Eur. Phys. J. B **53**, 143–154 (2006)
DOI: 10.1140/epjb/e2006-00359-6

THE EUROPEAN PHYSICAL JOURNAL B

Polaron effects and boundary conditions in cylindrical wires

G. Iadonisi[a], F. Trani, G. Cantele, and D. Ninno

Coherentia CNR-INFM and Università di Napoli "Federico II" - Dipartimento di Scienze Fisiche, Complesso Universitario Monte S. Angelo, via Cintia, 80126 Napoli, Italy

Received 12 June 2006 / Received in final form 24 July 2006
Published online 4 October 2006 –

Abstract. In this work we show that the polaron effects in cylindrical quantum wires are function of the cylinder radius R_0 through the boundary conditions for both the ionic and the electronic motion and through the size dependence of the static and high frequency dielectric constants. We find that the dielectric constants are increasing functions of R_0. This fact and the different boundary conditions for the ions and the electrons have the final consequence that polaron self-energy can either be an increasing or a decreasing function of R_0.

PACS. 71.38.-k Polarons and electron-phonon interactions – 73.21.Hb Quantum wires – 63.22.+m Phonons or vibrational states in low-dimensional structures and nanoscale materials

1 Introduction

In the last years a large number of experimental techniques have been used to fabricate confined semiconductors nanostructures with different shapes [1–8]. These systems are interesting for both the basic physics and the opto-electronic devices. The electronic, optical and transport properties have been investigated both in quantum dots [10–14] and in quantum wires [15–19]. Many-body effects have been taken into account [20,21]. In particular, the first quasi-analytical solution of the Schrödinger equation in the ellipsoidal geometry [22] has induced studies on the shape dependence of electronic, optical and correlation properties [23,24]. Furthermore, the possibility to find bound electronic states in cylindrical deformed wires [16,25–27] stimulated the study of the correlated and localized two-electrons states [28].

There are two different ways to confine the particles (electrons and/or holes) in a volume: (a) using a suitable localization potential in two or three dimensions; (b) assuming that the particles are confined because two materials are in contact so that confining forces come out at the interface. For what concerns polaron effects, these different kinds of localizations require different electron-phonon interactions. In the first case the polaron effects are calculated using a three-dimensional model (for example the Fröhlich interaction [29]) where the electron localization is due to a confining potential; in the second case, depending on the materials at contact, suitable boundary conditions at the interface must be imposed for both the electronic and the ionic motion. In this last case it seems that polaronic effects are described with more details. In any case, although the results of the models could be different when the dimension of the system is small with respect to the polaron radius, a physical requirement is that they must be the same when the system dimension increases.

In confined systems, the phonon modes have been calculated using both the continuous dielectric model [30–40] and the microscopic description [41–44], even in regular cylindrical wires and spherical dots with multi-shells materials [45,46]. In the most simple cases, the optical longitudinal phonon mode is that of the bulk material, but in some calculations in the continuous dielectric model [47,48], the motion of the ions with reliable boundary conditions has been considered explicitly in cylindrical wires of GaAs plunged in AlAs. When the dimension of the system is small, both the longitudinal and transverse optical phonon frequencies are lower than the asymptotic ones, but they tend to the asymptotic limit when the radius becomes larger than almost 20 Å. Furthermore the explicit form of both the electron-phonon and the electron-interface phonon interaction have been calculated in the regular cylinder [45] in the framework of the Fröhlich polaron theory, assuming that the longitudinal optical phonon mode is that of the bulk material. Using this form for the electron-phonon interaction and an electronic wave function completely localized in the cylinder, the polaron self-energy is an increasing function of the cylinder radius R_0 and it becomes the bulk self-energy when $R_0 \gg R_p$ [49] (R_p is the polaron radius). On the other hand, using a localization potential and the Fröhlich form of the electron-phonon interaction it is found that

[a] e-mail: giuseppe.iadonisi@na.infn.it

the polaron self-energy is a decreasing function of R_0 and becomes that of the bulk when $R_0 \gg R_p$ [50,51].

In this work we study the polaron effects when a particle (electron or hole) is forced to be in a quantum wire of cylindrical shape. The medium is treated in the continuous approximation, but we impose different boundary conditions for the motion of ions and electrons. We discuss also the origin of the dependence of the static and high frequency dielectric constants on the cylinder radius using as a starting point the self-consistent calculation of the dielectric constants in an ellipsoidal dot [22,23,54] when $\chi = c/a \to \infty$ (c and a are respectively the rotational and transverse axis). The result is that the dielectric constants increase as a function of R_0 because the induced charges on the surface tend to screen the polarization effects. This fact and the use of different boundary conditions for the ion and the electron motion have the final result that the polaron self-energy can increase or decrease as a function of R_0.

The work is organized as it follows: in Section 2 we discuss, in the continuum model, the features of the dispersive dielectric function in a cylindrical quantum wire and how it depends on the radius and on the boundary condition for the ionic motion; in Section 3 we write the polaron Hamiltonian using different forms of the electron-phonon interaction; in Section 4 we calculate, using a self-consistent variational method, the self-energy of the polaron and show how it depends on the type of the electron-phonon interaction used; finally in Section 5 we present the conclusions.

2 The dielectric function of a cylindrical quantum wire

The polaron effects in a polar material can be studied starting from the set of equations

$$\frac{d^2\mathbf{u}}{dt^2} = -\omega_0^2\mathbf{u} + \frac{e}{\mu}\mathbf{E}_{loc} - \beta_l^2\nabla(\nabla\cdot\mathbf{u}) + \beta_t^2\nabla\times(\nabla\times\mathbf{u}) \quad (1)$$

$$\mathbf{P} = ne\mathbf{u} + n\alpha_p\mathbf{E}_{loc} \quad (2)$$

$$\mathbf{E}_{loc} = \mathbf{E} + \frac{4}{3}\pi\mathbf{P} \quad (3)$$

where μ is the reduced mass of the ions in the unit cell and $\mathbf{u}$, $\mathbf{E}$, $\mathbf{P}$, ω_0 describe, respectively, their relative displacements, the electric field, the polarization field and the ions oscillation frequency, n is the number of ionic dipoles per unit volume and α_p the polarizability of the atoms in the unit cell. In equation (1), that concerns the equation of motion for the ionic displacement, non-local contributions are taken into account. In equation (3) local field effects are included through the Lorentz rule for an homogeneous and isotropic material, although this could be avoided using more complicated linear relations. With the substitution of equation (3) in (2), we obtain

$$\mathbf{P} = b_{21}\mathbf{u} + b_{22}\mathbf{E} \quad (4)$$

with

$$b_{21} = \frac{ne}{1-\frac{4}{3}\pi n\alpha_p}$$
$$b_{22} = \frac{n\alpha_p}{1-\frac{4}{3}\pi n\alpha_p}. \quad (5)$$

By inserting equations (3) and (4) in the spatial Fourier transform of equation (1), we obtain

$$\frac{d^2\tilde{\mathbf{u}}}{dt^2} = -\left(\omega_0^2 - \frac{4}{3}\pi\frac{e}{\mu}b_{21} - \beta_t^2k^2\right)\tilde{\mathbf{u}} - \left(\beta_t^2-\beta_l^2\right)(\mathbf{k}\cdot\tilde{\mathbf{u}})\mathbf{k} + b_{12}\tilde{\mathbf{E}} \quad (6)$$

with

$$b_{12} = \frac{e}{\mu}\left(1+\frac{4}{3}\pi b_{22}\right). \quad (7)$$

We assume that the above equations can be used both in the bulk material and in the cylinder; the only difference is that the values of the constants could depend on the cylinder radius. If the ionic motion is transverse, i.e. $\mathbf{k}\perp\tilde{\mathbf{u}}$, we find for the frequency of the transverse mode

$$\omega_t^2(k) = \omega_0^2 - \frac{4}{3}\pi\frac{e}{\mu}b_{21} - \beta_t^2k^2. \quad (8)$$

On the other hand, taking also the time Fourier transform of equation (6), we obtain for the longitudinal motion

$$\tilde{\mathbf{u}} = \frac{b_{12}}{\omega_t^2(k) + \left(\beta_t^2-\beta_l^2\right)k^2 - \omega^2}\tilde{\mathbf{E}} \quad (9)$$

and equation (4) becomes

$$\tilde{\mathbf{P}} = \left(b_{22} + \frac{b_{12}b_{21}}{\omega_t^2(k) + \left(\beta_t^2-\beta_l^2\right)k^2 - \omega^2}\right)\tilde{\mathbf{E}}. \quad (10)$$

