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Polaron in cylindrical and spherical quantum dots

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Polaron states in cylindrical and spherical quantum dots with parabolic confinement potentials are investigated applying the Feynman variational principle. It is observed that for both kinds of quantum dots the polaron energy and mass increase with the increase of Fröhlich electron-phonon coupling constant and confinement frequency. In the case of a spherical quantum dot, the polaron energy for the strong coupling is found to be greater than that of a cylindrical quantum dot. The energy and mass are found to be monotonically increasing functions of the coupling constant and the confinement frequency.

Key words: *polaron, polaron energy, polaron mass, parabolic confinement, Fröhlich electron-phonon coupling constant, quantum dot*

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1. Introduction

Recent advances in the technology of fabrication of quasi-2D, -1D, -0D nanocrystals have stimulated the theoreticians' interest in formulating models describing physical phenomena associated with nanocrystals [1–12]. These structures are attractive both for scientific investigation and for the development of a new generation of electronic devices.

Nowadays not only perfect planar multilayer structures but also cylindrical and spherical structures are being intensively investigated [7–13]. Polaron energy is evaluated in [13–15] using perturbation theory, in [16] using the weak coupling approximation, in [17] using the dielectric continuum model and in [18] using the Feynman variational principle.

The polaron concept was introduced by Landau [19] as the autolocalised state of a charge carrier in a homogeneous polar medium. The quantum dot is one of the simplest quantum confined systems. For the strong electron-phonon interaction an electron localises at a small region. A polaron is a quasi particle that arises due to the conduction electron (or hole) together with its self-induced polarization in an ionic crystal or in a polar semiconductor [20]. To classify polarons, the Fröhlich electron-phonon coupling constant value, α is weak-coupling if $\alpha < 1$, strong-coupling if $\alpha \geqslant 7$ and intermediate-coupling between these ranges. The majority of crystals are weak or intermediate-coupling polarons. Strong coupling is not attained even in strong ionic crystals such as alkaline halides. The polaron character is well pronounced only for strong coupling [21].

It is possible to reduce the lower bound of the electron-phonon coupling constant's threshold value in nanocrystals to within weak or intermediate-coupling range. When investigating the polaron in nanocrystals, we should consider both the electron and the phonon confinements. The electron confinement is described in [1,22–27].

The present investigation also arises from the recent advances in fabrication of nanocrystal with strong ionic coupling [28]. The spectra of polar optical vibrations in 0D and 1D structures are investigated in [29]. [30] investigated the bulk and interface polarons in quantum wires and dots. Polaron in a spherical quantum dot is studied in [7,31–33] and in a cylindrical quantum dot in [34,35]. It is known that for decreasing dimensionality of a structure ($3D \to 2D \to 1D \to 0D$) polaron effects are enhanced, but the number of independent directions of charge transport decreases [36]. Thus, quasi 1D present certain interest as structures with maximal polaron effect under the condition of the existence of at least one charge transport direction. Quantum dot systems attract much attention in electronics and optics [8,37].

In this paper the polaron states in spherical and cylindrical quantum dots are investigated applying the Feynman variational principle. This results in the upper bound polaron ground state energy for an arbitrary Fröhlich electron-phonon-coupling constant. The electronic confinement is selected for the spherical and cylindrical quantum dots in the form of a parabolic confinement potential. For the parabolic confinement, rigid interface boundaries are absent and interface-like phonon modes are smoothly distributed in space rather than localized near a sharp boundary. Then we examine the electron interaction only with 3D longitudinal polar optical phonons (3D-phonon approximation). Interaction between electrons is described by 3D coulomb potentials of corresponding symmetries and the Fröhlich 3D Hamiltonian is chosen to describe electron-phonon interaction. Consequently, interface phonons may not be considered. This approach seems to be adequate since the integral polaron effects resulting from the summation over all phonon modes appear to be weakly dependent on the details of the phonon spectra. In the phenomena with integral phonon effects we resort to numerical results.

In [33,38] interface-type longitudinal polar optical phonons have no contribution to polaron effects. In [7,30] bulk-type phonons play the dominant role in the polaron energy shift.

