POLARON STATES AT ARBITRARY COUPLING REGIMES IN RECTANGULAR POTENTIAL WELL

E. P. Pokatilov, M. I. Andrieş, A. A. Barsuk

State University of Moldova, str. Mateevici 60, MD-2009, Chishinau, Republic of Moldova

Abstract

We report here a new approach to the confined polaron problem at arbitrary coupling regimes. It is shown, that developed theory permits calculation of polaron energy without use of parabolic potential barriers.

1. Introduction

Modern optoelectronic technologies permit fabrication of low-dimensional structures in which electron is confined within narrow quantum wells. In their fabrication, besides Si and Ga crystals, polaronic compounds of type A_3B_5 and A_2B_6 and alkali-haloid's crystals are widely used. In future it is not inconceivable use of liquid components with great values of permittivity. In this situation redefinition of electron's parameters due to polaronic effect becomes of a great importance. Taking into consideration polaronic states is necessary in all fundamental problems of optoelectronics, like laser emission, luminescence, electroconductivity and others. Final goal of the theoretical investigations in this direction is to find effective methods of calculation of polaronic states and their optimization.

Today we have a great number of publications devoted to polaron effect investigation in different structures. Polaron states at arbitrary coupling regimes were investigated in [1] for the bulk crystals and in [2] for 2D and 1D systems. The polaron ground-state energy and the polaron effective mass were obtained in [3] at arbitrary values of the electron-phonon coupling constant α. A great interest is shown to more realistic quasi-2D (quantum well), quasi-1D (quantum wire) and quasi-0D (quantum dot) structures. Polarons in a slab of a finite width for the weak coupling regime were considered in [4, 5]. Polarons in a cylindrical quantum wire were considered in [6]. In all the above-mentioned papers, the increase of the polaron ground-state energy and of the effective mass with confinement strengthening was obtained. Thus, polaron effect role increases in nanostructures as compared with 3D systems.

Most of work on polarons is based on Feynman variational theory founded on path integration, which allows one to investigate polaron parameters at arbitrary coupling regime. However Feynman variational method possibilities are strictly confined by the parabolic potentials. In the present paper we are trying to surmount this restriction, extending variational procedure over non-parabolic potentials.

For showing the essence of this new approach we shall simplify the model, although in principle these simplifications are not necessary and we shall not use them in future. Fundamental is that we can use potential wells of different confinements and real phonon spectra.

In this paper we examine a quasi-2D structure – quantum layer with infinite barriers. Electron motion is described by x, y coordinates (in layer's plane) and z coordinate (in the direction perpendicular to layer's plane). We consider that "fictitious" particle moves in

layer's plane and is described only by x, y coordinates. We apply bulk-phonon approximation (3D phonons).

2. Feynman variational theory

The Lagrange function of the polaron problem under consideration has the form

$$L = -\frac{m}{2\hbar^2}\left(\dot{z}_\tau^2 + \dot{\rho}_\tau^2\right) - V(z_\tau) - \frac{1}{2}\sum_{\vec{k}}\left[\frac{\dot{q}_k^2}{\hbar^2} + \omega_k^2 q_k^2\right] + \sum_{\vec{k}}\gamma_k(\rho, z)\, q_{\vec{k}}\,, \tag{1}$$

where $\overline{\rho} = (x, y)$ and z are coordinates of an electron, $q_{\vec{k}}$ are the vibrational normal coordinates for LO phonons of wave vector $\vec{k}$ with frequency ω_0, $V(z_\tau)$ is quantum potential well. Amplitudes of the electron-phonon interaction are given by the expression

$$\gamma_{\vec{k}}(\vec{r}) = 2\sqrt{\frac{2\pi\hbar\omega_0\alpha_F}{V}}\,\frac{\omega_0}{k}\left(\frac{\hbar}{2m\omega_0}\right)^{1/4} e^{i\vec{k}\vec{r}} = \gamma_{\vec{k}}^{\,0}\, e^{i\vec{k}\vec{r}}\,, \tag{2}$$

where the Fröhlich coupling constant is

$$\alpha_F = \frac{e^2}{2\hbar\omega_0}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\left(\frac{2m\omega_0}{\hbar}\right)^{1/2}, \tag{3}$$

ε_∞ and ε_0 are high-frequency and static dielectric constants, respectively.