This last equation allows the definition of the longitudinal spatial and frequency dependent dielectric function

$$\frac{\varepsilon(k,\omega)-1}{4\pi} = b_{22} + \frac{b_{12}b_{21}}{\omega_t^2(k) + \left(\beta_t^2-\beta_l^2\right)k^2 - \omega^2} \quad (11)$$

from which it immediately follows that

$$\varepsilon_\infty = 1 + 4\pi b_{22} \quad (12)$$

$$\varepsilon(k,0) = \varepsilon_\infty + 4\pi\frac{b_{12}b_{21}}{\omega_t^2(k) + \left(\beta_t^2-\beta_l^2\right)k^2}. \quad (13)$$

We can therefore rewrite equation (11) as

$$\varepsilon(k,\omega) = \varepsilon_\infty + \frac{\left(\varepsilon(k,0)-\varepsilon_\infty\right)\left(\omega_t^2(k) + \left(\beta_t^2-\beta_l^2\right)k^2\right)}{\omega_t^2(k) + \left(\beta_t^2-\beta_l^2\right)k^2 - \omega^2}. \quad (14)$$

From this equation we can derive the longitudinal frequency ω_l as the solution of $\varepsilon(k,\omega) = 0$

$$\omega_l^2 = \frac{\varepsilon(k,0)}{\varepsilon_\infty}\left(\omega_0^2 - \frac{4}{3}\pi\frac{e}{\mu}b_{21} - \beta_l^2k^2\right). \quad (15)$$

Using equation (14) and considering only terms up to k^2, this frequency can be rewritten as

$$\omega_l^2(k) = \frac{\varepsilon(0,0)}{\varepsilon_\infty}\left(\omega_0^2 - \frac{4}{3}\pi\frac{e}{\mu}b_{21}\right) - \frac{\varepsilon(0,0)}{\varepsilon_\infty}\beta_l^2 k^2 + \frac{\varepsilon(k,0)-\varepsilon(0,0)}{\varepsilon_\infty k^2}\left(\omega_0^2 - \frac{4}{3}\pi\frac{e}{\mu}b_{21}\right)k^2. \quad (16)$$

If, as we assume, $\lim_{k\to 0}\frac{\varepsilon(k,0)-\varepsilon(0,0)}{k^2} = \beta$ (finite number), we obtain

$$\omega_l^2(k) = \omega_L^2 - \beta_L^2 k^2 \quad (17)$$

where

$$\omega_L^2 = \frac{\varepsilon(0,0)}{\varepsilon_\infty}\omega_t^2(0) \quad (18)$$
$$\beta_L^2 = \frac{\varepsilon(0,0)}{\varepsilon_\infty}\beta_l^2 - \frac{\beta}{\varepsilon_\infty}\left(\omega_0^2 - \frac{4}{3}\pi\frac{e}{\mu}b_{21}\right).$$

This last equation gives the Lyddane-Sachs-Teller relation and the spatial dispersion of the longitudinal optical phonon frequency. In our hypothesis, for example, the Lyddane-Sachs-Teller has the same form in the bulk and in the confined system, but the values of $\varepsilon(0,0)$, ε_∞, β_l^2, β, ω_0^2 and b_{21} can depend on the cylinder radius.

We now want to consider how to adapt the dispersive dielectric function to the case of a cylindrical quantum wire. It is well known that the longitudinal phonon mode can be described through the equation [47,52,53]

$$\left[\nabla^2 + \frac{\omega_L^2 - \omega^2}{\beta_L^2}\right]\mathbf{u} = 0 \quad (19)$$

where we are taking $\nabla\times\ \mathbf{u} = 0$. The cylinder axis is oriented along the z-axis, so that the system is invariant for translations and rotations around the z-direction, so that we can write

$$u_z = C_m \exp(iqz)\exp(im\varphi)F_m(\rho) \quad (20)$$

where z, φ and ρ are the cylindrical coordinates and q and m are the wavenumber along the z-direction and an integer number such that $u_z(\varphi) = u_z(\varphi + 2\pi)$. Since u_z must satisfy equation (19), we find that

$$F_m(\rho) = J_m\left(\sqrt{\gamma^2 - q^2}\rho\right) \quad (21)$$

with $\gamma^2 = \frac{\omega_L^2-\omega^2}{\beta_L^2}$. The condition $\nabla\times\ \mathbf{u} = 0$ implies that

$$u_\varphi = \frac{m}{q\rho}u_z \quad (22)$$
$$u_\rho = -i\frac{\sqrt{\gamma^2-q^2}}{q}C_m\exp(iqz)\exp(im\varphi)J_m'\left(\sqrt{\gamma^2-q^2}\rho\right).$$

We use these results to determine a complete set of longitudinal polarization modes. This is an important tool for the development of the theory in the next Sect., because we can adapt the form of the electron-phonon interaction to the physical situation of our system. For example, if we determine the frequencies of the normal modes through the equation $J_m\left(\sqrt{\gamma^2-q^2}R_0\right) = 0$, we have that the displacements and the strains of the modes satisfy on the surface the conditions $u_z = u_\varphi = 0$, $u_\rho \neq 0$, $S_{\varphi z} = \frac{1}{2}\left(\frac{1}{\rho}\frac{\partial u_z}{\partial\varphi} + \frac{\partial u_\varphi}{\partial z}\right) = 0$, $S_{zz} = \frac{\partial u_z}{\partial z} = 0$, $S_{\varphi\varphi} = \frac{\partial u_\varphi}{\partial\varphi} = 0$, $S_{\rho\varphi} = \frac{1}{2}\left(\frac{\partial u_\varphi}{\partial\rho} + \frac{1}{\rho}\frac{\partial u_\rho}{\partial\varphi} - \frac{u_\varphi}{\rho}\right) \neq 0$, $S_{\rho\rho} = \frac{\partial u_\rho}{\partial\rho} \neq 0$, $S_{\rho z} = \frac{1}{2}\left(\frac{\partial u_\rho}{\partial z} + \frac{\partial u_z}{\partial\rho}\right) \neq 0$. On the other hand if we impose that $J_m'\left(\sqrt{\gamma^2-q^2}R_0\right) = 0$, we have normal modes such that on the surface the displacement $u_\rho = 0$, $u_\varphi \neq 0$, $u_z \neq 0$, and that only the strain $S_{\rho z} = 0$. Finally if we impose $b\sqrt{\gamma^2-q^2}R_0 J_m'\left(\sqrt{\gamma^2-q^2}R_0\right) + aJ_m\left(\sqrt{\gamma^2-q^2}R_0\right) = 0$, where a and b are fixed numbers independent of m, we have normal modes with mixed boundary conditions with all displacements and strain not zero (except the case $b/a = -1$, when the strain $S_{\rho\varphi} = 0$). In all the described cases the dispersive longitudinal frequencies are given by

$$\omega_{l,mi}^2 = \omega_L^2 - \beta_L^2\left(\frac{\chi_{mi}^2}{R_0^2} + q^2\right) \quad (23)$$

where the numbers χ_{mi} are found through specific equations. The conclusion is that the space and time dispersive dielectric function has a form much more complicated than that given by equation (14). The general form should be written as

$$\varepsilon(q,\omega) = \varepsilon_\infty(q) + \sum_{m,i}\frac{C_{mi}(q)\omega_{0,mi}^2(q)}{\omega_{0,mi}^2(q) - \omega^2} \quad (24)$$

whose zero are given by the frequencies of equation (23)

$$\varepsilon_\infty(q) + \sum_{m,i}\frac{C_{mi}(q)\omega_{0,mi}^2(q)}{\omega_{0,mi}^2(q) - \omega_{l,mi}^2} = 0 \quad (25)$$

and

$$\varepsilon(q,0) = \varepsilon_\infty(q) + \sum_{m,i}C_{mi}(q). \quad (26)$$

Numerical calculations have shown that in nanowires $\varepsilon_\infty(q)$ is smaller than that in the bulk [22,23,54] and such size dependence is not due to the dispersive terms of the bulk dielectric function. We can therefore assume that the dielectric function depends on the system size through two independent factor: the dispersive term and the size dependence of $\varepsilon_\infty(q)$. This allows us to make the following approximation: we neglect the dispersive terms in the bulk dielectric function and consider the limit $q \to 0$, so that the second term to the right of equation (24) reduces to the bulk case. We obtain for the frequency dependent dielectric function

