EFFECT OF THE SCREENING ON THE POLARON MASS IN A SEMICONDUCTOR HOLLOW NANOCYLINDER

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Abstract

The effect of the screening effect of the electron–phonon interaction on a weakly coupling Frohlich polaron mass has been investigated in a semiconductor hollow nanocylinder (HNC). General analytical expressions for the polaron mass have been obtained in arbitrary values of nanocylinder radius r_0, taking into account screening as well as considering transitions between the subbands of dimensional quantization. The dependence of the polaron mass for the ground and excited states on nanocylinder radius has been represented on the basis of our numerical calculations. According to research carried out, it has been established that the screening contribution to polaron mass taking into account the virtual transitions from the ground state to subbands n = ±1, ±2, ±3, as well as the transitions from the polaron excited state with n = 1 to subbands n = −1, ±2,±3, is significant for $a = r_0/r_p < 1$ values, where r_p is the polaron radius. For values of the parameter a > 1 the screening contribution to polaron mass decreases with increasing r_0, but the decrease of the polaron correction to the mass due to screening is still more than 30 %.

1. Introduction

One of the main characteristic parameters of the polaron is its effective mass, which can be determined from the experiments on the cyclotron and magneto-phonon resonance. In [1], the valence intraband transitions in p-doped InAs quantum dots (QDs) were studied by means of far-infrared resonance (FIR) magneto-optical technique. It was shown that a model taking into account the hole-LO phonon coupling is able to predict the experimental results. The experiments demonstrate the fact that the intraband magneto-optical transitions occur between hole polaron states.

A number of theoretical and experimental works concern the problem of the effect of the screening of electron-phonon interaction on the magnitude of the polaron cyclotron- resonance (CR) mass. Klimin and Devreese have theoretically investigated cyclotron-resonance spectra for a polaron gas in a GaAs/AlAs quantum well taking into account the screening of the electron-phonon coupling [2]. In [3] it was shown that, including the screening, the polaron cyclotron-resonance mass correction is reduced as compared to a calculation without taking into account the effect of screening. It was concluded that the static screening approach gives good results for the polaron cyclotron-resonance mass renormalization in the relevant magnetic field region. CR data of the 3D bulk system n-GaAs and of the 2D electron system of AlGaAs-GaAs heterojunction were presented in [4]. Polaron effects are found to be significant in both system; however, the polaron effect is found to be weaker in the 2D electron gas of an AlGaAs-GaAs heterojunction than in 3D bulk n-GaAs crystal.

In recent years the rapid development of nanotechnology has made it possible to design a low-dimensional system of complex geometric shapes in the form of rings, spirals, tubes, etc. [5, 6]. This situation has aroused interest in new theoretical and experimental studies of low-dimensional systems. Among them, the nanotubes (NT) present the great interest.

Our recent paper [7] was devoted to the effect of screening of the electron-phonon interaction with weak coupling on the polaron binding energy in a semiconductor NT. To solve this problem, we used the results of computation of the electron dielectric permeability for an infinitely long semiconductor NT given in [8]. Here we use the same technique to calculate the polaron correction to the mass in NT, which is essentially a hollow nanocylinder (HNC).

Thus, the aim of the present study is to theoretically investigate the effect of the screening of the electron-phonon interaction on the Fröhlich polaron mass in a semiconductor HNC, taking into account transitions between the subbands of dimensional quantization just as is done in calculating the binding energy of the polaron.

2. Energy states, electron wave functions and the matrix element of the electron-phonon coupling

We consider an HNC with radius r_0 on the surface of which there is a 2D gas of mobile electrons. According to the results of [9], the quantized energy spectrum and normalized wave function in a one-particle approximation are given as follows:

$$\varepsilon_{nk} = \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2 n^2}{2m r_0^2}, \tag{1}$$

$$\psi_{nk}(Z,\varphi) = \frac{1}{\sqrt{2\pi L}} e^{i(kZ + n\varphi)}. \tag{2}$$

Here m is the effective mass of an electron, φ and Z are the cylindrical co-ordinates, L is the length of the cylinder along NC-axis in the Z-direction, and $n = 0, \pm 1, \pm 2, \ldots$ are the number of subband of dimensional quantization. Quasi-momentum $\hbar\vec{k}$ corresponds to the motion of electrons on a cylinder surface along the Z-axis.