2. Feynman variational principle

The Feynman variational principle is one of the most effective methods when investigating the polaron problem for arbitrary values of the electron-phonon-coupling constant α. To evaluate the polaron energy and the effective mass, the Feynman variational principle [27] is used:

$$\ln Z \geqslant \ln Z_{\mathrm{F}} = \ln Z_0 - \langle S[\vec{r}\,] - S_0[\vec{r}\,]\rangle\,, \tag{2.1}$$

where the angle brackets in 2.1 denote averaging over electron paths and are defined as follows:

$$\langle F[\vec{r}\,]\rangle = \frac{Sp\int \mathrm{D}\vec{r}\, F[\vec{r}\,]\exp\{S_0[\vec{r}\,]\}}{Sp\int \mathrm{D}\vec{r}\, \exp\{S_0[\vec{r}\,]\}},$$

where $\mathrm{D}\vec{r}$ denotes path integration, Sp is the spur, $S_0[\vec{r}\,]$ is the model action functional with:

$$S_0[\vec{r}\,] = \int L_0 \mathrm{d}t;$$

then $S[\vec{r}\,]$ is the exact action functional of the exact system:

$$S[\vec{r}\,] = \int L \mathrm{d}t,$$

where $\vec{r}$ is the radius vector, L and L_0 are the Lagrangians of the exact and model systems respectively. In 2.1, the quantity Z_0 is the statistical sum of the model system andZ_{F} is the Feynman statistical sum defined respectively as follows:

$$\begin{aligned} Z_0 &= Sp\int \mathrm{D}\vec{r}\, \exp\{S_0[\vec{r}\,]\}, \\ Z &= Sp\int \mathrm{D}\vec{r}\, \exp\{S[\vec{r}\,]\}. \end{aligned} \tag{2.2}$$

The functions S and S_0 in 2.1 are obtained after the path integration over phonon variables and coordinates of the “fictitious” particles, respectively.

The thermodynamic energy E of a system is expressed through Z by the formula:

$$E = -\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln Z, \qquad \lambda = \frac{1}{T}, \tag{2.3}$$

from where

$$E \leqslant E_{\mathrm{F}}\,, \tag{2.3'}$$

where

$$E_{\mathrm{F}} = -\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln Z_{\mathrm{F}}\,.$$

Here T is the absolute temperature (in units of the Bolztman’s constant) and E_{F} is the Feynman energy. The lowest energy level of the system is obtained as a limiting case of 2.3 as $T \to 0$, i.e. $\lambda \to \infty$. Thus, the upper bound ground state energy may be obtained without solving any wave equation.

3. Feynman polaron in a cylindrical quantum dot

Consider the motion of an electron in a cylindrical quantum dot with a symmetric parabolic confinement potential. The Hamiltonian that describes the electron and phonon subsystem including their interaction with lattice vibrations is:

$$\hat{H} = \hat{H}_{\mathrm{e}} + \hat{H}_{\mathrm{ph}} + \hat{H}_{\mathrm{e-ph}}\,, \tag{3.1}$$

where $\hat{H}_{\mathrm{e}}$ is the electron Hamiltonian in cylindrical coordinates:

$$\hat{H}_{\mathrm{e}} = \frac{\hat{P}_{\perp}^2}{2m_{\perp}} + \frac{\hat{P}_{||}^2}{2m_{||}} + \frac{m_{\perp}\Omega_{\perp}^2}{2}\rho^2 + \frac{m_{||}\Omega_{||}^2}{2}z^2.$$