$$\varepsilon(\omega) = \varepsilon_\infty(0) + \frac{[\varepsilon(0,0) - \varepsilon_\infty(0)]\,\omega_t^2}{\omega_t^2 - \omega^2} \quad (27)$$

where ω_t is the transverse frequency. In this equation the dependence of $\varepsilon_\infty(0)$ on the wire radius is known, but not

that of $\varepsilon(0,0)$. Since equation (27) can be written in the form

$$\varepsilon(\omega) = \varepsilon_\infty(0)\left[1 + \frac{\left(\frac{\varepsilon(0,0)}{\varepsilon_\infty(0)} - 1\right)\omega_t^2}{\omega_t^2 - \omega^2}\right] \tag{28}$$

we see that in the limit $R_0 \to \infty$ it occurs that $\frac{\varepsilon(0,0)}{\varepsilon_\infty(0)} = \frac{\varepsilon_0}{\varepsilon_\infty}$, where ε_0 and ε_∞ are the static and high frequency dielectric constant, $\varepsilon_\infty(0) = \varepsilon_\infty$ and ω_t is the bulk transverse frequency. Our final approximation is that even if ω_t and $\varepsilon_\infty(0)$ do not assume the asymptotic value, this occurs for the ratio $\frac{\varepsilon(0,0)}{\varepsilon_\infty(0)}$. It seems that numerical calculations reported in [47] support this fact, at least for not very small radii ($R_0 \lesssim 10$ Å).

We consider now a quantum wire embedded in a second material with dielectric constant ε_d. Our model is developed starting from the above equations with $\beta_l = \beta_t = 0$. In this case equations (9) and (10) can be written in real space: the condition $\nabla \times \mathbf{u} = 0$ implies that $\mathbf{E} = -\nabla\phi(\mathbf{r})$ and consequently

$$\mathbf{P} = -\frac{\varepsilon(\omega) - 1}{4\pi}\nabla\phi(\mathbf{r}). \tag{29}$$

Since $\nabla \cdot \mathbf{D} = \varepsilon(\omega)\nabla \cdot \mathbf{E} = \nabla \cdot (\mathbf{E} + 4\pi\mathbf{P}) = 0$, we have for the potential $\phi(\mathbf{r})$

$$\begin{aligned} \varepsilon(\omega)\nabla^2\phi(\mathbf{r}) &= 0 \quad r < R_0 \\ \varepsilon_d\nabla^2\phi(\mathbf{r}) &= 0 \quad r > R_0. \end{aligned} \tag{30}$$

Equations (29) and (30) allow to understand the features of $\phi(\mathbf{r})$ and $\mathbf{P}(\mathbf{r})$ considering reasonable physical conditions for the system:

(I) we could assume that inside the wire $\varepsilon(\omega) = 0$, i.e. $\omega = \omega_l = (\varepsilon_0/\varepsilon_\infty)^{\frac{1}{2}}\omega_t$. Since the normal component of the displacement vector $\mathbf{D}$ is continuous on the surface we must have

$$\varepsilon(\omega)\frac{\partial\phi}{\partial n}|_{in} = \varepsilon_d\frac{\partial\phi}{\partial n}\,|_{out} \tag{31}$$

and, consequently, $\frac{\partial\phi}{\partial n}\,|_{out} = 0$. From that it follows that $\phi(\mathbf{r})$ is arbitrary inside the wire while outside it satisfies the Poisson equation with the boundary condition that it is zero at infinite and its normal derivative is zero on the wire surface: i.e. $\phi(\mathbf{r}) = 0$ outside the wire. Since the potential $\phi(\mathbf{r})$ must be continuous across the surface, we must choose the arbitrary function $\phi(\mathbf{r})$ in the wire with the boundary condition $\phi(\mathbf{r})\,|_{\mathbf{r}\in S} = 0$. Since the surface charge is given by

$$\sigma_s = -\frac{\partial\phi}{\partial n}\,|_{in} \tag{32}$$

we conclude that the adopted boundary conditions implies the presence of induced surface charge;

(II) we could also assume $\frac{\partial\phi}{\partial n}\,|_{in} = 0$ and that $\phi(\mathbf{r})$ is discontinuous at the surface (in any case $\phi(\mathbf{r}) = 0$ for $r > R_0$). We have the new physical situation that on the surface there is a distribution of microscopic dipoles;

(III) we could finally assume that there is an unique polar medium of dispersive frequency $\varepsilon(\omega)$. In this case we must consider only the first of equations (30) in all the space with the boundary condition $\phi(\mathbf{r}) \to 0$ when $r \to \infty$. Since in this case there is no discontinuity in the medium, the surface charges or dipoles distribution are not present.

Before ending this section we note that other different problems can be solved in this theoretical scheme. The first one is obtained requiring that inside and outside the wire $\nabla^2\phi = 0$. The regular solution of the Laplace equation inside and outside the wire and the continuity of the normal component of the vector $\mathbf{D}$ allows to determine the frequency ω_s of the polarization modes, that are surface modes, because in the wire $\nabla \cdot \mathbf{P} = -\frac{\varepsilon(\omega_s)-1}{4\pi}\nabla^2\phi = 0$. The second problem that it can be treated is that of a cylinder deformed (for example having a bulge) or containing an impurity, when localized phonon modes arise.

We do not enter here in the details of these new situations because the work could become more involved from the mathematical point of view. In any case in the Section 4.2 we discuss qualitatively the contribution of the surface polarization mode to the polaron effect.

3 Quantum wire polaron Hamiltonians and boundary conditions

In our first case, we take $\varepsilon(\omega) = 0$, $\mathbf{D} = 0$, $\mathbf{E} = -4\pi\mathbf{P}$ and consequently $\mathbf{E}_{loc} = -\frac{8}{3}\pi\mathbf{P}$ inside the wire. Since the energy of the free oscillations is given by

$$H_{ph} = \frac{1}{2}\int d\mathbf{r}\left[n\mu\dot{\mathbf{u}}^2 + n\mu\omega_0^2\mathbf{u}^2 - ne\mathbf{u}\cdot\mathbf{E}_{loc}\right] \tag{33}$$

we obtain

$$H_{ph} = \frac{1}{2}\int d\mathbf{r}\left[n\mu\left(\frac{1 + \frac{8}{3}\pi n\alpha}{ne}\right)^2\left(\dot{\mathbf{P}}^*\cdot\dot{\mathbf{P}} + \omega_L^2\mathbf{P}^*\cdot\mathbf{P}\right)\right]. \tag{34}$$

Since (see Eq. (29))

$$\mathbf{P}(\mathbf{r}) = \frac{1}{4\pi}\nabla\phi(\mathbf{r}) \tag{35}$$

we write for the potential inside the wire

$$\begin{aligned} \phi(\mathbf{r}) &= \sum_{m=0}^{\infty}\sum_{i=1}^{\infty}\sum_q \frac{c_{miq}}{R_0}J_m\left(\chi_{mi}\frac{\rho}{R_0}\right)\frac{\exp(iqz)}{\sqrt{L}}\exp(im\varphi) \\ &= \sum_{m=0}^{\infty}\sum_{i=1}^{\infty}\sum_q \phi_{miq}(\rho, z, \varphi) \end{aligned} \tag{36}$$

where c_{miq} are coefficients to be fixed, χ_{mi} are the zeros of the Bessel function J_m labelled by the index i, ρ is the component of the vector $\mathbf{r}$ in the plane perpendicular to

the z-axis, φ the azimuthal angle and L the length of the wire in the z-direction, such that

$$\frac{1}{L}\int_{-\infty}^{\infty} dz \exp(-iqz)\exp(iq^{'}z) = \delta_{q,q'} \tag{37}$$

with $\delta_{q,q'}$ the Kronecker function. The potential $\phi(\mathbf{r})$ satisfies the boundary condition $\phi(\mathbf{r}) = 0\ |_{r=R_0}$ and it is written as a sum of terms orthogonal in the volume of the wire. We see that also $\mathbf{P}$ can be written as a sum of terms $\mathbf{P}_{miq}$ given by