According to Feynman variational theory (FVT), the electron-phonon interaction is simulated by an elastic interaction of the electron with a "fictitious" particle of M_f mass. The trial Lagrange function is written as

$$L_0 = -\frac{m\dot{\rho}^2}{2\hbar^2} - \frac{M_f\dot{R}^2}{2\hbar^2} - \frac{M_f{\omega_f}^2}{2}\left(\vec{\rho} - \vec{R}\right)^2 - \frac{m\dot{z}^2}{2\hbar^2} - V_0(z)\,, \tag{4}$$

where M_f and ω_f are the variational parameters, $R(x, y)$ are the coordinates of a "fictitious" particle, $V_0(z)$ is approximating quantum well potential function that includes, in principle, polaron effect and therefore depends on variational parameters.

We shall consider motion in x, y plane using standard Feynman approach. Following the path-integral method, statistical sum is written as

$$Z = Sp\int e^{S} D\vec{r}Dq = Sp\int e^{S_0} D\vec{r}Dq\,\frac{Sp\int e^{S-S_0} D\vec{r}Dq}{Sp\int e^{S_0} D\vec{r}Dq} = Z_0\left\langle e^{S-S_0}\right\rangle_{S_0}, \tag{5}$$

where

$$Z_0 = Sp\int e^{S_0} D\vec{r}Dq\,, \tag{6}$$

and

$$\left\langle F[\vec{r},q]\right\rangle_{S_0} = \frac{Sp\int F[\vec{r},q]e^{S_0} D\vec{r}Dq}{Sp\int e^{S_0} D\vec{r}Dq}.$$

Using Jensen-Feynman inequality

$$\left\langle e^{S}\right\rangle_{S_0} \geq e^{\langle S\rangle_{S_0}}\,, \tag{7}$$

from Eqs. (5) and (7) we find

$$Sp\int e^{S} D\vec{r}Dq \;\geq\; Z_0 e^{<S-S_0>_{S_0}}. \tag{8}$$

Finding the logarithm of Eq. (7) we obtain

$$\ln Z \geq \ln Z_0 + \left\langle S[\vec{r}] - S_0[\rho,z]\right\rangle_{S_0}. \tag{9}$$

Thus, statistical sum is given by Eq. (9) where Z_0 is a statistical sum of a system with Lagrangian L_0, S and S_0 are the exact and trial electron action functionals obtained as a result of the elimination of the phonon coordinates and the coordinates of the "fictitious" particle, respectively.

Path integral with action S_0 can be obtained accurately

$$Sp\int e^{S_0[\rho,R,z]} D\vec{\rho}D\vec{R}Dz = \frac{L^2 m\alpha^2}{2\pi\hbar^2\lambda}\cdot\left(2\;\; sh\frac{\lambda\hbar v}{2}\right)^{-2} Sp\int e^{S_0[z]}Dz\,,$$

where

$$\alpha^2 = \frac{M_f + m}{m}, \quad v = \alpha^2\omega_f, \quad \lambda \equiv 1/T\,,$$

and

$$Sp\int e^{S_0[z]}Dz = Sp\int \exp\left(\int_0^{\lambda}\left[-\frac{m\dot{z}_\tau^{\,2}}{2\hbar^2} - V_0(z_\tau)\right]Dz\right) = \sum_n e^{-\lambda E_n}\,.$$

Here E_n are the eigenvalues of the Hamiltonian derived from $L_0(z)$. In case of low temperatures $(T\to 0)$, $\lambda\to\infty$

$$Sp\int e^{S_0[z]}Dz = e^{-\lambda E_0}\,,$$

where E_0 is the ground state of an electron in $V_0(z)$ potential. As a result we obtain

$$\ln Z_0 = \ln\left[\frac{L^2 m\alpha^2}{2\pi\hbar^2\lambda}\cdot\frac{1}{\left(2sh\frac{\lambda\hbar v}{2}\right)^2}\right]-\lambda E_0 .$$

