Effect of screening on the phonon–polaron states in a nanotube of diluted magnetic semiconductor

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We report the calculation results of the effect of screening on weakly coupling Fröhlich polaron binding energy of the ground state and polaron contribution to the mass for the lowest spin-down subband of the conduction band in a diluted magnetic semiconductor nanotube. The expressions for the energy of the polaron and the polaron contribution to the effective mass was obtained as a function of the magnetic field and the radius of the nanotube, taking into account the screening effect as well as virtual transitions from the ground state with \( n = 0 \) to the size-quantized subbands with \( n' = \pm 1, \pm 2, \ldots, \pm 10 \). The performed numerical calculations demonstrate that the effect of screening decreases the polaronic binding energy and polaronic contribution to the effective mass about 35 and 25\%, respectively, for the value of the magnetic field equal 0.1 T. It has been established that the effect of screening reduces polaron binding energy of the ground state approximately by 30–15\% and also reduces the polaron contribution to the effective mass by 25–10\% with increase of the nanotube radius in the range about 10–40 nm.

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1. Introduction

Diluted magnetic semiconductors (DMS) or semimagnetic semiconductors are ternary semiconducting compounds. Lattice of these compounds is made up in part of substitutional magnetic ions. In other words, DMS are one of the best materials to combine semiconductor properties with magnetism.

The presence of magnetic ions leads to localization of its spins in DMS materials [1]. Spin-dependent phenomena of the DMS have attracted considerably attention in low-dimensional structures as they have found a lot of applications in the spintronics. DMS give a possibility to appearance of the spin splitting and spin polarization due to the sp–d exchange interaction between electrons and local magnetic ions in the external magnetic field [2]. It should be noticed that the most characteristic feature of DMS is giant splitting [2], which increases the spin polarization of the electrons. Recently, it was found that the incorporation of Mn ions into the crystal matrix of various \( A^2B^6 \) semiconductor compounds led to the fabrication of DMS quantum dots and hybrid DMS structures [3–6].

The physical properties of all structures are mainly determined by electronic processes occurring in them. These processes also include electron–phonon interaction. One of the evidences of the electron–phonon coupling is polaron effect. Especially, considerable interest exists in the study of the phonon–polaron states in the nanotube (NT) on DMS-based materials. DMS-based \( A^2B^6 \) compounds are usually weakly polar materials. Therefore, Fröhlich polaron of the large radius will be realized in such magnetic compounds.

Recently, there is growing interest in fundamental properties of the 2D electron gas, such as the screening of the electron–phonon interaction. The theoretical calculations based on the one-electron approximation predict an enhancement of the polaron parameters in the bulk structures. However, it is experimentally found that the polaron parameters in 2D GaAs–Al\(_x\)Ga\(_{1-x}\)As heterostructures are smaller than those in the three dimensional GaAs system. The theoretical [7–9] and experimental [10–13] studies have demonstrated that many-particle effects, i.e., screening effects, reduce the polaron renormalization of the electron effective mass.

The screening effect also changes the polaron energy. Far infrared absorption probes directly the polaron energy levels instead of the purely electronic states. The electron polarons have been extensively studied by intraband magneto-optical transitions in \( n \)-doped quantum dots [14,15].
The results of relevant experimental studies show that the screening effect should reduce the value of both basic polaron parameters such as the binding energy and the effective polaron mass \( m_p \). From the foregoing follows that the effect of screening also will change the parameters of the phonon–polaron in quasi-2D DMS structures.

Present paper is devoted to theoretical study of the influence of the screening effect on phonon–polaron parameters in DMS-based NT, taking into account the exchange interaction as well as the transitions to the size-quantized subbands in the external uniform magnetic field.

2. Energy states, electron wave functions and matrix element of the electron–photon coupling

It is considered NT of DMS with radius \( r_0 \) on the surface of which there is 2D gas of mobile noninteracting electrons threaded by a longitudinal magnetic field. The energy spectrum of the similar structure has been obtained for DMS-type CdSe\(_{1−x}\)Mn\(_x\)Te quantum dot with cylindrical symmetry [16].