$$\begin{aligned}
\mathbf{P}_{miq} &= \frac{1}{4\pi}\left(\frac{\partial\phi_{miq}}{\partial\rho}\mathbf{e}_\rho + \frac{1}{\rho}\frac{\partial\phi_{miq}}{\partial\varphi}\mathbf{e}_\varphi + \frac{\partial\phi_{miq}}{\partial z}\mathbf{e}_z\right)\\
\mathbf{P}_{miq}\cdot\mathbf{e}_\rho &= \frac{c_{miq}}{4\pi}\frac{\chi_{mi}}{R_0^2}J_m^{'}(\chi_{mi}u)\frac{\exp(iqz)}{\sqrt{L}}\exp(im\varphi)\\
\mathbf{P}_{miq}\cdot\mathbf{e}_\varphi &= \frac{c_{miq}}{4\pi}\frac{im}{\rho R_0}J_m(\chi_{mi}u)\frac{\exp(iqz)}{\sqrt{L}}\exp(im\varphi)\\
\mathbf{P}_{miq}\cdot\mathbf{e}_z &= \frac{c_{miq}}{4\pi}\frac{iq}{R_0}J_m(\chi_{mi}u)\frac{\exp(iqz)}{\sqrt{L}}\exp(im\varphi)
\end{aligned} \tag{38}$$

where $u = \frac{\rho}{R_0}$, $J_m^{'}(x) = \frac{dJ_m(x)}{dx}$ and $\mathbf{e}_\rho$, $\mathbf{e}_\varphi$, $\mathbf{e}_z$ indicate respectively the unit vector in the direction of ρ, in the direction perpendicular to ρ and to the z-axis and finally along the z-axis. Since $\mathbf{u}$ is proportional to $\mathbf{P}$, we see that the boundary condition on the potential ϕ becomes boundary condition for the displacement $\mathbf{u}$. The modes $\mathbf{P}_{miq}$ are normalized as

$$\begin{aligned}
\int_V d\mathbf{r}\mathbf{P}^*_{m'i'q'}\cdot\mathbf{P}_{miq} &= \delta_{m'm}\delta_{i'i}\delta_{q'q}\frac{J_m^{'}(\chi_{mi})^2}{16\pi}\\
&\times\left(\frac{\chi_{mi}^2}{R_0^2}+q^2\right)c_{miq}^2.
\end{aligned} \tag{39}$$

The coefficients c_{miq} are fixed assuming

$$n\mu\left(\frac{1+\frac{8}{3}\pi n\alpha}{ne}\right)^2\frac{J_m^{'}(\chi_{mi})^2}{16\pi}\left(\frac{\chi_{mi}^2}{R_0^2}+q^2\right)c_{miq}^2 = 1. \tag{40}$$

We can therefore conclude that equation (34) gives the energy of the free polarization modes as the sum of independent harmonic oscillators, all with the same frequency ω_L. With the transformations

$$\mathbf{P} = \sum_{miq}\left(\frac{\hbar}{2\omega_L}\right)^{\frac{1}{2}}\left(a_{miq}+a_{miq}^\dagger\right)\mathbf{P}_{miq} \tag{41}$$

$$\dot{\mathbf{P}} = -i\sum_{miq}\left(\frac{\hbar\omega_L}{2}\right)^{\frac{1}{2}}\left(a_{miq}-a_{miq}^\dagger\right)\mathbf{P}_{miq} \tag{42}$$

where the boson operators a_{miq} ($a_{miq}^\dagger$) destroy (create) the modes with the labels (miq), we obtain from (34) the free phonon Hamiltonian

$$H_{ph} = \sum_{miq}\hbar\omega_L\left(a_{miq}^\dagger a_{miq}+\frac{1}{2}\right). \tag{43}$$

The electron-phonon interaction is given by

$$\begin{aligned}
H_{el-ph} &= e\int d\mathbf{r}^{'}\mathbf{P}(\mathbf{r}^{'})\cdot\nabla^{'}\frac{1}{\mid\mathbf{r}^{'}-\mathbf{r}\mid}\\
&= -\frac{e}{4\pi}\int d\mathbf{r}^{'}\nabla^{'}\phi(\mathbf{r}^{'})\cdot\nabla^{'}\frac{1}{\mid\mathbf{r}^{'}-\mathbf{r}\mid}\\
&= \frac{e}{4\pi}\int d\mathbf{r}^{'}\phi(\mathbf{r}^{'})\nabla_{\mathbf{r}^{'}}^2\frac{1}{\mid\mathbf{r}^{'}-\mathbf{r}\mid}\\
&= -e\int d\mathbf{r}^{'}\phi(\mathbf{r}^{'})\delta\left(\mathbf{r}^{'}-\mathbf{r}\right) = -e\phi(\mathbf{r})
\end{aligned} \tag{44}$$

with $\nabla^{'}\equiv\nabla_{\mathbf{r}^{'}}$. Using the expressions of c_{miq} derived from equation (40) we find for the polaron Hamiltonian

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + H_{ph} + H_{el-ph} \tag{45}$$

with H_{ph} given by equation (43) and

$$\begin{aligned}
H_{el-ph} = -\sum_{miq}\Bigg[V_{miq}\frac{\exp(iqz)}{R_0}J_m\left(\chi_{mi}\frac{\rho}{R_0}\right)\\
\times\exp(im\varphi)a_{miq}^\dagger + h.c.\Bigg]
\end{aligned} \tag{46}$$

where

$$V_{miq} = e\sqrt{\frac{2\hbar\omega_l}{L}}\sqrt{\frac{1}{\varepsilon^*}}\frac{1}{\left[J_m^{'}(\chi_{mi})^2\left(\frac{\chi_{mi}^2}{R_0^2}+q^2\right)\right]^{\frac{1}{2}}} \tag{47}$$

with $\frac{1}{\varepsilon^*} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}$. We have inserted the normalization factor L in the expression of the electron-phonon interaction.

Considering the case when there is a distribution of electric dipoles on the surface, we take the same expression (36) for the potential $\phi(\mathbf{r})$, but the numbers χ_{mi} are replaced by $\chi_{mi}^{'}$, the zeros of $J_m^{'}(x)$. This choice allows us to show that the normalization condition is replaced by

$$\begin{aligned}
\int_V d\mathbf{r}\mathbf{P}^*_{m'i'q'}\cdot\mathbf{P}_{miq} &= \delta_{m'm}\delta_{i'i}\delta_{q'q}\frac{J_m(\chi_{mi}^{'})^2}{16\pi}\\
&\times\left(1-\frac{m^2}{\chi_{mi}^{'2}}\right)\left(\frac{\chi_{mi}^{'2}}{R_0^2}+q^2\right)c_{miq}^2.
\end{aligned} \tag{48}$$

We can follow the same procedure as before to write the final Hamiltonian. The only difference occurs in the calculation of the electron-polarization interaction since now $\phi(\mathbf{r})\neq 0$ on the surface. We have

$$\begin{aligned}
H_{el-ph} = -e\sum_{m=0}^{\infty}\sum_{i=1}^{\infty}\sum_q\frac{c_{miq}}{R_0}\frac{\exp(iqz)}{\sqrt{L}}\exp(im\varphi)\\
\cdot\Bigg[J_m\left(\chi_{mi}\frac{\rho}{R_0}\right) - J_m(\chi_{mi})I_m(qR_0)\\
\times qR_0K_m^{'}(qR_0)\Bigg]
\end{aligned} \tag{49}$$

where $I_m(x)$ and $K_m(x)$ are the modified Bessel functions and $K_m^{'}(x) = \frac{dK_m(x)}{dx}$. The new electron phonon interaction becomes

$$H_{el-ph} = -\sum_{miq}\Bigg[U_{miq}\frac{\exp(iqz)}{R_0}\exp(im\varphi)a^{\dagger}_{miq} \cdot\Bigg\{J_m\left(\chi^{'}_{mi}\frac{\rho}{R_0}\right) - J_m\left(\chi_{mi}\right)I_m(qR_0) \times qR_0K^{'}_m(qR_0)\Bigg\} + h.c.\Bigg] \quad (50)$$

where

$$U_{miq} = e\sqrt{\frac{2\hbar\omega_L}{L}}\sqrt{\frac{1}{\varepsilon^*}}\frac{1}{\left[J_m(\chi^{'}_{mi})^2\left(1-\frac{m^2}{\chi^{'2}_{mi}}\right)\left(\frac{\chi^{'2}_{mi}}{R_0^2}+q^2\right)\right]^{\frac{1}{2}}}. \quad (51)$$

We have found that the expression of the electron-phonon interaction depends on the basis used to calculate it. The choice of the basis depends on the physical boundary conditions acting on the wire.