In order to derive $S_0[\vec{r}]$ it is necessary to integrate $Z_0 = Sp\int e^{S_0[\vec{r},R]}D\rho DzD\vec{R}$ by paths R of the "fictitious" particle. Having integrated we obtain

$$S_0[\vec{\rho},z]=\int_0^\lambda\left[-\frac{m\dot{\rho}^2}{2\hbar^2}-\frac{M_f{\omega_f}^2\rho_\tau^2}{2}\right]d\tau+\int_0^\lambda\left[-\frac{m\dot{z}^2}{2\hbar^2}-V_0(z_\tau)\right]d\tau+$$
$$\Phi_0[\rho_\sigma,\rho_\tau]-2\ln\left[2sh\frac{\lambda\hbar\omega_f}{2}\right],$$

where

$$\Phi_0[\rho_\sigma,\rho_\tau]=\frac{\hbar M_f\omega_f^3}{4}\int\int_0^\lambda\vec{\rho}_\tau,\vec{\rho}_\sigma\,\frac{ch\left[\hbar\omega_f\left(|\tau-\sigma|-\lambda/2\right)\right]}{sh\left(\lambda\hbar\omega_f/2\right)}.$$

Functional $S[\vec{r}]$ could be found integrating by path the phonons $q_k(\tau)$

$$S[\vec{\rho},z]=\int_0^\lambda\left[-\frac{m\dot{\rho}^2}{2\hbar^2}--\frac{m\dot{z}^2}{2\hbar^2}-V(z)\right]d\tau+\Phi\left[\vec{r}_\tau,\vec{r}_\rho\right].$$

Here

$$\Phi\left[\vec{r}_\tau,\vec{r}_\rho\right]=\sum_{\vec{k}}\Phi_k\left[\vec{r}_\tau,\vec{r}_\rho\right],$$

$$\Phi_k\left[\vec{r}_\sigma,\vec{r}_\tau\right]=\frac{\hbar}{4\omega_k}\left(\gamma_k^0\right)^2\int\int_0^\lambda e^{i\vec{k}(\vec{r}_\tau-\vec{r}_\sigma)}\;\frac{ch\left[\hbar\omega_{\vec{k}}\left(|\tau-\sigma|-\lambda/2\right)\right]}{sh\left(\lambda\hbar\omega_{\vec{k}}/2\right)}\;d\tau\;\;d\sigma .$$

$$\langle\Phi_k\left[\vec{r}_\sigma,\vec{r}_\tau\right]\rangle_{S_0}=\frac{\hbar}{4\omega_k}\left(\gamma_k^0\right)^2\int\int_0^\lambda\langle e^{i\vec{\eta}(\vec{\rho}_\tau-\rho_\sigma}\rangle_{S_0[\rho]}\;\frac{ch\left[\hbar\omega_{\vec{k}}\left(|\tau-\sigma|-\lambda/2\right)\right]}{sh\left(\lambda\hbar\omega_{\vec{k}}/2\right)}\langle e^{ik(z_\tau-z_\sigma)}\rangle_{S_0[z]}\;d\tau\;\;d\sigma .$$

A particular feature of our new approach consists in the integral calculation method by z paths. Due to a non-parabolic potential well in $L_0(z)$, there are no standard representations for output (exact) calculations of

$$\left\langle e^{i\kappa(z_\tau-z_\sigma)}\right\rangle_{S0}\equiv\frac{Sp\int e^{i\kappa(z_\tau-z_\sigma)}\;e^{S\,0[z]}\;Dz}{Sp\int e^{S\,0[z]}\;Dz}.$$

We shall make use of transition amplitude representation for a time-independent Hamiltonian, suitable at any shape of potential well, using $\psi_n(z)$ eigenfunctions of trial Hamiltonian

$$\int_{z_\sigma}^{z_\tau} e^{S_0[z_{\tau'}]} Dz_{\tau'} = K_0\left[z_\tau, \tau;\ z_\sigma, \sigma\right] = \sum_n \psi_n\left(z_\tau\right)\ \psi_n^*(z_\sigma) e^{-(\tau-\sigma)\,E_n}\,. \tag{10}$$

By τ and σ points $\lambda - 0$ interval is divided into three parts $\lambda - \tau$, $\tau - \sigma$ and $\sigma - 0$, and on each of them electron moves in a potential well without interacting with phonons and can be described by amplitude of transition $K_0[z_\tau, \tau; z_\sigma, \sigma]$ (10), determined by that potential well. Interaction with phonons occurs in points of time τ and σ.