Here $\rho^2 = x^2 + y^2$; $\hat{P}_{\perp}$, $m_{\perp}$ and $\hat{P}_{||}$, $m_{||}$ are components of the operator of the momentum and electron band mass in the transversal and longitudinal directions respectively; Ω is the frequency characterizing the parabolic confinement potential; and

$$\left.\begin{aligned} \hat{H}_{\mathrm{ph}} &= \sum_{\vec{q}} \hbar\,\omega_{\vec{q}}\,\hat{b}_{\vec{q}} + \hat{b}_{\vec{q}} \\ \hat{H}_{\mathrm{e-ph}} &= \sum_{\vec{q}} \left[\gamma_{\vec{q}}\,\hat{b}_{\vec{q}}\,\mathrm{e}^{\mathrm{i}\vec{q}\,\vec{r}} + \gamma_{\vec{q}}\,\hat{b}_{\vec{q}}\,\mathrm{e}^{-\mathrm{i}\vec{q}\,\vec{r}}\right] \end{aligned}\right\} \tag{3.2}$$

are respectively the phonon contribution and electron-phonon interaction Hamiltonians. Here $\gamma_{\vec{q}}$ is the amplitude of the electron-phonon interaction numbered by the wave vector $\vec{q}$:

$$\gamma_{\vec{q}} = \left[\frac{\alpha\pi}{V}\left(\frac{\hbar\,\omega_o}{q}\right)^2 R_p\right]^{\frac{1}{2}}, \qquad R_p = \left(\frac{\hbar}{2m_{\mathrm{e}}\omega_o}\right)^{\frac{1}{2}}, \qquad q^2 = q_{\perp}^2 + q_{||}^2$$

and ω_0 is the non-dispersional phonon frequency.

Considering the Hamiltonian 3.1, the model lagrangian L_0 for the system (considering the ground state) is selected in the one-oscillatory approximation:

$$\begin{aligned} L_0 = \;& -\frac{m_{\perp}\dot{\rho}^2}{2\hbar^{\,2}} - \frac{m_{||}\dot{z}^2}{2\hbar^{\,2}} - \frac{m_{\perp}\Omega_{\perp}^2}{2}\rho^2 - \frac{m_{||}\Omega_{||}^2}{2}z^2 - \frac{M_{\perp}\dot{R}^2}{2\hbar^{\,2}} - \frac{M_{||}\dot{Z}^2}{2\hbar^{\,2}} \\ & - \frac{\kappa_{\perp}}{2}(R-\rho)^2 - \frac{\kappa_{||}}{2}(z-Z)^2; \qquad \kappa_j = M_j\omega_{jf}, \quad j = \perp, \end{aligned} \tag{3.3}$$

where $R$and Z are the coordinates of the model particle and ρ with z are the coordinates of the electron, respectively. The quantities $M_{\perp}, M_{||}, \kappa_{\perp}$, and $\kappa_{||}$ serve as variational parameters. ω_f is the elastic coupling frequency.

From the Lagrangian in 3.3, the transverse and longitudinal equations of motion for the model system are independent. In 3.3 the time $t = -\mathrm{i}\hbar\,\tau$ and $\dot{\psi} = \mathrm{d}\psi/\mathrm{d}\tau$. The model Lagrangian in 3.3 simulates the interacting electron-phonon system.

From the equation of motion the eigen frequencies are obtained:

$$\omega_{ij}^2 = \frac{1}{2}\left(\frac{\kappa_j}{m_j} + \Omega_j^2\right) - (-1)^i\frac{1}{2}\left[\left(\frac{\kappa_j}{m_j} + \Omega_j^2\right)^2 - \frac{4\kappa_j\Omega_j^2}{m_j}\right]^{\frac{1}{2}}, \qquad i = 1, 2, \qquad j = \perp, ||\,. \tag{3.4}$$

Considering 2.1 and 2.3, the polaron dimensionless energy E is evaluated:

$$E=\sum_{j=1}^{2}\left(\frac{1}{2}\right)^{j}\left[\Omega_j\left(\frac{1}{2}\right)^{-1}+\frac{(\Omega_j-\omega_{1j})^2(\Omega_j-\omega_{2j})^2}{\Omega_j^2(\omega_{1j}+\omega_{2j})}\right]-\alpha\int\limits_0^\infty F(A_\perp,A_{||})\mathrm{e}^{-\tau}\mathrm{d}\tau,$$

$$j=1\to\perp,\qquad j=2\to||\,. \quad (3.5)$$

The dimensionless effective mass M is conveniently obtained:

$$M=\sum_j\frac{\left(\Omega_j^2-\omega_{2j}^2\right)\left(\omega_{1j}^2-\Omega_j^2\right)}{\omega_{1j}^2\omega_{2j}^2}, \quad (3.6)$$