Taking into account the expression for Fourier component of scalar potential $\Phi_{\vec{q}}$ [9]

$$\Phi_{q_\perp q_Z} = i\sqrt{\frac{2\pi\hbar\omega_L}{\in^* V}} \frac{1}{\sqrt{q_\perp^2 + q_z^2}} e^{-i\left(q_\perp r_0 \cos\varphi + q_z z\right)}$$

the matrix element $M_{n-n', q_\perp q_Z}$ for the energy $(-e\sum_{\vec{q}} \Phi_{\vec{q}})$ of the electron-phonon coupling is calculated with wave function (2) for any n, n'

$$M_{n-n', q_\perp q_Z} = -\hbar\omega_L \sqrt{\frac{4\pi\alpha\, r_p}{V}} \frac{i^{(n-n'+1)}}{\sqrt{q_\perp^2 + q_Z^2}} J_{|n-n'|}(q_\perp r_0). \tag{3}$$

Here $q_\perp, q_Z$ are the transverse and longitudinal phonon wave vector of $\vec{q}, \omega_L$ is the limiting LO phonon frequency, $\alpha = \sqrt{\frac{m}{2\hbar\omega_L}} \frac{e^2}{\hbar}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)$ is the electron-phonon coupling parameter, $r_p = \sqrt{\hbar / 2m\omega_L}$ is the polaron radius; $\varepsilon_0, \varepsilon_\infty$ is the static and high-frequency dielectric permeability, respectively, and $J_{|n-n'|}(q_\perp r_0)$ is the Bessel function of the index $\Delta n = n - n'$. In deriving (3) it was taken into account that the phonon-electron interaction at low temperatures leads to virtual electron transitions with the emission of one LO-phonon.

3. Polaron mass

Using the perturbation theory, a task with regard to a weak coupling Fröhlich polaron has been solved in the quasi-two-dimensional systems [10]. In this paper, an analytical expression for the polaron correction to the effective electron mass is calculated taking into account the intersubband transitions.This analytical expression for the polaron contribution to the mass gives the well-known value $\Delta m / m\alpha = \pi/8$ in the limit of a two-dimensional case. Here $\Delta m = m_p - m$, m and m_p are the electron and polaron effective masses.

In this study, we will investigate the effect of screening on the Fröhlich polaron mass at low temperatures on the semiconductor HNC surface. To obtain an analytical expression for the polaron effective mass, it is necessary to calculate the correction to the electron energy $\Delta E_{n,\vec{k}}$ due to its interaction with the LO-phonons. The calculation is carried out within the framework of the standard perturbation theory.

Taking into account the screening effect, the expression for the polaron correction to the energy $\Delta E_{n,\vec{k}}$ in the second-order perturbation theory, is defined as follows [7]:

$$\Delta E_{n,\vec{k}} = \sum_{n',\vec{q}} \frac{\left|M_{n-n',q}\right|^2}{(\varepsilon_{n\vec{k}} - \varepsilon_{n'\vec{k}-\vec{q}} - \hbar\omega_L) \in^2_{|n-n'|}(q)}. \quad (4)$$

Here $\in_{|n-n'|}(q)$ is determined by the expression [7]

$$\in_{|n-n'|}(q) = 1 - \frac{2me^2}{\pi\hbar^2 \in_0 q} I_{|n-n'|}(qr_0) K_{|n-n'|}(qr_0) \sum_{n=-n_F}^{n_F} \ln\left[\frac{(n+n')(n-n') - q(q-2k_F)r_0^2}{(n+n')(n-n') - q(q+2k_F)r_0^2}\right]. \quad (5)$$

Here $I_{|n-n'|}(qr_0)$, $K_{|n-n'|}(qr_0)$ are the modified Bessel functions of the first and second kind, respectively.

