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# INFLUENCE OF THE MEDIUM POLARIZATION ON THE ENERGY OF AN ELECTRON IN A QUANTUM DOT

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*The Buimistrov–Pekar method has been applied to calculate the polaronic shift of the electron energy level in a quantum dot. In the framework of the parabolic confinement approximation, the differential equation for the phonon amplitude is exactly solved, by using the Green's function method. The results of various approximations have been compared.*

*K e y w o r d s*: polaron, quantum dot, confining potential, ground-state energy, Buimistrov–Pekar method, Green's function method, all-coupling approximation.

## 1. Introduction

In recent years, new physical properties of semiconductor nanostructures have been a subject of intense researches. Owing to the localization of charge carriers in nano-sized objects, the energy is quantized. In this connection, a particular attention is paid to studying the influence of phonons on the electron spectrum in low-dimensional semiconductor structures (i.e. nanostructures) [1–3]. In polar crystals, the interaction between charge carriers and polar optical phonons is strong. Therefore, the study of polaron effects typical of low-dimensional systems is of considerable interest. To calculate the polaronic effects in nanostructure materials, researchers take advantage of various approximations [4–9]. In so doing, along with the Feynman method of path integration, the methods of canonical transformations (CTs) are also applied [8–10].

In the method of parametrized CTs [8, 9], the Lee–Low–Pines transformation and the transformation of a phonon amplitude displacement are applied consecutively by introducing certain variational parameters. In the Buimistrov–Pekar method [10], the differential equation for the phonon displacement amplitude was obtained with the use of the CT method. However, since the solution of this equation is cumbersome, the phonon displacement amplitudes were chosen as linear combinations of the limiting expressions corresponding to the cases of weak and strong couplings.

In this work, the polaronic shift of the electron level in a quantum dot is calculated with the use of the method developed in works [10, 11]. The differential equation for the phonon displacement amplitude is solved exactly, by using the Green's function (GF) method. To simplify the problem, the confinement potential is considered to be parabolic. The results obtained in various approximations are compared with one another.

## 2. Model

The Hamiltonian of an interacting electron-phonon system in nanostructures can be written in the form

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

where $m$ is the band mass of an electron, $b^+_{\mathbf{q}}$ and $b_{\mathbf{q}}$ are the creation and annihilation, respectively, operators of a phonon with the momentum $\mathbf{q}$, $\omega_0$ is

the frequency of optical phonons, $v_{\mathbf{q}}$ the form factor of the electron-phonon interaction, $V(r)$ the confinement potential, and

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

Averaging Hamiltonian (1) in the basis

$$\Psi = \Phi_{\rm ph}\phi(r) = U\,|0\rangle\,\phi(r),$$
$$U = \exp\left[\sum_{\mathbf{q}}\left(F_{\mathbf{q}}(r)b^+_{\mathbf{q}} - F^*_{\mathbf{q}}(r)b_{\mathbf{q}}\right)\right], \tag{3}$$
$$U^+U = 1, \langle 0\mid 0\rangle = 1,$$

we obtain the functional

$$J\left[F_{\mathbf{q}}(r),\phi(r)\right] = E_0 + \sum_{\mathbf{q}}\int d\mathbf{r}\phi^2\left[\frac{\hbar^2}{2m}\left|\nabla F_{\mathbf{q}}\right|^2 + \right.$$
$$\left. + \hbar\omega_0\left|F_{\mathbf{q}}\right|^2 + v_{\mathbf{q}}F_{\mathbf{q}}e^{i\mathbf{qr}} + \ v^*_{\mathbf{q}}F^*_{\mathbf{q}}e^{-i\mathbf{qr}}\right], \tag{4}$$
$$E_0 = \frac{\hbar^2}{2m}\int d\mathbf{r}\left(\nabla\phi\right)^2 + \int d\mathbf{r}V(r)\phi^2. \tag{5}$$

By varying functional (4) with respect to $F_q$, we obtain the inhomogeneous differential equation

$$-\frac{\hbar^2}{2m}\nabla^2 F_{\mathbf{q}}(r) - 2\frac{\hbar^2}{2m}\frac{\nabla\phi}{\phi}\nabla F_{\mathbf{q}}(r) +$$
$$+\hbar\omega_0 F_{\mathbf{q}}(r) + v^*_{\mathbf{q}}e^{-i\mathbf{qr}} = 0. \tag{6}$$