Finally, to treat the case of an electron constrained to move in a quantum wire embedded in the infinite medium of the same material, we start from the Fröhlich Hamiltonian in the three-dimensional space

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + \hbar\omega_l\sum_{\mathbf{k}}a^{\dagger}_{\mathbf{k}}a_{\mathbf{k}} + \sum_{\mathbf{k}}\left[\frac{Z}{k}\exp\left(i\mathbf{k}\cdot\mathbf{r}\right)a_{\mathbf{k}} + h.c.\right] \quad (52)$$

where $Z = -i\left(4\pi\alpha R_p/L^3\right)^{\frac{1}{2}}\hbar\omega_L$, $\mathbf{k}$ and $\mathbf{r} = (\rho, z)$ are the wave vector and the electron position respectively and L is the linear dimension of the polar medium. We write the polaron Hamiltonian in cylindrical coordinates through the unitary transformation

$$a_{\chi,k_z,n} = \sqrt{\frac{\chi}{2\pi}}\int_0^{2\pi}d\varphi\exp(in\varphi)a_{\mathbf{k}} \quad (53)$$

with $\mathbf{k}\equiv(\chi\cos\varphi, \chi\sin\varphi, k_z)$. It is found that

$$a_{\mathbf{k}} = \frac{1}{\sqrt{2\pi\chi}}\sum_{n=-\infty}^{\infty}\exp(-in\varphi)a_{\chi,k_z,n} \quad (54)$$

and

$$\left[a_{\chi,k_z,n}, a^{\dagger}_{\chi^{'},k^{'}_z,n^{'}}\right] = \delta(\chi-\chi^{'})\delta(k_z-k^{'}_z)\delta_{n,n^{'}} \quad (55)$$

where $\delta(x)$ and $\delta_{n,n^{'}}$ are the Dirac and Kronecker δ functions. In this representation the polaron Hamiltonian becomes

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + \hbar\omega_L\sum_{\chi,k_z,n}a_{\chi,k_z,n}a^{\dagger}_{\chi,k_z,n} + \sum_{\chi,k_z,n}\Bigg[\sqrt{2\pi}Z\frac{\sqrt{\chi}}{\sqrt{\chi^2+k_z^2}}i^n\exp(ik_zz) \times J_n\left(\chi\varrho\right)a_{\chi,k_z,n} + h.c.\Bigg] \quad (56)$$

where $\sum_{k_z}\rightarrow\frac{L}{2\pi}\int dk_z$ and $\sum_{\chi}\rightarrow\left(\frac{L}{2\pi}\right)^2\int d\chi$.

In all the cases discussed we find that $\nabla\cdot\mathbf{P} = \frac{1}{4\pi}\nabla^2\phi \neq 0$ in the wire, indicating that the induced charges concern all the material. These cases are different from the surface polarization discussed at the end of the previous section.

4 The polaron ground state

4.1 The calculation of the polaron energy

Since the interaction Hamiltonians (46), (50) and (56) have similar forms, we proceed to the explicit calculation of the polaron energy only in the first case. The Hamiltonian (45) is transformed using two unitary transformation: the first one $\exp(S)$ takes into account the rotational symmetry of the system while the second one $\exp(S_1)$ is a coordinate dependent Lee, Low and Pines transformation [55,56]

$$S = i\varphi\sum_{miq}ma^{\dagger}_{miq}a_{miq}. \quad (57)$$

and

$$S_1 = \sum_{miq}\left(g^*_{miq}(\rho,z)a_{miq} - g_{miq}(\rho,z)a^{\dagger}_{miq}\right) \quad (58)$$

In Appendix A we present the details of the calculation and write the polaron energy E_p

$$\begin{aligned}E_p &= \langle\Phi(\rho,z)\mid H_p\mid\Phi(\rho,z)\rangle \\ &= \frac{\hbar^2}{2m^*}\Bigg[\langle\Phi\mid -\frac{\partial^2}{\partial\rho^2} - \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{\partial^2}{\partial z^2}\mid\Phi\rangle \\ &\quad +\langle\Phi\mid\left(\sum_{miq}\left|\frac{\partial g_{miq}(\rho,z)}{\partial\rho}\right|^2 + \sum_{miq}\left|\frac{\partial g_{miq}(\rho,z)}{\partial z}\right|^2\right)\mid\Phi\rangle \\ &\quad +\langle\Phi\mid\frac{1}{\rho^2}\sum_{miq}m^2\mid g_{miq}(\rho,z)\mid^2\mid\Phi\rangle\Bigg] \\ &\quad +\hbar\omega_L\langle\Phi\mid\sum_{miq}\mid g_{miq}(\rho,z)\mid^2\mid\Phi\rangle \\ &\quad +\langle\Phi\mid\sum_{miq}\Bigg[V_{miq}J_m\left(\chi_{mi}\frac{\rho}{R_0}\right)\frac{f_{miq}(z)}{R_0} \times g^*_{miq}(\rho,z) + c.c\Bigg]\mid\Phi\rangle. \end{aligned} \quad (59)$$

We determine the polaron ground state energy through the variational method using a trial wave function $\Phi(\rho,z)$ defined only in the wire, independent of φ and such that $\Phi\left(R_0,z\right) = 0$. Its form will be specified later. The procedure we follow is as follow. From the explicit form of $E_p = \langle\Phi(\rho,z)\mid H_p\mid\Phi(\rho,z)\rangle$, we write the Euler equations

$$\frac{\delta E_p}{\delta g^*_{miq}(\rho,z)} = 0 \quad (60)$$

whose solutions give $g_{miq}(\rho, z)$. Inserting these in the expression of E_p and using a suitable form for the wave function $\Phi(\rho, z)$, we can minimize the total energy with respect to the parameters contained in $\Phi(\rho, z)$. The explicit form of the Euler equations is

$$-\frac{\hbar^2}{2m^*}\left[\frac{\partial^2 g_{miq}}{\partial\rho^2}+\left(\frac{1}{\mid\Phi\mid^2}\frac{\partial\mid\Phi\mid^2}{\partial\rho}+\frac{1}{\rho}\right)\frac{\partial g_{miq}}{\partial\rho}+\frac{\partial^2 g_{miq}}{\partial z^2}+\frac{1}{\mid\Phi\mid^2}\frac{\partial\mid\Phi\mid^2}{\partial z}\frac{\partial g_{miq}}{\partial z}-\frac{m^2}{\rho^2}g_{miq}\right]+\hbar\omega_L g_{miq}=-V_{miq}J_m\left(\chi_{mi}\frac{\rho}{R_0}\right)\frac{\exp(iqz)}{R_0}. \quad (61)$$

An important point is that these equations depend on the electronic wave function, indicating that there is an influence of the electron state on the phonons distribution functions and vice versa. The trial wave function is taken of the form

$$\Phi(\rho,z)=\frac{1}{R_0}\left[c_1 J_0\left(\chi_1\frac{\varrho}{R_0}\right)+c_2 J_0\left(\chi_2\frac{\varrho}{R_0}\right)\right]\frac{\exp(i\bar{Q}z)}{\sqrt{L}} \quad (62)$$

where χ_1 and χ_2 are the first two zeros of $J_0(x)$ and c_1 and c_2 are normalization factors given by

$$c_1=\pm\frac{1}{|J_0'(\chi_1)|}\left[\frac{1}{\pi}-\left(c_2 J_0'(\chi_2)\right)^2\right]^{\frac{1}{2}}$$
$$|c_2|\le\frac{1}{\sqrt{\pi}|J_0'(\chi_2)|}. \quad (63)$$

The form (62) of the wave function contains contributions from higher energy electronic subbands. However, in all our calculations we have systematically found that the lowest energy is obtained when $c_2 = 0$; in other words, the best trial wave function is

$$\Phi(\rho,z)=\frac{1}{R_0}\frac{1}{\sqrt{\pi}}\frac{1}{|J_0'(\chi_1)|}J_0\left(\chi_1\frac{\varrho}{R_0}\right)\frac{\exp(i\bar{Q}z)}{\sqrt{L}}. \quad (64)$$