Energy spectrum of the electron on the surface of the nanotube has the form [17]

\[
\varepsilon_{n,k} = 6\alpha \sigma + \frac{\hbar^2 k^2}{2M \varepsilon_{\sigma}} + \frac{\hbar^2}{2M \varepsilon_{\perp}} \left[ n + \frac{1}{2} \left( \frac{\varepsilon_{\sigma}}{R} \right)^2 \right]^2.
\]

Here \( r_0 \) is the radius of nanotube, \( h \) is the magnitude of a magnetic field directed along \( z \) axes, \( \sigma = \pm 1/2 \) for spin up \( \uparrow \) and spin down \( \downarrow \), correspondingly, \( k \) is the wave vector characterizing an electron motion along \( z \) axis of the NT, \( n = 0, \pm 1, \pm 2, \ldots \) is the azimuthal quantum number, \( R = \sqrt{\hbar/m_e \omega_c} \), \( \omega_c = eH/m_e c \) are the magnetic length and the cyclotron frequency, respectively. The longitudinal and transverse effective masses of an electron in an external uniform magnetic field are determined by the following expressions:

\[
\frac{1}{M_{\perp}} = \frac{1}{m_e} \varepsilon_g + 2\varepsilon_g (3A - B),
\]

\[
\frac{1}{M_{\perp}} = \frac{\varepsilon_g}{4m_e} \left[ \frac{3}{\varepsilon_g + 6\sigma(A - B)} + \frac{1}{\varepsilon_g + 2\sigma(3A + B)} \right],
\]

where \( \varepsilon_g \), \( m_e = 3h^2 \varepsilon_g/4\hbar^2 \) are the band gap and the effective mass of conduction electrons in the absence of magnetic field, respectively.

The terms \( A = (\alpha/\beta)B \) and \( B = (N_0 \beta \langle S_\sigma \rangle)/6 \) determine Zeeman splitting of the conduction and valence bands, respectively. Here \( N_0 \beta \) is a magnetic ion concentration; \( P \) is the Kane’s parameter. The contribution of the exchange interaction to the energy of the band electrons are characterized by the exchange constants \( \alpha = \langle S \mid J \mid S \rangle \) and \( \beta = \langle X \mid J \mid X \rangle \). The spin of magnetic ion \( \langle S_\sigma \rangle = -S B_g(Y) \) averaged along the direction of the magnetic field, is determined by the Brillouin function \( B_g(Y) \) under neglecting of the interaction between the magnetic ions:

\[
B_g(Y) = \frac{2S + 1}{2S} \coth \left( \frac{2S + 1}{2S} Y \right) - \frac{1}{2S} \coth \left( \frac{1}{2S} Y \right),
\]

where \( Y = \xi \mu_B SH/(k_B T) \), \( S = 5/2 \), \( \xi = 2 \). \( T \) is an absolute temperature, \( k_B \) is the Boltzmann constant, and \( \mu_B \) is the Bohr magneton.

The expression of the normalized wave function of an electron, moving freely on the cylindrical surface of NT with the length \( L \), has the following form [18,19]:

\[
\psi_{n,k}(z,\phi) = \frac{1}{\sqrt{2\pi L_z}} e^{(ikz+n\phi)} S_{\sigma},
\]

where \( S_{\sigma} \) is the spin part of wave function, where

\[
S_{\sigma} = \left\{ \begin{array}{ll}
1 & ; S = 0 \\
0 & \end{array} \right. .
\]

Earlier the expression for the matrix element \( M_{n-n',q} \) of the potential energy \( (-\varepsilon \sum_{q} \Phi_q) \) was obtained by taking into account only transitions within subband which is suitable only for the limiting case of small NT radius \( r_0 \).