After integration over the polar angle φ in (4), we obtain the following expression for the correction to the polaron energy in the new dimensionless variables $x = r_p q_\perp$, $z = r_p q$, $\kappa = r_p k$, $a = r_0/r_p$:

$$\Delta E_{n,\kappa} = -\frac{\alpha\hbar\omega_L}{\pi} \sum_{n'} \int_0^\infty \int_{-\infty}^\infty \frac{\left|J_{n-n'}(ax)\right|^2}{(x^2+z^2)\left(z^2 + 2\kappa z + a^{-2}(n'^2 - n^2) + 1\right)} \frac{1}{\in^2_{|n-n'|}(z)} x\,dx\,dz. \quad (6)$$

Limiting ourselves to second-order terms we expand the integrand of (6) in powers of κ:

$$\Delta E_{n,\kappa} = \Delta E_{n,0} + A_n \kappa^2 \tag{7}$$

The integration over x in (11) leads to the following results:

$$\Delta E_{n,0} = -\frac{2\alpha}{\pi}\hbar\omega_L \sum_{n'}\int_0^\infty \frac{I_{|n-n'|}(az)K_{|n-n'|}(az)}{\left(z^2 + a^{-2}(n'^2 - n^2)+1\right)\in^2_{|n-n'|}(z)}dz\,, \tag{8}$$

$$A_n = -\frac{8\alpha}{\pi}\hbar\omega_L \sum_{n'}\int_0^\infty \frac{z^2 I_{|n-n'|}(az)K_{|n-n'|}(az)}{\left(z^2 + a^{-2}\left(n'^2 - n^2\right)+1\right)^3\in^2_{|n-n'|}(z)}dz, \tag{9}$$

Where: $I_{|n-n'|}(az)$ и $K_{|n-n'|}(az)$ are the modified Bessel functions of the first and second kind, respectively.

Let us write the expression for the polaron mass taking into account the second term in the (7), which transform as follows:

$$A_n\kappa^2 = \frac{A_n}{\hbar\omega_L}\frac{\hbar^2 k^2}{2m}\,,\quad \frac{1}{m_p} = \frac{1}{m}\left(1+\frac{A_n}{\hbar\omega_L}\right),\quad m_p = m(1 - A_n/\hbar\omega_L)\;. \tag{10}$$

Polaron mass calculations were performed by means of equations (5), (9), and (10) for GaAs with the following values of the parameters:

$r_p = 4nm$; $e = 1.6\times10^{-19}C$; $m = 0.067\,m_0$,
$m_0 = 9.1\times10^{-31}kg$, $\in_0 = 12.8$, $\hbar = 6.6\times10^{-34}Js$, $\kappa_F = 0.1a^{-1}$.

The results of numerical calculations for dependences ($\Delta m/m\alpha$) on the ratio $a = r_0/r_p$ are presented in Fig. 1 for the band state with $n = 0$. Here it is assumed that the Fermi level is located in the zero band.

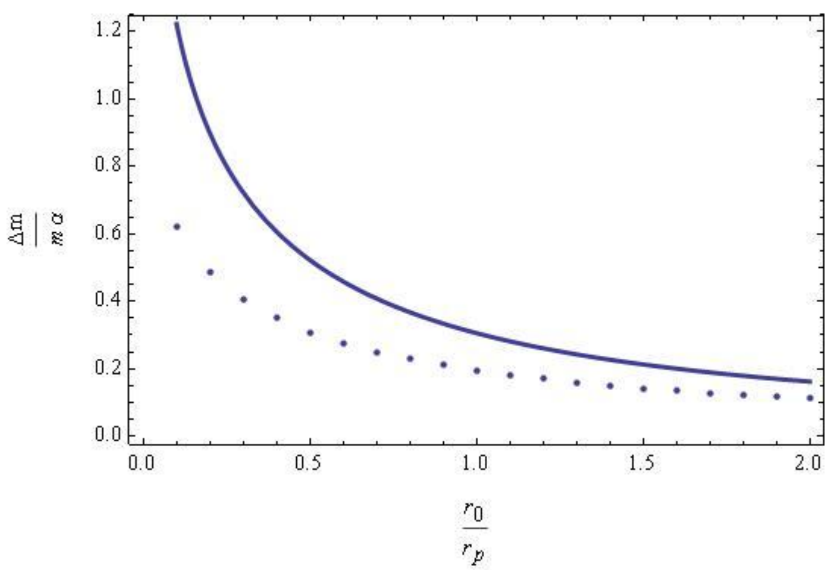

Fig. 1. Dependence of $\Delta m/m\alpha$ on the r_0/r_p ratio for the ground band state with $n = 0$: (a) solid curve is obtained without screening and (b) dotted curve is obtained taking into account screening. Here the Fermi level is located in the zero band.

The solid curve in Fig. 1 corresponds to the case without screening, but the dotted curve is obtained taking into account the screening effect. In both cases, transitions between subbands of dimensional quantization are not considered.