where

$$F(A_\perp,A_{||})=\sqrt{\frac{2}{\pi}}\frac{1}{\left(|A_{||}-A_\perp|\right)^{1/2}}\begin{cases}Ar\sinh\left(\frac{A_{||}}{A_\perp}-1\right)^{1/2}, & A_{||}>A_\perp\,,\\ \arcsin\left(1-\frac{A_{||}}{A_\perp}\right)^{1/2}, & A_{||}>A_\perp\,,\end{cases}$$

$$A_j=\sum\frac{a_{ij}}{\omega_{ij}}\left(1-\mathrm{e}^{-\omega_{ij}\tau}\right),\quad j=\perp,||\,,\quad a_1=\frac{\omega_1^2-\omega_f^2}{\omega_1^2-\omega_2^2},\quad a_2=\frac{\omega_f^2-\omega_2^2}{\omega_1^2-\omega_2^2}\,. \quad (3.7)$$

4. Feynman polaron in a spherical quantum dot

Consider the motion of an electron in a spherical quantum dot with a spherical symmetric parabolic confinement potential. The model Lagrangian L_0 of the system is selected:

$$L_0=-\frac{m\,\dot{\vec{r}}^2}{2\hbar^{\,2}}-\frac{M_f\dot{\vec{R}}^2}{2\hbar^{\,2}}-\frac{m\Omega^2\vec{r}^{\,2}}{2}-\frac{M_f\omega_f^2\left(\vec{R}-\vec{r}\right)^2}{2}, \quad (4.1)$$

where $\vec{R}$ is the coordinate of the fictitious particle. The quantities M_f and ω_f are the mass and the elastic coupling frequencies of the fictitious particle, respectively. Both of them serve as variational parameters. From the equation of motion of the model system there follow the eigen frequencies:

$$\omega_j^2=\frac{1}{2}\left[\frac{\kappa}{\mu}+\Omega^2-(-1)^i\sqrt{\left(\frac{\kappa}{\mu}+\Omega^2\right)^2-\frac{4\Omega^2\kappa}{\mu}}\right],$$

$$j=1,2,\quad \mu=\frac{mM}{m+M},\quad \kappa=M_f\omega_f^2\,. \quad (4.2)$$

From 2.1 and 2.3, the Feynman polaron variational energy E is given by:

$$E=\frac{3}{2}\Omega+\frac{3}{4}\frac{(\omega_1-\Omega)^2(\Omega-\omega_2)^2}{\Omega^2(\omega_1+\omega_2)}-\frac{\alpha}{\sqrt{\pi}}\int\frac{\mathrm{e}^{-\tau}\mathrm{d}\tau}{A^{1/2}}, \quad (4.3)$$

where

$$A = \sum_{j=1}^{2} \frac{a_j}{\omega_j} \left(1 - \mathrm{e}^{-\omega_j \tau}\right).$$

The polaron effective mass M may be conveniently evaluated from the equation of the eigen frequencies 4.2:

$$M = \frac{\left(\omega_1^2 - \Omega^2\right)\left(\Omega^2 - \omega_2^2\right)}{\omega_1^2 \omega_2^2}.$$

5. Conclusions

Figures 1 and 2 show the plot of the polaron energy (absolute value) versus Fröhlich electron-phonon-coupling constant for the cylindrical and spherical quantum dots, respectively. The plots slightly deviate from a linear relation. Here, the polaron energy increases with the increase of the electron-phonon-coupling constant. From the plots, the confinement strengthening enhances the electron-phonon interaction. The Polaron energy for the case of the spherical quantum dot is greater than that of the cylindrical quantum dot. For example, if we consider $\alpha = 8.25$ then for the cylindrical quantum dot we have the following values for the energy $E_{\mathrm{c}} = 25.1072; 20.50333; 15.711$. These values of the energy correspond, respectively, to the confinement frequencies $\Omega = 7; 5; 3$. For the case of the spherical quantum dot for $\alpha = 8.25$ we have$E_{\mathrm{s}} = 25.29462; 20.66347; 15.84761$ that correspond, respectively, to the following confinement frequencies $\Omega = 7; 5; 3$. We have also examined the polaron energies at the confinement frequency $\Omega = 10.3$. For the case of the cylindrical quantum dot we have $E_{\mathrm{c}} = 29.75767; 25.58428; 21.48544$ that correspond, respectively, to $\alpha = 7; 5; 3$. For the case of the spherical quantum dot we have $E_{\mathrm{s}} = 29.90701; 25.64913; 21.50619$ that correspond, respectively, to $\alpha = 7; 5; 3$. This also shows that the polaron energy for the case of the spherical quantum dot is greater than that of the cylindrical quantum dot. This confirms the results in [36].