Here taking into account the expression for Fourier component of the scalar potential \( \Phi_q \)

\[
\Phi_q = i \frac{2\pi \hbar \omega_z}{\varepsilon^* V} \frac{1}{\sqrt{q_z^2 + q_\perp^2}} e^{-(iq_\perp r_0 \cos \phi + q_z z)},
\]

where \( q_\perp \) is the magnetic part of \( q \), \( r_0 \) is the radius of the NT. The matrix element \( M_{n-n',q} \) of the electron–photon coupling is calculated with the wave function (4) for any \( n, n' \) [17]:

\[
M_{n-n',q} = -i \frac{4\pi \alpha_F \hbar}{\sqrt{q_z^2 + q_\perp^2}} \int_{q\perp} J_{n-n'}(q_\perp r_0) q_z.
\]

Here \( V \) is the NT volume, \( \alpha_F \) is the Fröhlich coupling parameter and \( r_p \) is the polaron radius, given as

\[
\alpha_F = \frac{m_e \varepsilon^*}{2 \hbar \omega_z} \left( \frac{1}{\varepsilon_{\sigma}} - \frac{1}{\varepsilon_0} \right), \quad r_p = \sqrt{\frac{2m_e \omega_z}{\hbar}}.
\]

The effective dielectric constant \( \varepsilon^* \) is determined by the expression \( (\varepsilon^*)^{-1} = \varepsilon_{\sigma} - \varepsilon_0 \), where \( \varepsilon_0 \) and \( \varepsilon_\infty \) are the static and high-frequency dielectric constants, respectively. \( J_{n-n'}(q_\perp r_0) \) is the Bessel function of index \( n-n' \), \( \omega_z \) is the longitudinal optical-phonon (LO) frequency.

The matrix element \( M_{n-n',q} \) is calculated under the condition that an electron–photon interaction leads to the virtual transitions of an electron with emission of one LO phonon at sufficiently low temperatures. In this work the upper temperature limit is determined by the condition \( k_B T < |\Delta E_{0,0}| \), where \( \Delta E_{0,0} \) is the polaron binding energy of the ground state. In accordance with our estimates for NT with diameter of 20 nm, polaron binding
energy is given by the order 1.9 meV, which approximately corresponds to the temperature 12 K.

3. Dielectric permeability in a nanotube of the DMS

In semiconductors with the sufficiently high carriers concentration, the electron–phonon interaction is screened. According to [20], the potential of the electron–phonon interaction is screened by replacing the matrix element (6) with the following expression:

\[ M_{n\rightarrow n'}, q ightarrow M_{n\rightarrow n'}, q' / \varepsilon_n (q, \omega) . \]  

(7)

Here \( \varepsilon_n (q, \omega) \) is the electron dielectric function. The expression for the dielectric function is mainly defined by electron energy spectrum of the considered system.

Our recent paper [21] was devoted to influence of screening of electron–phonon interaction on the polaron binding energy in a semiconductor NT. In those paper it is used the results of a computation of the electron dielectric permeability for an infinitely long semiconductor NT [22].

In order to solve the similar problem for NT of DMS, we first calculate the dielectric function for energy spectrum (1), using the same technique [22,23].

\[
\Pi_{|p-n'|, \sigma}(z,0) = -\frac{r_p L_z}{2\pi \hbar^2 z^2} n_{F, \sigma} \sum M_{z, \sigma} \log \left| \frac{m_e}{M_{z, \sigma}'} - z^2 \frac{m_e}{M_{\perp, \sigma}'} + \frac{m_e}{M_{\perp, \sigma}'} a^{-2} (n-n') \left( n+n' + \left( \frac{\hbar^2}{R} \right)^2 \right) \right|
\]

(10)

Here \( k_F \) is the Fermi wave vector. Then by means of expressions (8), (9) we obtain the following expression for the dielectric function:

\[
\varepsilon_{n|p-n'|, \sigma}(z,0) = 1 - \frac{2e^2}{L_z \varepsilon_0} I_{|p-n'|}(za) K_{|p-n'|}(za) \Pi_{|p-n'|, \sigma}(z,0).
\]

(11)

4. Phonon–polaron energy and its mass

In the present paper we investigate the influence of screening effect on the basic phonon–polaron parameters on NT surface of the DMS. In order to obtain the analytical expression for the polaron parameters it is necessary to calculate the contribution to the electron energy due to electron interaction with the LO-phonons. The calculation is carried out within the framework of the standard perturbation theory.