In Appendix B we show how to solve equation (61) using the trial wave function (64). Since $\frac{\partial|\Phi|^2}{\partial z}=0$, the main technical difficulty is the complicated electron coordinates dependence of the coefficient of the terms $\frac{\partial g_{miq}}{\partial\rho}$. A way to address this problem is the substitution of $\frac{R_0}{|\Phi|^2}\frac{\partial|\Phi|^2}{\partial\rho}$ with $\langle\Phi|\frac{R_0}{|\Phi|^2}\frac{\partial|\Phi|^2}{\partial\rho}|\Phi\rangle$. What we are doing is a sort of mean field approximation for taking into account the influence of the electron wave function on the phonon distribution functions. In the framework of the Fröhlich electron-phonon interaction, the same approximation has been used, with success, in the calculation of the ground state and of some excited states both in the polaronic exciton and bipolaron problems [56]. The final result is

$$g_{miq}(u,z)=V_{miq}\frac{2m^*}{\hbar^2}\exp(iqz)R_0 v_{mi}(u) \quad (65)$$

where

$$v_{mi}(u)=u^{|m|}\exp\left(\frac{\Gamma-\Lambda}{2}u\right)\frac{\Gamma(a)}{\Gamma(b)\Lambda^{1-b}}\cdot[-M(a,b,\Lambda u)\times\int_u^1 dy y^{b-|m|}\exp\left[-\left(\frac{\Gamma+\Lambda}{2}y\right)\right]U(a,b,\Lambda y)\times J_m(\chi_{mi}y)+\frac{U(a,b,\Lambda)}{M(a,b,\Lambda)}M(a,b,\Lambda u)\times\int_0^1 dy y^{b-|m|}\exp\left[-\left(\frac{\Gamma+\Lambda}{2}y\right)\right]M(a,b,\Lambda y)\times J_m(\chi_{mi}y)-U(a,b,\Lambda u)\times\int_0^u dy y^{b-|m|}\exp\left[-\left(\frac{\Gamma+\Lambda}{2}y\right)\right]M(a,b,\Lambda y)\times J_m(\chi_{mi}y)] \quad (66)$$

and where

$$\Gamma=-\langle\frac{R_0}{\mid\Phi\mid^2}\frac{\partial\mid\Phi\mid^2}{\partial\rho}\rangle, Q^2=\frac{R_0^2}{R_p^2}+(qR_0)^2$$
$$R_p=\left(\frac{\hbar}{2m^*\omega_L}\right)^{\frac{1}{2}}, a=\mid m\mid+\frac{1}{2}+\frac{\Gamma}{2\Lambda}$$
$$b=2\mid m\mid+1, \Lambda=\sqrt{\Gamma^2+4Q^2}. \quad (67)$$

Here $M(a,b,x)$, $U(a,b,x)$ and $\Gamma(x)$ are two independent hypergeometric confluent functions and $\Gamma(x)$ the Gamma function [57] respectively. Since $g_{miq}(u,z)$ is calculated through an inhomogeneous differential equation, we need additional boundary conditions; in this case we imposed in equation (66) that $v_{mi}(u)$ is regular at $u = 0$ and $v_{mi}(1) = 0$

A similar procedure can be used to calculate the ground state energy of the Hamiltonian (56). We find

$$E_p=-\frac{\hbar^2}{2m^*}\langle\Phi|\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{\partial^2}{\partial z^2}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right]|\Phi\rangle+\langle\Phi|V_p(\rho,z)|\Phi\rangle \quad (68)$$

where the effective potential V_p is defined as

$$V_p(\rho,z)=\frac{\hbar^2}{2m^*}\sum_{\chi,k_z,n}\left(\left|\frac{\partial g_{\chi,k_z,n}(\rho,z)}{\partial\rho}\right|^2+\left|\frac{\partial g_{\chi,k_z,n}(\rho,z)}{\partial z}\right|^2\right)+\hbar\omega_l\sum_{\chi,k_z,n}\mid g_{\chi,k_z,n}(\rho,z)\mid^2+\sum_{\chi,k_z,n}[V_{\chi,k_z,n}J_n(\chi\rho)\exp(ik_z z)\, g_{\chi,k_z,n}(\rho,z)+c.c.] \quad (69)$$

with

$$V_{\chi,k_z,n}=i^{n+1}\left(\frac{8\pi^2\alpha R_p}{L^3}\right)^{\frac{1}{2}}\hbar\omega_L\frac{\sqrt{\chi}}{\sqrt{\chi^2+k_z^2}}. \quad (70)$$

We can write and solve the Euler equations in the same approximation obtaining

$$g_{\chi,k_z,n}(\rho,z)=\frac{2m*}{\hbar^2}R_0^2 V^*_{\chi,k_z,n}\exp(-ik_z z)v_n(u) \quad (71)$$

with

$$v_n(u) = \exp\left(\frac{\Gamma-\Lambda}{2}u\right)\Gamma(a) \cdot \left[-M(a,1,\Lambda u)\int_u^\infty dyy\exp\left[-\left(\frac{\Gamma+\Lambda}{2}y\right)\right] \times U(a,1,\Lambda y)J_n(\chi R_0 y) \times -U(a,1,\Lambda u)\int_0^u dyy\exp\left[-\left(\frac{\Gamma+\Lambda}{2}y\right)\right] \times M(a,1,\Lambda y)J_n(\chi R_0 y)\right] \quad (72)$$

where a, Γ, Λ and u defined above as the hypergeometric functions $M(a,1,x)$ and $U(a,1,x)$. In this case we solve equation (72) with the boundary conditions that $v_n(u)$ is regular at $u = 0$ and $v_n(\infty) = 0$. In the case of the Hamiltonian (49) with the electron-phonon interaction given by equation (50) the solution is similar to that obtained in equation (66).

4.2 Numerical results

We have calculated the polaron self-energy using the Hamiltonian (45) both with the electron-phonon given by the equations (46) and (50), and the Hamiltonian (56) using always the trial wave function of equation (64). If we calculate the quantity $\frac{2m^*E_p}{\hbar^2}$, the geometric and material polarity parameters entering in the Hamiltonian are the cylinder radius R_0, the electron-phonon coupling constant α and the polaron radius R_p. In such units the free electron first subband is given by χ_{01}^2/R_0^2. In Figure 1 we show the main result of the work, i.e. the quantity $\frac{\Delta E_p}{\alpha} = -\frac{1}{\alpha}\left(E_p - \frac{\chi_{01}^2}{R_0^2}\right)$ as function of R_0 for a fixed value of R_p using the different polaron Hamiltonians described in the previous sections. In particular, the full line gives $\frac{\Delta E_p}{\alpha}$ using the electron-phonon interaction (46) with the boundary condition $g_{miq}(R_0,z) = 0$; the dashed line gives the same quantity with the same Hamiltonian and boundary condition, but taking into account the dependence on R_0 of the bulk high frequency dielectric constant (see later); the dash-dotted line gives $\frac{\Delta E_p}{\alpha}$ calculated with the Hamiltonian (56) with the boundary condition $g_{\chi,k_z,n}(R_0,z) = 0$ and finally the dotted line gives the same quantity with the same Hamiltonian and the boundary condition

$$g_{\chi,k_z,n}(\infty,z) = 0.$$

We find the following features: (a) $\frac{\Delta E_p}{\alpha}$ is an increasing function of R_0 when we use the the electron-phonon interaction (46) and the boundary condition $g_{miq}(R_0,z) = 0$; (b) the asymptotic value of all lines is the bulk polaron self-energy; (c) $\frac{\Delta E_p}{\alpha}$ is an increasing (decreasing) function for $R_0 \lesssim R_p$ ($R_0 \gtrsim R_p$) when we use the Hamiltonian (56) with the boundary condition $g_{\chi,k_z,n}(R_0,z) = 0$; (d) $\frac{\Delta E_p}{\alpha}$ is a decreasing function of R_0 when we use the Hamiltonian (56) with the boundary condition $g_{\chi,k_z,n}(\infty,z) = 0$;

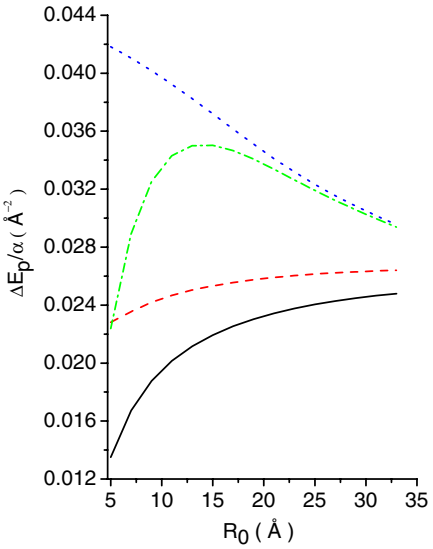

Fig. 1. The quantity $\frac{\Delta E_p}{\alpha}$ (in units Å^{-2}) as function of R_0 for $R_p = 5.11$ Å using: (a) the Hamiltonian (45) and the boundary conditions $g_{miq}(R_0,z) = 0$ (full line); (b) the same as (a), but taking into account the dependence on the dimension of the dielectric constants (dashed line); (c) Hamiltonian (56) and the boundary conditions $g_{miq}(R_0,z) = 0$ (dash-dotted line); (d) the same as (c) with the boundary condition $g_{miq}(\infty,z) = 0$ (dotted line).