Now, the extreme value of functional (4) looks like

$$J\left[\phi(r)\right] = E_0 + \sum_{\mathbf{q}} v_{\mathbf{q}}\int d\mathbf{r}\phi^2(r)F_{\mathbf{q}}(r)e^{i\mathbf{qr}}. \tag{7}$$

The solution of Eq. (6) describes the dependences of the phonon field displacement amplitudes on the electron coordinate. In the weak-coupling limit, $\alpha \to 0$, i.e. when the electron cloud size is rather big, we may neglect the gradient of the electron function (the second term in Eq. (6)). Then, assuming $\phi^2(r) \sim 1$ in Eq. (7) (in the absence of a confinement), we obtain the known result

$$F_{\mathbf{q}}(r) = -\frac{v^*_{\mathbf{q}}e^{-i\mathbf{qr}}}{\hbar^2q^2/2m + \hbar\omega}, \quad J = -\alpha\hbar\omega_0. \tag{8}$$

Buimistrov and Pekar [10] used the linear combination $F_{\mathbf{q}}(r) = f_{\mathbf{q}} + g_{\mathbf{q}}e^{-i\mathbf{qr}}$. When determining the parameters $f_{\mathbf{q}}$ and $g_{\mathbf{q}}$ by minimizing functional (4), they obtained a result that approximates the polaron energy at an arbitrary coupling strength $\alpha$.

Following Gross [11], let us introduce the notation $F_{\mathbf{q}} = V^*_{\mathbf{q}}\Phi_{\mathbf{q}}/\phi$ and rewrite Eqs. (6) and (7) in the form

$$-\frac{\hbar^2}{2m}\Delta\Phi_{\mathbf{q}}(r) + \frac{\hbar^2}{2m}\frac{\Delta\phi}{\phi}\Phi_{\mathbf{q}}(r) +$$
$$+\hbar\omega_0\Phi_{\mathbf{q}}(r) + \phi(r)e^{-i\mathbf{qr}} = 0, \tag{9}$$
$$J\left[\phi(r)\right] = E_0 + \sum_{\mathbf{q}}\left|V_{\mathbf{q}}\right|^2\int d\mathbf{r}\ \phi(r)\Phi_{\mathbf{q}}(r)e^{i\mathbf{qr}}. \tag{10}$$

Introducing the GF for Eq. (9),

$$\Phi_{\mathbf{q}}(r) = -\int d\mathbf{r}'\ G(r,r')\phi(r')e^{-i\mathbf{qr}'} \tag{11}$$

and considering the relation

$$\sum_{\mathbf{q}}\left|V_{\mathbf{q}}\right|^2 e^{i\mathbf{q}(\mathbf{r}-\mathbf{r}')} = \frac{\alpha l_0(\hbar\omega_0)^2}{|\mathbf{r}-\mathbf{r}'|}, \tag{12}$$

we obtain from Eqs. (9) and (10) that

$$\left[-\frac{\hbar^2}{2m}\Delta + \frac{\hbar^2}{2m}\frac{\Delta\phi}{\phi} + \hbar\omega_0\right]G(r,r') = \delta(\mathbf{r}-\mathbf{r}'), \tag{13}$$
$$J\left[\phi(r)\right] = E_0 - \alpha l_0(\hbar\omega_0)^2\int d\mathbf{r}d\mathbf{r}'\frac{\phi(r)G(r,r')\phi(r')}{|\mathbf{r}-\mathbf{r}'|}. \tag{14}$$