Taking into account the screening effect, in accordance with (7), the expression for the polaron contribution to the electron energy \( \Delta E_{n,k,\sigma} \) in the second-order perturbation theory is defined as follows:

\[
\Delta E_{n,k,\sigma} = \sum_{n',q} \left| M_{n-n',q} \right|^2 \left( \varepsilon_{n|p-n'|, \sigma} - \varepsilon_{n', k-q, \sigma} - \hbar \omega_L \right) \right|^2 \varepsilon_{|p-n'|, \sigma}(q_z).
\]

(12)

Equations (6) and (12) yield the following expression for the polaron binding energy:

\[
\Delta E_{n,k,\sigma} = \frac{4\pi \alpha_F (\hbar \omega_L)^2 r_p}{V} \times \left( \frac{q_z^2}{q_z^2 + q_{\perp}^2} \right) (\varepsilon_{n|k-q, \sigma} - \varepsilon_{n', k-q, \sigma} - \hbar \omega_L) \varepsilon_{|p-n'|, \sigma}(q_z).
\]

(13)

We transform the summation in Eq. (13) into integration in cylindrical coordinates \((q_{\perp}, q_z, \phi) \rightarrow (x, z, \phi)\) taking into account of expression (1), and after integrating over the polar angle \( \phi \), one gets the expression for the polaron binding energy in the new dimensionless variables \( x = q_{\perp} r_p / z = q_z r_p / \kappa = k r_p \).
The notation $b_{nn'}$ introduced into Eq. (14) is defined by the following expression:

$$b_{nn'} = \left[1 - \frac{m_e}{M_{\perp \sigma}} \alpha^2 (n - n') \ n + n' + h\right]^{-1/2}.$$  

Integration over $x$ in Eq. (13) yields the following expression:

$$\int_{0}^{\infty} \left| J_{nn'}(xa) \right|^2 x dx = I_{nn'}(\varepsilon a) K_{nn'}(\varepsilon a).$$  

By means of the Eq. (16) we obtain for (14)

$$\Delta E_{n,k,\sigma} = -\frac{\alpha_F \hbar \omega_L}{\pi} \sum_{n'} \int_{-\infty}^{\infty} \frac{I_{nn'}(\varepsilon a) K_{nn'}(\varepsilon a)}{z^2 \frac{m_e}{M_{\perp \sigma}} + 2z\kappa \frac{m_e}{M_{\perp \sigma}} + b_{nn'}^2} \left(\varepsilon_{nn'}(\varepsilon a)\right)^2 dz.$$  

Restricting ourselves to second-order terms, we expand the integrand in Eq. (17) over powers of $\kappa$:

$$\Delta E_{n,k,\sigma} = \Delta E_{n,0,\sigma} + A_{n,\sigma} \kappa^2.$$  

Here the first term in the brackets corresponds to the polaron binding energy $\Delta E_{n,0}$ and the second term does to the polaron kinetic energy, i.e., expression (18) can be presented as follows:

$$\Delta E_{n,k,\sigma} = \Delta E_{n,0,\sigma} + A_{n,\sigma} \kappa^2.$$  

From (18), (19), the polaron binding energy $\Delta E_{n,0,\sigma}$ and polaron factor $A_{n,\sigma}$ for the correction to the kinetic energy are determined as