(e) the reduction of the high frequency dielectric in the confined systems implies an increase of the electron-phonon interaction. We conclude that the polaron effects are strongly dependent on the boundary condition imposed at the surface. These results are coherent with those found in the literature [51,49]. We remark that in principle even R_p and α depend on R_0 through ω_L, but we did not consider this point. Both α and R_p are decreasing function of R_0 so that ΔE_p should show a greater derivative as function of R_0.

We have also calculated the same quantity $\frac{\Delta E_p}{\alpha}$ as function of R_0 for the same value of R_p of Figure 1 using the Hamiltonian (49) with the electron-phonon given by the equation (50). The result, shown in Figure 2, is found considering the boundary condition $g_{miq}(R_0,z) = 0$. We find that the self-energy is lower than those shown in Figure 1, because the discontinuity at the surface of $\phi(\mathbf{r})$ determines an extra potential acting on the electron.

The good convergence of the numerical procedures has been checked varying m_m (the largest index of the Bessel functions taken into account, for example, in Eq. (36)) and i_m (the largest number of zeros for each Bessel function considered). In the cases of Figures 1 and 2 we have found that an excellent convergence is obtained with $m_m = 20$ and $i_m = 20$. However, bad convergence is obtained if the polaron radius R_p becomes largest than 10 Å.

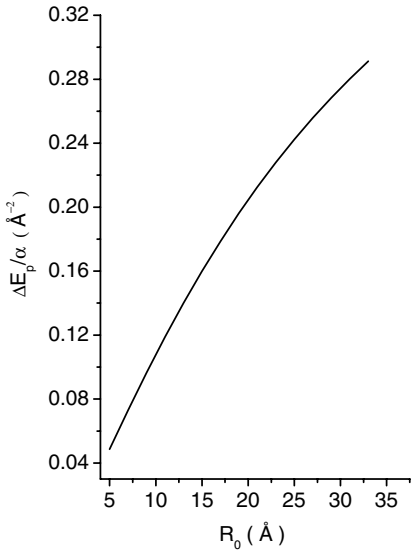

Fig. 2. $\frac{\Delta E_p}{\alpha}$ (in units Å^{-2}) as function of R_0 for R_p = 5.11 Å using the Hamiltonian (50) with the boundary condition $g_{miq}(R_0, z) = 0$.

For what it concerns the dependence of $\varepsilon_\infty(0,0)$ on the wire radius, we have used the empirical formula

$$\varepsilon_\infty(0,0) = \varepsilon_\infty \left(1 - \frac{a}{R_0} - \frac{b}{R_0^2}\right)$$

which well fits numerical results [54]. In our explicit calculation we take $a = 2$ Å and $b = 0.2$ Å^2.

This formula has been obtained from the numerical results for the electronic dielectric constants (transverse and longitudinal) of a rotational ellipsoid with axes c (rotational axis) and a, where these are calculated as function of the parameter $\chi = \frac{c}{a}$ with fixed value of a. When $\chi \to \infty$ we obtain the dielectric constants of the wire of radius a. We have also verified that the calculation done on the wire gives the same result (unpublished). A large work has been done on the ellipsoidal dot [22,23,54], because in the range $1 \leq \chi < \infty$ and a fixed we have the crossover from the spherical dot to the cylindrical one and in the range $0 \leq \chi \leq 1$ and c fixed we have the crossover from a slab of material with thickness $2c$ to the spherical dot. We have solved the Schrödinger equation for an electron localized in the ellipsoidal dot and we have studied how the ground and the excited states depend on χ. Moreover, since $\nabla \cdot \mathbf{P} = \frac{1}{4\pi}\nabla^2\phi \neq 0$ in the wire, we can say that the dielectric constants of an ellipsoidal dot, changing with care the geometrical parameters, can describe all the situation from that of a slab to that of the cylinder, included that of the sphere. We stress that in Section 2 we found that for the surface polarization modes $\nabla \cdot \mathbf{P} = 0$ in the wire, so that the dielectric constant should show, in this case, a crossover between the two-dimensional and the one-dimensional features [58].

A complete analysis of the polaron effect in a cylindrical wire should include also the contribution coming out from the surface polarization modes, as it was done in the work [59]. We have not done explicit calculations for this last contribution, but we can give a qualitative conclusion on this point, since in the work [49] we considered this point. We found that the volume polaron effects increases with R_0, whereas the surface ones decreases. In this work we have found the same features for the volume polaron, so that we think that same should occur also for the surface contributions. In any case explicit calculations could be done, considering also different boundary condition for the phonon distribution function.

We summarize the results obtained in this section saying that the results of Figure 2 regard the polaron effects in a cylindrical sample when on the surface there is a distribution of microscopic dipoles and that the phonon distribution function is zero on the surface. The results of Figure 1 regard a more common physical situation in which we have an electron constrained to be in a wire embedded in a matrix of the same material. In the first case we have induced charges on the surface and in the wire and in the second one we have induced charges in all the space. These two situations are described by suitable boundary conditions for the distribution function of the phonons. If the wire is embedded in a different material, the polaron self-energy is first an increasing and then a decreasing function of R_0; if the wire is embedded in a matrix of the same material, the polaron selfenergy is a decreasing function of R_0. Furthermore we have found that the dependence on the cylinder radius of the dielectric constants increases the polaron selfenergy.

5 Conclusion

In this work we have shown that in the continuous model of a cylindrical confined system, the dispersive dielectric function depends on the cylinder radius. A first contribution comes from the spatial dispersive terms of the bulk dielectric function and a second one has been found in the high frequency dielectric function, even if the spatial dispersive terms are neglected. In any case, the ratio between the full dielectric constant and the high frequency one does not depend on the wire dimension. The consequence of these facts is that the Fröhlich electron-phonon coupling increases on decreasing the cylinder radius.

We have calculated the electron-phonon interaction considering different boundary conditions on polarization field showing that one may have different polaron Hamiltonian. We have calculated polaron self-energies taking also into account the contribution of the boundary condition on the phonon distribution and the electronic wave function. The final result is that the self-energy can increase or decrease as a consequence of both the boundary condition and the dimension dependent electron-phonon coupling.

Appendix A

We consider the polaron Hamiltonian given in equation (45). Since the Hamiltonian is invariant for rotation around the z-axis, we perform the unitary transformation

$$H_1 = \exp(-S) H \exp(S) \tag{73}$$

with

$$S = i\varphi \sum_{miq} m a^{\dagger}_{miq} a_{miq}. \tag{74}$$

We obtain

$$\begin{aligned} H_1 = &-\frac{\hbar^2}{2m^*}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial z^2}\right. \\ &\left. + \frac{1}{\rho^2}\left(\frac{\partial^2}{\partial\varphi^2} + 2\frac{\partial S}{\partial\varphi}\frac{\partial}{\partial\varphi} + \left(\frac{\partial S}{\partial\varphi}\right)^2\right)\right] \\ &+ \sum_{miq} \hbar\omega_L \left(a^{\dagger}_{miq} a_{miq} + \frac{1}{2}\right) \\ &- \sum_{miq}\left[V_{miq} J_m\left(\chi_{mi}\frac{\rho}{R_0}\right)\right. \\ &\left. \times \frac{\exp(iqz)}{R_0} a\,\dagger_{miq} + h.c.\right]. \end{aligned} \tag{75}$$

We introduce now the generalized Lee, Low and Pines unitary transformation [52] to extract the polaron effects in the self-energy through

$$H_2 = \exp(-S_1) H_1 \exp(S_1) \tag{76}$$

with

$$S_1 = \sum_{miq}\left(g^*_{miq}(\rho, z) a_{miq} - g_{miq}(\rho, z) a^{\dagger}_{miq}\right). \tag{77}$$