The equation for the amplitude $\Phi_q$ in Eq. (13) and the functional of the polaron state (14) depend only on the electron trial function. It is hard to find analytical solutions of the inhomogeneous equation (13) for an arbitrary given trial function $\phi(r)$. However, if the ground-state function of a three-dimensional oscillator,

$$\phi(r) = \frac{1}{\pi^{3/4}}\frac{1}{a_s^{3/2}}\exp\left(-\frac{r^2}{2a_s^2}\right), \quad \omega_s^2 = \frac{k}{m},$$
$$a_s = \sqrt{\frac{\hbar}{m\omega_s}}, \quad E_{\mathbf{n}} = \hbar\omega_s\left(n_1+n_2+n_3+3/2\right), \tag{15}$$

with the variational parameter $a_s$ is taken as a trial function, Eq. (13) can be solved by expanding the GF

in a series of oscillator eigenfunctions,

$$G(r,r') = \sum_{\mathbf{n}} \frac{\Psi_{\mathbf{n}}(r)\Psi_{\mathbf{n}}(r')}{E_{\mathbf{n}} + W} =$$
$$= \hbar\omega_s \sum_{\mathbf{n}} \frac{\Psi_{\mathbf{n}}(r)\Psi_{\mathbf{n}}(r')}{n_1 + n_2 + n_3 + W_0}, \quad (16)$$
$$W_0 = \frac{3}{2} + \frac{W}{\hbar\omega_s}.$$

Here, $\Psi_{\mathbf{n}}(r)$ is the basis set of functions for a three-dimensional oscillator,

$$\Psi_{\mathbf{n}}(r) = \Psi_{n_1}(x)\Psi_{n_2}(y)\Psi_{n_3}(z),$$
$$\Psi_{n_1}(x) = \frac{1}{\pi^{1/4}} \frac{1}{a_s^{1/2}} \frac{1}{(n!)^{1/2}} \frac{1}{(2^{n_1})^{1/2}} \times \quad (17)$$
$$\times \exp\left(-\frac{x^2}{2a_s^2}\right) H_{n_1}\left(\frac{x}{a_s}\right).$$

Using the relation

$$\frac{1}{c} = \int_0^\infty dt \exp(-tc) \quad (18)$$

and the Mehler formula for the summation of Hermite polynomials [12],

$$\sum_{n_1=0}^{\infty} \left(\frac{e^{-t}}{2}\right)^{n_1} \frac{H_{n_1}(x/a_s)\, H_{n_1}(x'/a_s)}{n_1!} =$$
$$= \frac{1}{\sqrt{1-e^{-2t}}} \exp\left(\frac{2xx'e^{-t} - (x^2 + x'^2)e^{-2t}}{a_s^2(1-e^{-2t})}\right), \quad (19)$$

we obtain

$$G(r,r') = \frac{1}{\hbar\omega_s \pi^{3/2} a_s^3} \exp\left(-\frac{r^2 + r'^2}{2a_s^2}\right) \times$$
$$\times \int_0^\infty dt \frac{e^{-tW_0}}{[1-e^{-2t}]^{3/2}} \exp\left(\frac{2\mathbf{r}\mathbf{r}'e^{-t} - (r^2 + r'^2)e^{-2t}}{a_s^2(1-e^{-2t})}\right). \quad (20)$$

Substituting this expression into functional (14) and integrating over $r$ and $r'$, we obtain the final formula for the polaron energy (in $\hbar\omega_0$ units),

$$\varepsilon_p = \frac{3}{2}\mu^2 + \frac{3\gamma^2}{8\mu^2} - \alpha\sqrt{\frac{2}{\pi}}\mu \int_0^\infty dt \frac{e^{-t}}{\sqrt{1-\exp(-2\mu^2 t)}}, \quad (21)$$
$$\mu = \frac{l_0}{a_s}, \quad \gamma = \frac{\Omega}{\omega_0}, \quad \Omega^2 = \frac{\chi}{m}.$$

Here, the coefficient $\gamma$ characterizes the dimensionless confinement strength. In the adiabatic strong-coupling limit, holding only one term in Eq. (16) or expanding the integrand in Eq. (21) in the limit $\mu \to \infty$, we obtain

$$\varepsilon_p = \frac{3}{2}\mu^2 + \frac{3\gamma^2}{8\mu^2} - \alpha\sqrt{\frac{2}{\pi}}\mu. \quad (22)$$