Convolving path integrals on each of these segments in transition amplitudes, and integrating by z_0 and z_λ one can obtain

$$\begin{aligned}
&\left\langle e^{i\kappa(z_\tau - z_\sigma)} \right\rangle_{S_0} = \int \delta(z_\lambda - z_0) dz_\lambda dz_0 \int dz_\tau dz_\sigma \times \\
&\left(\sum_m \psi_m\left(z_\lambda\right) \psi_m^*\left(z_\tau\right) e^{-(\lambda-\tau)E_m} \right) \left(\sum_n \psi_n\left(z_\tau\right) \psi_n^*\left(z_\sigma\right) e^{-(\tau-\sigma)E_n} \right) \times \\
&\sum_l \psi_l\left(z_\sigma\right) \psi_l^*\left(z_0\right) e^{-\sigma E_l} e^{i\kappa(z_\tau - z_\sigma)} \Big/ \int e^{S_0} Dz = \\
&\sum_n \left| \left\langle \psi_n^*\left(z_\tau\right) \right| e^{i\kappa z_\tau} \left| \psi_0\left(z_\tau\right) \right\rangle \right|^2 e^{-(\tau-\sigma)(E_n - E_0)}
\end{aligned} \tag{11}$$

Wave functions ψ_n are here the eigenfunctions, and E_n - eigenvalues of the Schrödinger equation with a variational potential

$$\left(\frac{p_z^2}{2m} + V_0(z) \right) \psi_n = E_n \psi_n\,.$$

We shall choose a potential well with infinite barriers

$$V(z) = \begin{cases} 0, & |z| \le L/2; \\ \infty, & |z| \ge L/2. \end{cases}$$

Under such conditions polaron effect couldn't influence the shape and the height of potential well, therefore $V(z) = V_0(z)$. As a result, we obtain

$$\left\langle S - S_0 \right\rangle_{S_0} = \left\langle \Phi\left[\vec{r}_\sigma, \vec{r}_\tau\right] \right\rangle_{S_0} - \left\langle \Phi_0\left[\vec{r}_\sigma, \vec{r}_\tau\right] \right\rangle_{S_0} + \frac{M_f \omega_f^{\,2}}{2} \int_0^\lambda \left\langle \rho_\tau \right\rangle^2 \ d\tau + 2\ln\left[2sh \frac{\lambda \hbar \omega_f}{2} \right].$$

Using the following thermodynamic formula

$$E = -\frac{\partial}{\partial \lambda} \ln Z ,$$

in case of $\lambda \to 0$, polaron energy is found to be

$$E = \int \psi_0^* \hat{H}(z) \psi_0 dz + \frac{hv}{2}\left(1 - \frac{1}{\alpha}\right)^2 - \\ - \frac{\hbar}{2\omega_0} \sum_{\vec{k}} \left(\gamma_{\vec{k}}^0\right)^2 \sum_n \left| \left\langle \psi_n \left| e^{i\kappa z} \right| \psi_0 \right\rangle \right|^2 \int_0^\infty d\tau \, e^{-(E_n - E_0 + \hbar\omega_0)\tau} e^{-\eta^2 A(\tau)}, \tag{12}$$

where

$$\gamma_{\vec{k}}^0 = 2\sqrt{\frac{2\pi\hbar\omega_0\alpha_F}{V}} \frac{\omega_0}{k} \left(\frac{\hbar}{2m\omega_0}\right)^{1/2},$$

and

$$A(\tau) = \frac{\hbar^2 a_1}{2m}\tau + \frac{\hbar a_2}{2mv}\left(1 - e^{-\hbar v \tau}\right), \ \left(a_1 = 1/\alpha^2, a_2 = 1 - 1/\alpha^2\right).$$

3. Analytical analysis

We shall turn to the non-dimensional variables. For the energy we have $\varepsilon = \frac{E}{\hbar\omega_0}$. For coordinates and variational parameters $\bar{z} = \frac{z}{R_p}$, $\bar{\kappa}_z = \kappa_z R_p$, $\bar{\eta} = \eta R_p$, $\bar{v} = \frac{v}{\omega_0}$ and $t = \hbar\omega_0 \, \tau$.