$$\Delta E_{n,0,\sigma} = \frac{2\alpha_F \hbar \omega_L}{\pi} \sum_{n'} \int_{0}^{\infty} I_{nn'}(\varepsilon a) K_{nn'}(\varepsilon a) \left[1 - \frac{z^2 \frac{m_e}{M_{\perp \sigma}} + b_{nn'}^2}{\varepsilon_{nn'}(\varepsilon a)}\right]^{-1} dz.$$  

$$A_{n,\sigma} = -\frac{8\alpha_F \hbar \omega_L}{\pi} \sum_{n'} \int_{0}^{\infty} I_{nn'}(\varepsilon a) K_{nn'}(\varepsilon a) \left[\frac{z^2 \frac{m_e}{M_{\perp \sigma}} + b_{nn'}^2}{\varepsilon_{nn'}(\varepsilon a)}\right]^{-2} dz.$$  

Taking into account the second term in expression (19) we obtain for the polaron contribution to the effective mass of electron, expressed in terms of $A_{n,\sigma}$ [17].
5. Numerical calculations

It is interesting to analyze the formulas (11), (20), (21) for the limiting case of small NT radius with condition \( a = n_0/r_p < 1 \). With the decreasing of the value of NT radius (that is the value of \( a < 1 \)) the distance between the levels of size quantization increases.

Then, from the expression of the integrand (11) follows that the main contribution to the integral comes from the region of the variable \( z < 1 \). As a result of this situation, we can limit ourselves with state \( n = 0 \). Contribution to the dielectric function due to the free carriers in this region is small compared with unity.

Taking into account weak logarithmic dependence of the dielectric function from the \( z \) variable which follows from the known asymptotics of modified Bessel functions, the average value of the dielectric function we can take out from the integrand expression. Integrals (20), (21) for the energy and mass in this case are analytically calculated and reduced to the Meyer functions.

It is known that the Meyer functions have logarithmic asymptotics for small values of \( a \). Therefore, as with the screening or without screening the binding energy and the polaron mass increases logarithmically with decreasing radius of the NT, that is observed below in Figs. 1(a) and 2(a).

Now in the further calculations we will be limited only the lowest conduction band with spin down \( \downarrow \). The dependences of the basic polaron parameters as the function of the magnetic field and the nanotube radius were calculated according to formulas (20), (21) and (10), (11). The calculations were performed at temperature \( T = 1 \) K taking into account the following specific features of the problem under consideration:

i) The Fermi level lies between the size-quantized subbands with \( n = 0 \) and \( n = -1 \) (also as well as below of spin up conduction band). Such position of location of the Fermi level we obtain at fixed concentration \( n_c = 1.5 \times 10^6 \) m\(^{-1}\) with \( k_F = 2\zeta r_p \), where \( \zeta = 0.1 \).

ii) With the increasing of the magnetic field the Fermi level rises. In order that the polaron band could be located below the bottom of the conduction band with spin down (i.e., in the band gap) the condition \( |\Delta E_{0,0} - \varepsilon_F| > k_0T \) should be realized.

For computation the following values of the parameters for Hg\(_{1-x}\)Mn\(_x\)Se compound with \( x = 0.066 \) are chosen: \( \hbar_0 L = 16.8 \) meV, \( \varepsilon_0 = 28.5, \varepsilon_x = 13, P = 5.09 \times 10^{-8} \) eV cm, \( N_0\alpha = -0.32 \) eV, \( N_0\beta = 0.92 \) eV, \( \varepsilon_g = 24 \) meV, \( \bar{g} = 2 \), \( S = 5/2, T = 1 \) K, \( r_p = 0.26 \) nm, \( m_b = 9.1 \times 10^{-31} \) kg, \( e = 1.6 \times 10^{-19} \) C, \( c = 3 \times 10^8 \) m/s [17].