In figures 3 and 4 the mass increases with the increase of the electron phonon coupling constant. This coincides with the results obtained in [30]. Figures 3 and 4 also show that though the graphs of the mass are lifted in the same fashion, the one for the cylindrical dot is greater in numerical value than that of the spherical quantum dot. From figures 1 to 4 it is observed that the polaron energy and mass are monotonically increasing functions of the coupling constant. It is observed that regions of weak and intermediate polarons overlap with those of strong coupling polarons (i.e., the regions of strong coupling polarons are shifted to those of weak and intermediate polarons).

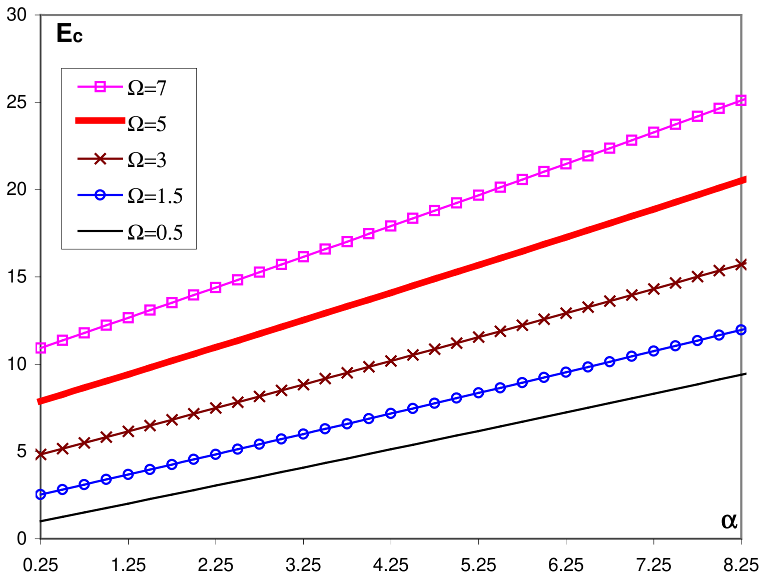

Figure 1. Plot of the polaron energy versus Fröhlich electron-phonon constant (cylindrical dot)

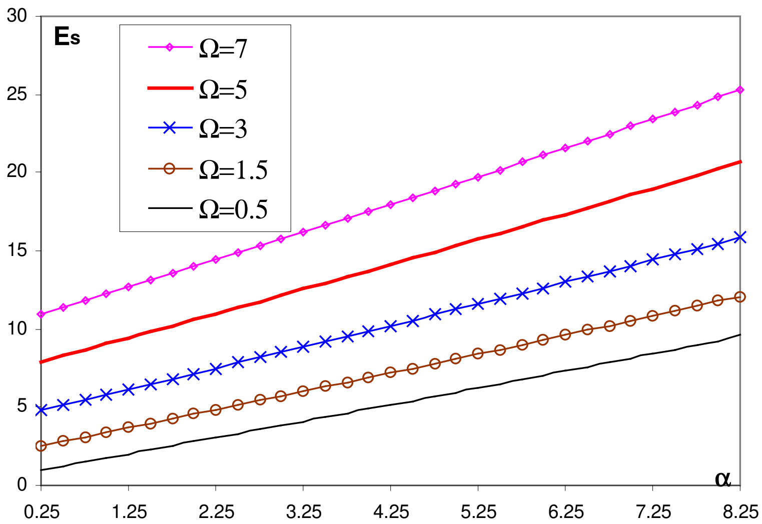

Figure 2. Plot of the polaron energy versus Fröhlich electron-phonon constant (spherical dot)