Dimensionless formula of energy is

$$\varepsilon\left(\alpha, \bar{v}, \alpha_F\right) = \varepsilon_0 + \frac{\bar{v}}{2}\left(1 - \frac{1}{\alpha}\right)^2 + \varepsilon_{e-ph}\left(\alpha, \bar{v}, \alpha_F\right), \tag{13}$$

Where electron-phonon part has the form

$$\varepsilon_{e-ph} = -\frac{\alpha_F}{\pi} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \left| \left\langle \psi_n \left| e^{i\bar{\kappa}\bar{z}} \right| \psi_0 \right\rangle \right|^2 d\bar{\kappa} \int_0^\infty e^{-(\varepsilon_n - \varepsilon_0 + 1)t} dt \int_0^\infty \frac{\bar{\eta} e^{-\bar{\eta}^2 \bar{A}(t)}}{\bar{\eta}^2 + \bar{\kappa}^2} d\bar{\eta} . \tag{14}$$

In (13) and (14) energy depends on non-dimensional variational parameters α and $\bar{v}$, as well as on Fröhlich coupling constant α_F. Integration variables are also dimensionless. Function $\bar{A}(t)$ has the form

$$\overline{A}(t) = a_1 t + \frac{\overline{a}_2}{\overline{\nu}}\left(1 - e^{-\overline{\nu}t}\right).$$

Using the well known expressions for energy levels and eigenfunctions for a particle in $V(z)$ potential [8], one can obtain the matrix element $\left\langle \psi_n \left| e^{i\overline{\kappa}\,\overline{z}} \right| \psi_0 \right\rangle$ in an explicit form

$$\left\langle \psi_n \left| e^{i\overline{\kappa}\,\overline{z}} \right| \psi_0 \right\rangle = \frac{4}{\overline{L}^2}\left(I_1^2 + I_2^2\right),$$

where

$$I_1 = -\frac{4\overline{L}^2\pi^2 n\,\overline{\kappa}\sin^2 n\pi/2 \sin \overline{L}\overline{\kappa}/2}{\left((n-1)\pi - \overline{L}\overline{\kappa}\right)\left(\pi + n\pi - \overline{L}\overline{\kappa}\right)\left((n-1)\pi + \overline{L}\overline{\kappa}\right)\left(\pi + n\pi + \overline{L}\overline{\kappa}\right)},$$
$$I_2 = -\frac{4\overline{L}^2\pi^2 n\,\overline{\kappa}\cos^2 n\pi/2 \cos \overline{L}\overline{\kappa}/2}{\left((n-1)\pi - \overline{L}\overline{\kappa}\right)\left(\pi + n\pi - \overline{L}\overline{\kappa}\right)\left((n-1)\pi + \overline{L}\overline{\kappa}\right)\left(\pi + n\pi + \overline{L}\overline{\kappa}\right)}.$$

In order to calculate the double integral

$$J\left(\overline{\kappa}^2\right) = \int_0^\infty e^{-(\varepsilon_n - \varepsilon_0 + 1)t} dt \int_0^\infty \frac{\overline{\eta}\, e^{-\overline{\eta}^2 \overline{A}(t)}}{\overline{\eta}^2 + \overline{\kappa}^2} d\overline{\eta}\,, \tag{15}$$

we introduce the notation $\beta = \varepsilon_n - \varepsilon_0 + 1$ and make the following transformations of variables: $\overline{\eta} = \overline{\kappa}\, y$, $x = y^2\, \overline{A}(t)$. Accordingly, (15) takes the form

$$J\left(\overline{\kappa}^2\right) = \int_0^\infty e^{-\beta t} \int_0^\infty \frac{e^{-\overline{\kappa}^2 x}}{x + \overline{A}(t)} dx dt\,. \tag{16}$$

Taking into account, that asymptotical behavior of $\overline{A}(t)$ in the explicit form is

$$\overline{A}(t) = a_1 t + \frac{\overline{a}_2}{\overline{\nu}}\left(1 - e^{-\overline{\nu}t}\right) \approx t\,, \quad (t << 1)$$

we can write $\overline{A}(t) \equiv t + \left(\overline{A}(t) - t\right)$, and represent

$$\frac{1}{x + \overline{A}(t)} = \frac{1}{x + t} + \left(\frac{1}{x + \overline{A}(t)} - \frac{1}{x + t}\right) = \frac{1}{x + t} - \frac{\overline{A}(t) - t}{(x + t)\left(x + \overline{A}(t)\right)}. \tag{17}$$

Since $\overline{A}'(t) = a_1 + a_2\, e^{-\overline{\nu}\, t} > 0$, $\overline{A}(t)$ is a monotone increasing function. So, integral (16) using decomposition (17) can be represented in the form

$$J\left(\bar{\kappa}^2\right)=\frac{1}{2}\int_0^\infty e^{-\beta t}\int_0^\infty \frac{e^{-\bar{\kappa}^2 x}}{x+t}\,dxdt-\frac{1}{2}\int_0^\infty e^{-\beta t}\left(\bar{A}(t)-t\right)\int_0^\infty \frac{e^{-\bar{\kappa}^2 x}}{(x+t)\left(x+\bar{A}(t)\right)}\,dxdt\,. \tag{18}$$