Using equations (9) and (10), polaron correction to the mass for the band state with $n = 0$

was calculated taking into account transitions to the subbands $n = \pm1, \pm2, \pm3$.
In this case, the Fermi level is also placed in the zero band. The calculation results for the dependences $\Delta m/m\alpha$ on the parameter r_0/r_p are presented in Fig. 2. This figure shows the nonmonotonic dependence on the polaron radius. A slight minimum of the curve corresponds approximately to a value of $r_p = 2r_0$.

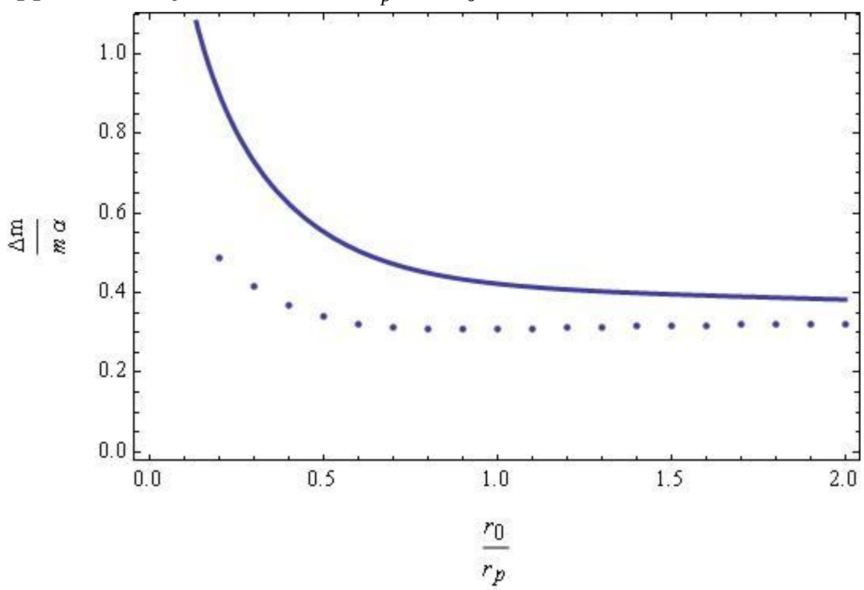

Fig. 2. Dependence of $\Delta m/m\alpha$ on the r_0/r_p ratio taking into account the transitions from the ground band state with $n = 0$ to subbands $n = \pm1, \pm2, \pm3$: (a) the solid curve is obtained without taking into account screening and (b) the dotted curve is derived taking into account screening. The Fermi level is placed in the zero band.

It is evident from the dotted curve in Fig. 2 that the value of $\Delta m/m\alpha$ approached its well-known value of $\pi/8$ with increasing value of the NC radius r_0/r_p [10]. As distinct from the solid curve in Fig. 1, the value of $\Delta m/m\alpha$ in this figure does not approach the value $\pi/8$ with increasing NC radius. According to these results, we conclude that, for deriving correct expressions for the polaron effective mass for any given values of r_0/r_p in 2D systems, it is necessary to take into account the intersubband transitions.

A comparison of the dotted curves of Figs. 1 and 2 suggests that the observed the slight minimum in the dotted curve of Fig. 2 is due to the intersubband transitions. By means of equations (9) and (10), similar calculations were for the excited polaron in the subband with $n = 1$. The results of these numerical calculations for the dependences $\Delta m/m\alpha$ on the r_0/r_p ratio are given below in Fig. 3. In this case, for the polaron being in $n = 1$ state, the intersubband transitions to the states with n = -1,±2, ±3 are taken into account. The Fermi level is placed in the zero band.

By means of equations (9) and (10), similar calculations were performed for the case of location of the Fermi level in the subband with $n = 1$. Fermi wave numbers κ_{F0} *and* κ_{F1} corresponding to the states $n = 0$ and $n = 1$ are related through the ratio

$$\kappa_{F0}^2 = \kappa_{F1}^2 + a^{-2} \tag{11}$$

The results of numerical calculations for the dependences $\Delta m/m\alpha$ on the r_0/r_p ratio are given in Fig. 4 for the polaron in the state $n = 1$ taking into account the intersubband transitions to the states with $n = -1, \pm 2, \pm 3$.