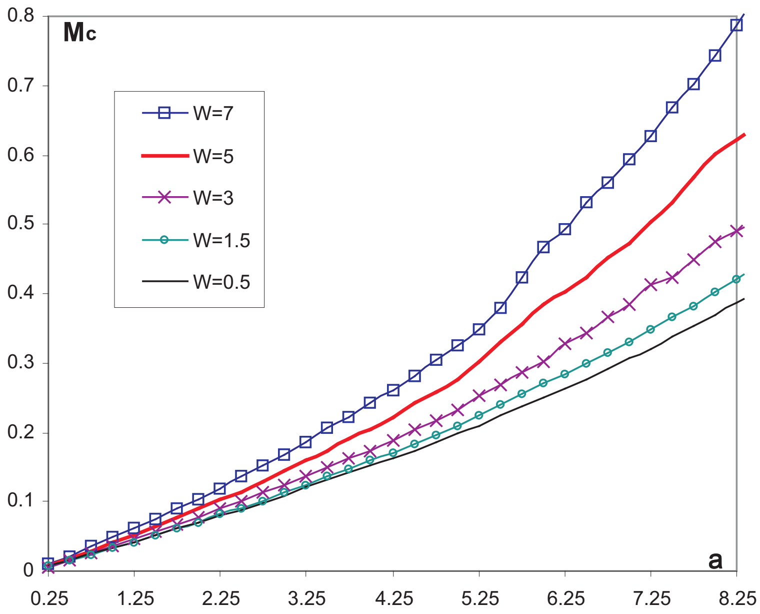

Figure 3. Plot of the polaron mass versus Fröhlich electron-phonon constant (cylindrical dot)

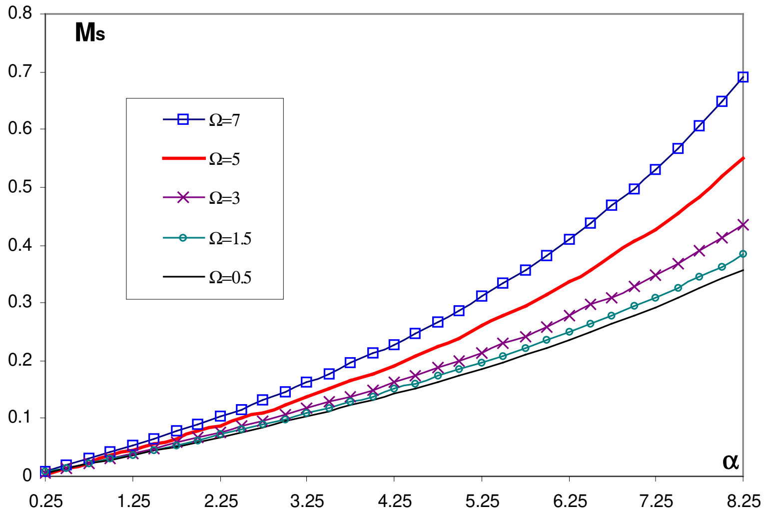

Figure 4. Plot of the polaron mass versus Fröhlich electron-phonon constant (spherical dot)

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Полярон в циліндричних і сферичних квантових крапках

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Досліджуються стани полярона в циліндричних і квантових крапках з параболічними обмежуючими потенціалами, використовуючи варіаційний принцип Фейнмана. Знайдено, що для обох типів квантових крапок енергія і маса полярона зростає з ростом постійної Фрьоліха електрон-фононного зв'язку і обмежуючої частоти. Показано, що у випадку сферичної квантової крапки енергія полярона для сильного зв'язку є більшою, ніж у випадку циліндричної квантової крапки. Знайдено, що енергія і маса є монотонно зростаючими функціями постійної зв'язку і обмежуючої частоти.

Ключові слова: *полярон, енергія полярона, параболічне обмеження, постійна Фрьоліха електрон-фононної взаємодії*

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