The first integral in (18) can be derived in an explicit form and is equal to

$$J_1\left(\bar{\kappa}^2\right)=\frac{1}{2}\int_0^\infty e^{-\beta t}\int_0^\infty \frac{e^{-\bar{\kappa}^2 x}}{x+t}\,dxdt=\frac{1}{2}\frac{\ln\bar{\kappa}^2-\ln\beta}{\bar{\kappa}^2-\beta}\,. \tag{19}$$

As for the second integral in (18)

$$J_2\left(\bar{\kappa}^2\right)=\frac{1}{2}\int_0^\infty e^{-\beta t}\left(\bar{A}(t)-t\right)\int_0^\infty \frac{e^{-\bar{\kappa}^2 x}}{(x+t)\left(x+\bar{A}(t)\right)}\,dxdt$$

we notice that it do not have any singularity by $\bar{\kappa}^2$. In particular, at $\beta=1$ and $\bar{\kappa}^2=0$

$$J_2(0)=\frac{1}{2}\int_0^\infty e^{-t}\left(t-\bar{A}(t)\right)\int_0^\infty \frac{dx}{(x+t)\left(x+\bar{A}(t)\right)}\,dxdt=\int_0^\infty e^{-t}\ln\frac{t}{\bar{A}(t)}dt\neq 0\,.$$

It means the uniform convergence of integral by x and we can change the integration order. For numerical calculations it is convenient to represent $J_2\left(\bar{\kappa}^2\right)$ in the following form

$$J_2\left(\bar{\kappa}^2\right)=\frac{1}{2}\int_0^\infty e^{-\bar{\kappa}^2 x}\int_0^\infty \frac{\left(t-\bar{A}(t)\right)e^{-\beta t}}{(x+t)\left(x+\bar{A}(t)\right)}\,dtdx\,. \tag{20}$$

As a result we obtain the following expression for $J\left(\bar{\kappa}^2\right)$

$$J\left(\bar{\kappa}^2\right)=\frac{1}{2}\left(\frac{\ln\bar{\kappa}^2-\ln\beta}{\bar{\kappa}^2-\beta}-\int_0^\infty e^{-\bar{\kappa}^2 x}\int_0^\infty \frac{\left(t-\bar{A}(t)\right)e^{-\beta t}}{(x+t)\left(x+\bar{A}(t)\right)}\,dtdx\right). \tag{21}$$

Collecting all together, we derive the final form for polaron energy

$$\begin{aligned}\varepsilon=\varepsilon_0+\frac{\bar{v}}{2}\left(1-\frac{1}{\alpha}\right)^2-16\alpha_F\bar{L}^2\pi^3\sum_{n=1}^\infty n^2\int_{-\infty}^\infty d\bar{\kappa}\,\frac{\bar{\kappa}^2\left(1+(-1)^n\cos\bar{\kappa}\,\bar{L}\right)}{M^2}\times\\ \left\{\frac{\ln\bar{\kappa}^2-\ln\beta}{\bar{\kappa}^2-\beta}-\int_0^\infty e^{-\bar{\kappa}^2 x}\int_0^\infty \frac{\left(t-\bar{A}(t)\right)e^{-\beta t}}{(x+t)\left(x+\bar{A}(t)\right)}\,dtdx\right\}.\end{aligned} \tag{22}$$

The further calculations can be performed only in the numerical form.

4. Numerical results and discussions

Results of numerical calculations of polaron energy $\Delta\varepsilon = \varepsilon - \varepsilon_0$ using (22) are represented in Fig.1. The function $\Delta\varepsilon(\alpha_F)$ is plotted at different values of well width $\bar{L}$. Curves corresponding to 3D and 2D limiting cases are also plotted here. It is clearly seen, that with confinement strengthening, curves are moving away from 3D limit case and draw near 2D limit case.

