KN R: *continuous line* - (5) the linkage which is obtained by approximation (5), the linkage which is obtained on the basis of LLPH method is shown in *dashed line* and the linkage which is obtained on the basis of the adiabatic strong linkage method is shown in the *bar-dashed* line.

It can be seen that the correction of the polaron effect to the energy levels increases under the strong localization conditions $R/l_0 << 0.5$, when the radius of the KN is much smaller than the polaron radius. This regime corresponds to adiabatic *strong linkage polaron*: the speed of movement of the electron in polarization field - are greater than the speed of movement of ions and ions cannot be synchronized to the electron.

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

As can be shown in Figures 2 and 3, the approximate function (15) allows calculating the polaron shift of the energy levels to the KN radius compared to other approximate methods.

The approximation of the LLPH ($a_x = a$ method can be shown that, when the value of the KH radius is $R/l_0 > 0.5$, the polaron shift of the levels remains constant in the order of α as the theory of Li-Lou-Pains - namely, it is almost independent of the KH radius (see the figure 3).

In the figure 4 is illustrated the linkage $1s$ and $1p$ energy levels of the electron which is calculated on the basis of approximation (5) to the KN radius R. The Fryolix constant is taken as $\alpha = 2.45$, this value corresponds approximately to the CuCl semiconductor.

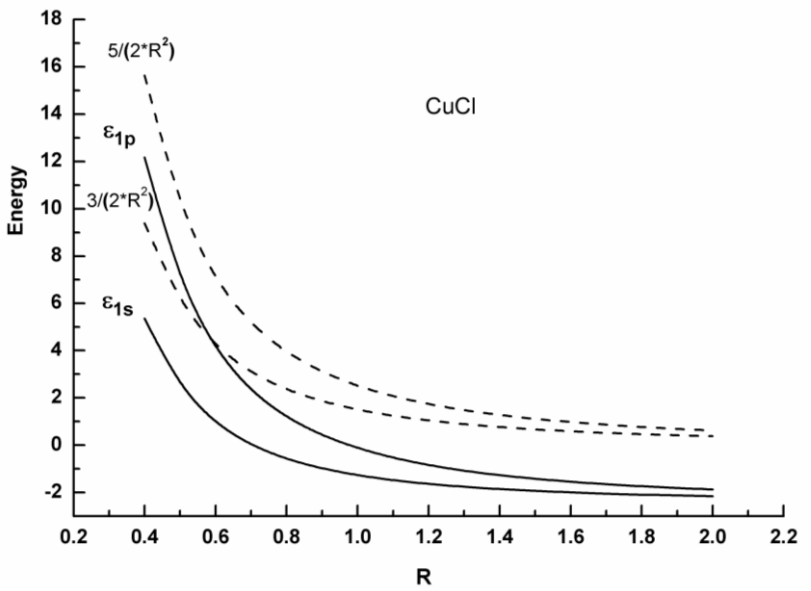


Figure 4. The linkage of 1s and 1p energy levels of electrons which are made of semiconductor CuCl ($\alpha = 2.45$) in KH to the KH radius R: continuous line - polyaronic effects are included, dashed line - polyaronic effects excluded.

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