## 3. Discussion of Results

The obtained functional (21) differs from other known results [8–10] in that the exact solution of Eq. (13) was used in its derivation. In the absence of a confinement ($\gamma = 0$, the free polaron), the critical point $\alpha_c \approx 5.8$ can be obtained for functional (21) in the meaning that, for $\alpha < \alpha_c$, the electron becomes delocalized. To compare the results, we consider a functional, which is obtained with the help of the CT parametrization method [9] (see formula (8) in work [9]),

$$E_p = \frac{3}{4}\mu^2 + \frac{3}{4}\frac{\omega^2}{\mu^2} - \frac{\alpha}{2\sqrt{2}\pi^2} \times$$
$$\times \int \frac{d\mathbf{q}}{q^2(1 + a^2q^2/2)} \exp\left[-\frac{(1-a)^2q^2}{2\mu^2}\right]. \quad (23)$$

Here, $\mu$ is the variational parameter of the electron trial function, and $\alpha$ is the variational parameter introduced in the CTs. Note that the denominator of the integrand in formula (8) in work [9] is wrong: $1 + aq^2/2$. Functional (23) can also be obtained from Eq. (4), by using the approximation $F_{\mathbf{q}}(r) = g_{\mathbf{q}}\exp(-ia\ \mathbf{qr})$, where the factor $g_{\mathbf{q}}$ is determined, by minimizing the total energy.

Making the substitutions $E_p \to \varepsilon_p$, $\mu \to \sqrt{2}\mu$, and $\omega \to \Omega$ in Eq. (23) and integrating over the angles, we obtain

$$\varepsilon_p = \frac{3}{2}\mu^2 + \frac{3}{8}\frac{\gamma^2}{\mu^2} - \frac{\sqrt{2}}{\pi}\alpha \times$$
$$\times \int_0^\infty \frac{dq}{1 + a^2q^2/2} \exp\left[-\frac{(1-a)^2q^2}{4\mu^2}\right]. \quad (24)$$

For a free polaron ($\gamma = 0$), functional (24) yields $\alpha_c \approx$ $\approx 8.5$. Hence, for $\alpha > 5.8$, the energy of a free polaron 21) is always lower than energy (24). Since the wave function of an electron is usually localized within the quantum dot, the critical point $\alpha_c$ is suppressed.

| $\alpha$ | Polaron energy $\varepsilon_p$ | | | |
|---|---|---|---|---|
| | $\gamma$ | (21) | (22) | (24) |
| 0.1 | 1 | 1.39 | 1.44 | 1.40 |
| | 26 | 38.70 | 38.71 | 38.71 |
| | 46 | 68.61 | 68.62 | 68.61 |
| 2 | 1 | −0.78 | 0.24 | −0.50 |
| | 26 | 32.85 | 33.14 | 33.03 |
| | 46 | 61.02 | 61.24 | 61.16 |
| 5.0 | 1 | −4.39 | −2.45 | −3.49 |
| | 26 | 23.21 | 23.89 | 23.64 |
| | 46 | 48.63 | 49.16 | 48.97 |

In Table, the results of calculations by formula (21) are compared with the adiabatic result (22) and functional (24). One can see that formula (21) provides the most accurate estimations of the energy. The results obtained with the use of formula (22) become more adequate at large $\gamma$, because the electron becomes "hotter" under the strong confinement condition, and the adiabatic approximation is satisfied better.

The obtained polaron functional (14) depends only on the trial electron function, with the phonon coordinates being completely excluded. For the trial oscillator function, there is a critical point $\alpha_c \approx 5.8$. According to Gross [11], this fact results from a strong localization of this function. For other choices of the trial electron function, e.g., $(1 + \gamma r)\exp(-\delta r)$, the solution of Eq. (13) becomes more complicated.

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ВПЛИВ ПОЛЯРИЗАЦІЇ
СЕРЕДОВИЩА НА ЕЛЕКТРОННУ ЕНЕРГІЮ
В КВАНТОВІЙ ТОЧЦІ

Р е з ю м е

Метод Буймістрова–Пекара застосовано до розрахунку поляронного зсуву електронного рівня в квантовій точці. З використанням параболічної апроксимації конфайнмента, диференціальне рівняння для амплітуди зміщень фононів точно вирішено методом функцій Гріна. Порівняно результати різних наближень.