A comparison of the results presented by the dotted curves in Figs. 3 and 4 suggests that the screening effect on the polaron correction to the mass increases with increasing Fermi level.

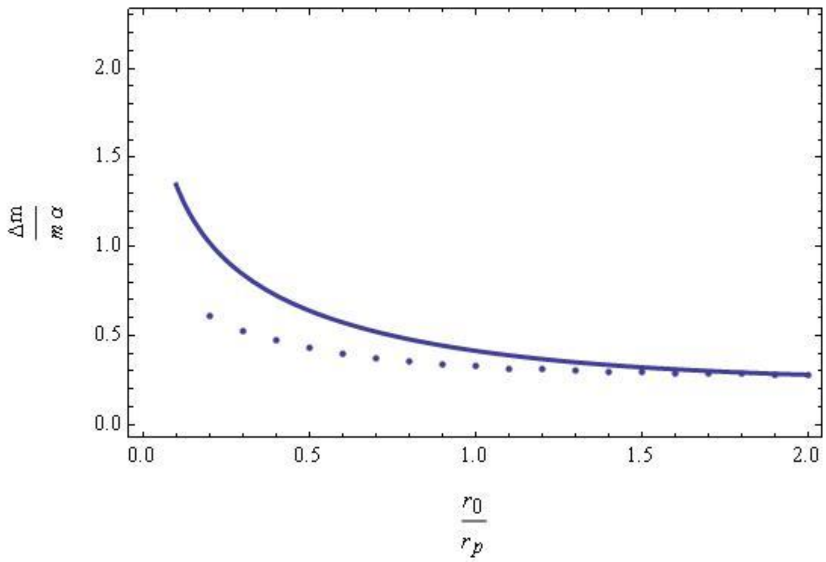

Fig. 3. Dependence of $\Delta m/m\alpha$ on the r_0/r_p ratio taking into account transitions from excited state with $n=1$ to subbands n = -1, ±2, ±3: (a) the solid curve is obtained without taking into account screening and (b) the dotted curve is derived taking into account screening. The Fermi level is placed in the zero band.

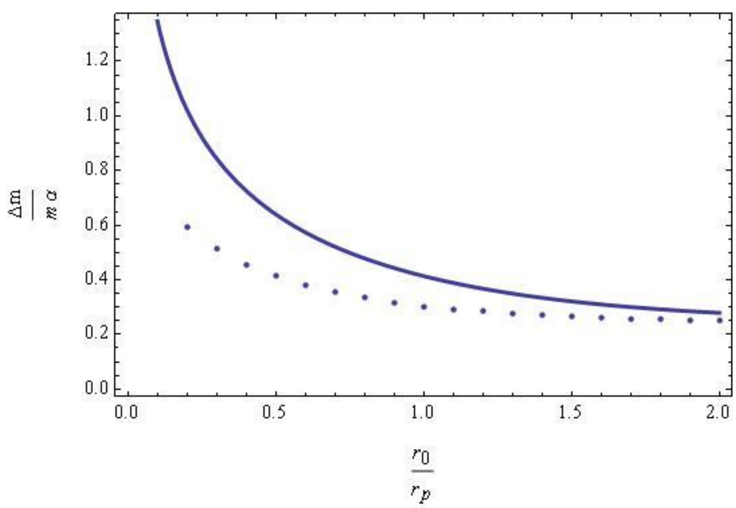

Fig. 4. Dependence of $\Delta m/m\alpha$ on the r_0/r_p ratio taking into account transitions from the excited state of the polaron with $n=1$ to subbands n =-1, ±2, ±3: (a) the solid curve is obtained without taking into account screening and (b) the dotted curve is derived taking into account screening. In this case, the Fermi level is placed in subband with $n=1$.

4. Conclusions

From the dependence of the polaron correction to the mass on the radius of HNC for the ground and excited states presented in Figs. 1-4, it follows that screening contribution to the polaron mass is significant for the values a < 1. For the specified value a = 0.5 in Fig. 2 the polaron correction to the mass decreases approximately by 35% in comparison with the case without screening. For the values of the parameter a > 1 the screening contribution to polaron mass decreases with increasing HNC-radius, but the decrease in the polaron correction to the mass due to screening is still more than 30%.

Thus, the obtained numerical calculation results confirmed the significance of the screening contribution to the polaron mass.

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