Fig.1. Dependences $\Delta\varepsilon(\alpha_F)$ plotted at different values of well width

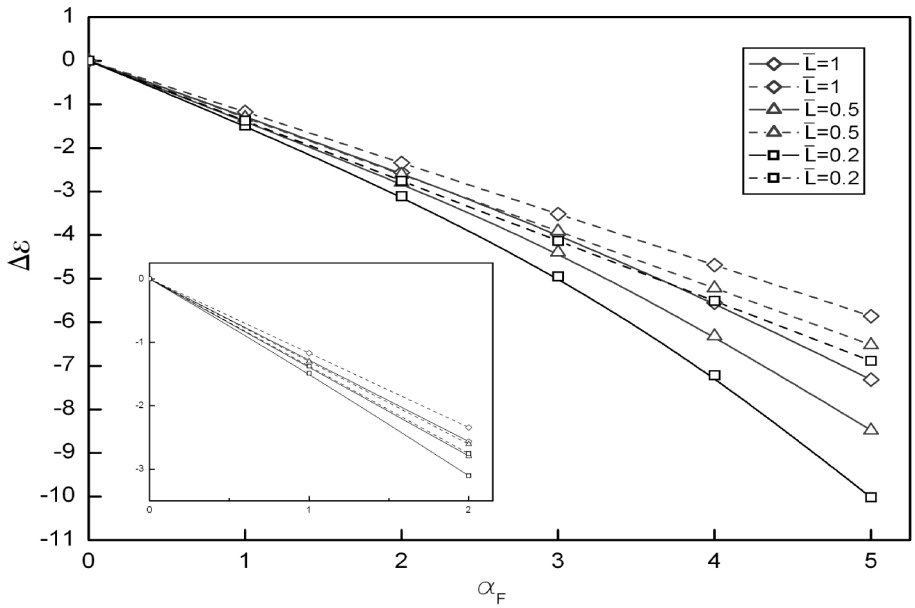


Fig. 2. Polaron energy dependences in weak-coupling limit.

In the weak-coupling limit, polaron energy is proportional to α_F for any confinement. But α_F factor depends on confinement. Polaron energy in weak-coupling limit for finite confinement is obtained using (22) and presented in Fig. 2. Dotted lines are plotted using perturbation theory. Firm lines denote results obtained using formula (22). Comparing these results one can see that for small α_F they coincide. In the linear approximation formula (22) can be written as $\Delta\varepsilon = -C\left(\bar{L}\right)\alpha_F$. Numerical values of the coefficients of the linear terms are $C(1,0)=1,02$, $C(0,5)=1,31$, $C(0,2)=1,43$. Comparing these values to the one obtained for 2D polarons in weak coupling limit $\left(\Delta\varepsilon = -\frac{\pi}{2}\alpha_F - 0,06397\,\alpha_F^2\right)$, we can clearly see theirs correct arrangement.

Thus we have: 1) our general formula (22) gives a correct weak-coupling limit; 2) expected dependence of weak-coupling region on confinement strength is obtained. It is observed that as coupling increases, straight-line region for energy shortens depending on coupling constant. It is worth noting the correct order of $\Delta\varepsilon(\alpha_F, \bar{L})$ curves.

5. Conclusions

A new approach to the polaron energy problem at arbitrary coupling regimes is proposed. Coupling energy for a polaron in a rectangular potential well with infinite barriers is calculated at different well widths. Thus, it is shown that developed theory permits calculation of polaron energy without use of parabolic potential barriers, for all electron-phonon coupling regimes.

Discussions with Professor J.T. Devreese and Professor V.M. Fomin are gratefully acknowledged.

The work was supported by the U.S. Civil Research and Development Foundation project MP2-3044.

References

[1] R.P. Feynman, Phys. Rev. 97, 660 (1955).
[2] V.M. Fomin, E.P. Pokatilov Phys. Rep. 158, 205 (1988).
[3] J.T. Devreese, Polarons, Encyclopedia of Applied Physics, VCH Publishers, New York, vol.14, 1966, pp. 383-413.
[4] Wu Xioaoguang, F.M. Peeters, J.T. Devreese, Phys. Rev. B 31, 3420 (1985).
[5] F.M. Peeters, J.T. Devreese Phys. Rev. B 36, 4442 (1987).
[6] P. Vansant, F.M. Peeters, M.A. Smondyrev, J.T. Devreese, Phys. Rev. B 52, 12743 (1995).
[7] E.P. Pokatilov, V.M. Fomin, J.T. Devreese, S.N. Balaban, S.N. Klimin, Phys. Rev. E 4, 156 (1999).
[8] L.D. Landau, E.M. Lifschitz: "Quantum Mechanics: Non-relativistic Theory", vol. 3, Nauka, Moscow, 1974.