Numerical calculation results for the dependences of the dimensionless polaron binding energy \( \Delta \varepsilon_{0,0} / \varepsilon_F h_0L \) and polaron contribution to the effective mass \( \Delta m_{c,p} / \alpha_M M_z \) on the dimensionless magnetic field \( h = r_p / R^2 \) (up to \( H = 0.1 \) T) are depicted in Fig. 1 for the value of \( a = n_0/r_p = 1/2 \). Computation of the basic polaron parameters is carried out taken into account the transitions from the ground state with \( n = 0 \) to the size-quantized subbands with \( n' = \pm 1, \pm 2, ..., \pm 10 \) are taken into account at \( n_0/r_p = 1/2 \).

From comparison of calculation results for the curves 1, 3 (Fig. 1) is followed that decreasing of polaron binding energy, as a result of the screening effect of polaron binding energy and polaron contribution to the effective mass, constitute about 35 and 25%, respectively, for the considered values of \( H \) up to 0.1 T.

The results of the calculations for the dependences of the dimensionless polaron binding energy \( \Delta \varepsilon_{0,0} / \varepsilon_F h_0L \) of the ground state and polaron contribution to the effective mass \( \Delta m_{c,p} / \alpha_M M_z \) on the dimensionless NT radius \( h_0/r_p \) are depicted in Fig. 2 at \( H = 0.1 \) T. From comparison of numerical data for the curves 2, 1 and 4, 3 it follows that the...
screening effect reduces a polaron binding energy of the ground state and polaron contribution to the effective mass about by 30–15% and 25–10% with increasing the values of the parameter \( a = \frac{\eta_0}{r_p} \) in the range about 0.5–2, respectively.

Comparison of curve 2 with 1 and curve 4 with 3 in Fig. 2 show that the screening effect considerably decreases polaron binding energy and polaron contribution to the effective mass on the NT radius in the presence of the magnetic field with increasing of NT radius.

From comparison of calculation results for the curves 2 and 1 presented in Fig. 2(a) is followed that as a result of the effect of the screening, the dimensionless polaron binding energy decreases approximately from 35 to 15% with an increasing of \( \eta_0/r_p \) from 0.5 to 2. As a result of comparative investigations of the curve 2 with curve 1 in Fig. 2(b), it has been established that with an increasing of the value of \( \eta_0/r_p \) from 0.5 to 2 the decrease in the polaron contribution to the mass owing to the screening effect constitutes about 25 to 15 %, respectively.

![Fig. 2](image)

Fig. 2. Dependences of the polaron binding energy (a) and polaron contribution to the electronic mass (b) on the radius of NT: in the absence of the exchange interaction and screening effect (1); taking into account of screening effect in the absence of exchange interaction (2); taking into account of the exchange interaction in the absence of screening effect (3); taking into account of screening effect in the presence of the exchange interaction (4). The transitions from the ground state \( n = 0 \) to the subbands \( n' = \pm 1, \pm 2, \ldots \pm 10 \) is taken into account at \( H = 0.1 \) T.

**Conclusion**

It has been presented a detailed description of the screening effect on the phonon–polaron states for the degenerate electron gas in NT of DMS type compounds.

The performed numerical calculations make possible to evaluate the influence of the screening effects on the polaron parameters. These evaluations were carried out for NT of Hg\(_{1-x}\)Mn\(_x\)Se compound with \( x = 0.066 \) at \( T = 1 \) K. The dependencies of the polaron binding energy and polaron contribution to the effective mass on the magnetic field and NT radius for the ground state were obtained. Owing to screening effect the decrease of polaron binding energy and polaron contribution to the effective mass constitute about 35 and 25%, respectively, for all the considered values of \( H \). The screening effect leads to a considerably decrease of the polaron binding energy for values of \( \eta_0/r_p \geq 0.5 \).

Moreover the screening effect is an important method for the interpretation of the magneto-optical, cyclotron resonance and far-infrared absorption experiments. Thus the obtained numerical calculation results confirmed the significance of screening effect for the polaron binding energy and polaron contribution to the effective mass.

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