We obtain

$$\begin{aligned} H_2 = &-\frac{\hbar^2}{2m^*}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + 2\frac{\partial S_1}{\partial\rho}\frac{\partial}{\partial\rho} + \frac{\partial^2 S_1}{\partial\rho^2} + \left(\frac{\partial S_1}{\partial\rho}\right)^2\right. \\ &+ \frac{\partial^2}{\partial z^2} + 2\frac{\partial S_1}{\partial z}\frac{\partial}{\partial z} + \frac{\partial^2 S_1}{\partial z^2} + \left(\frac{\partial S_1}{\partial z}\right)^2 \\ &\left. + \frac{1}{\rho^2}\left(\frac{\partial^2}{\partial\varphi^2} + 2\frac{\partial S_2}{\partial\varphi}\frac{\partial}{\partial\varphi} + \left(\frac{\partial S_2}{\partial\varphi}\right)^2\right)\right] \\ &+ \sum_{miq}\hbar\omega_L\left[\left(a^{\dagger}_{miq} - g^*_{miq}(\rho, z)\right)\left(a_{miq} - g_{miq}(\rho, z)\right)\right. \\ &\left. + \frac{1}{2}\right] - \sum_{miq}\left[V_{miq} J_m\left(\chi_{mi}\frac{\rho}{R_0}\right)\frac{\exp(iqz)}{R_0}\right. \\ &\left. \times \left(a\,\dagger_{miq} - g^*_{miq}(\rho, z)\right) + h.c.\right] \end{aligned} \tag{78}$$

with

$$\begin{aligned} S_2 &= \exp(-S_1) S \exp(S_1) \\ &= i\sum_{miq} m\varphi\left(a^{\dagger}_{miq} - g^*_{miq}(\rho, z)\right)\left(a_{miq} - g_{miq}(\rho, z)\right). \end{aligned} \tag{79}$$

In this work we are interested only to the ground state of the polaron, when no real phonon is present in the system. We define

$$\begin{aligned} H_p = \langle 0 \mid H_2 \mid 0\rangle = \\ &-\frac{\hbar^2}{2m^*}\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \sum_{miq}\left|\frac{\partial g_{miq}(\rho, z)}{\partial\rho}\right|^2 + \frac{\partial^2}{\partial z^2}\right. \\ &- \sum_{miq}\left|\frac{\partial g_{miq}(\rho, z)}{\partial z}\right|^2 \\ &\left. + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} - \sum_{miq} m^2 \mid g_{miq}(\rho, z) \mid^2\right] \\ &+ \hbar\omega_L \sum_{miq} \mid g_{miq}(\rho, z) \mid^2 \\ &+ \sum_{miq}\left[V_{miq} J_m\left(\chi_{mi}\frac{\rho}{R_0}\right)\frac{f_{miq}(z)}{R_0} g^*_{miq}(\rho, z) + c.c.\right]. \end{aligned} \tag{80}$$

This is the Hamiltonian of a particle with a potential due to the polarisation in the wire. We write

$$H_p = -\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial z^2} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right) + V_p(\rho, z) \tag{81}$$

where

$$\begin{aligned} V_p(\rho, z) = &\frac{\hbar^2}{2m^*}\sum_{miq}\left(\left|\frac{\partial g_{miq}(\rho, z)}{\partial\rho}\right|^2 + \left|\frac{\partial g_{miq}(\rho, z)}{\partial z}\right|^2\right) \\ &+ \left(\frac{\hbar^2}{2m^*}\frac{1}{\rho^2}\sum_{miq} m^2 \mid g_{miq}(\rho, z) \mid^2\right. \\ &\left. + \hbar\omega_L \sum_{miq} \mid g_{miq}(\rho, z) \mid^2\right) \\ &+ \sum_{miq}\left[V_{miq} J_m\left(\chi_{mi}\frac{\rho}{R_0}\right)\frac{\exp(iqz)}{R_0}\right. \\ &\left. \times g^*_{miq}(\rho, z) + c.c.\right]. \end{aligned} \tag{82}$$

The functions $g_{miq}(\rho, z)$ determine the distribution function of the polarization modes which contribute to the total polarization and consequently to the effective potential acting on the electron. We calculate the ground state energy through the variational method as described in Section 4.

Appendix B

To solve equation (61), we make the ansatz

$$g_{miq}(\rho, z) = R_0 \exp(iqz)\bar{g}_{miq}\left(\frac{\rho}{R_0}\right) \tag{83}$$

so that the substitution gives

$$-\frac{\hbar^2}{2m^*}\left[\left(\frac{d^2\bar{g}_{miq}}{du^2}+\frac{1}{R_0}\left(\frac{R_0}{\mid\Phi\mid^2}\frac{\partial\mid\Phi\mid^2}{\partial\rho}+\frac{1}{u}\right)\frac{d\bar{g}_{miq}}{du}\right)+\left(-q^2R_0^2+\frac{R_0^2}{\mid\Phi\mid^2}\frac{\partial\mid\Phi\mid^2}{\partial z}iq-\frac{m^2}{u^2}\right)\bar{g}_{miq}\right]\exp(iqz)+\hbar\omega_L R_0^2\exp(iqz)\bar{g}_{miq})=-V_{miq}J_m\left(\chi_{mi}u\right)\exp(iqz) \tag{84}$$

where $u=\frac{\rho}{R_0}$. It can be seen that the term $\frac{1}{\Phi^2}\frac{\partial\Phi^2}{\partial\rho}$ is a function of u. It is difficult to solve the equation (84); our approximation is to substitute the coefficients of $\bar{g}_{miq}$ and its derivatives with the average values on the trial electronic wavefunction. This is a mean field approximation already used in the polaron theory [56]. In this case, since $\frac{\partial|\Phi|^2}{\partial z}=0$, we have

$$\frac{d^2\bar{g}_{miq}(u)}{du^2}+\left(\frac{1}{u}-\Gamma\right)\frac{d\bar{g}_{miq}(u)}{du}-\left(Q^2+\frac{m^2}{u^2}\right)\bar{g}_{miq}(u)=\bar{V}_{miq}J_m\left(\chi_{mi}u\right) \tag{85}$$

where the quantity Γ, Q^2, $R_p=\left(\frac{\hbar}{2m^*\omega_L}\right)^{\frac{1}{2}}$ and $\bar{V}_{miq}=V_{miq}\frac{2m^*}{\hbar^2}$ are defined through equation (67). This equation is solved using standard mathematics, since the solution of the homogeneous equation associate to equation (85) can be written in terms of two independent hypergeometric functions.

References

1. U. Woggon, *Optical Properties of Semiconductors Quantum Dots* (Springer, Berlin, 1997)
2. L. Jack, P. Hawrylak, A. Wojs, *Quantum Dots* (Springer-Verlag, Berlin, 1998)
3. A. Eychmüller, A. Mews, H. Weller, Chem. Phys. Lett. **208**, 59 (1993); A. Mews, A. Eychmüller, M. Giersig, D. Schooss, H. Weller, J. Phys. Chem. **98**, 934 (1994); A. Eychmüller, T. Vossmeyer, A. Mews, H. Weller, J. Lumin. **58**, 223 (1994)
4. J. Del Castillo, V.D. Rodriguez, A.C. Yanes, J. Mendez-Ramos, M.E. Torres., Nanotechnology **16**, S300 (2005)
5. X. Peng, L. Manna, W. Wang, J. Wickham, E. Scher, A. Kadanavich, A.P. Alivisados, Nature **404**, 59 (2000)
6. J. Lee, H.N. Spector, J. Appl. Phys. **54**, 3921 (1983); J. Lee, H.N. Spector, J. Appl. Phys. **57**, 366 (1985); J. Lee, H.N. Spector, J. Appl. Phys. **97**, 43511 (2005)
7. M.H. Degani, O. Hipolito, Phys. Rev. B **35**, 9345 (1998)
8. K. Suenaga, C. Colliex, N. Demoncy, A. Loiseau, H. Pascard, F. Willaime, Science **278**, 653 (1997); Y. Zhang, K. Suenaga, C. Colliex, S. Iijima, Science **281**, 973 (1998)
9. L.L. Yang, Z.H. Yang, W.X. Cao, L. Chen, J. Xu, H.Z. Zhang, J. Phys. Chem. B **109**, 11501 (2005)
10. G.H. Wang, K.X. Guo, Physica E **28**, 14 (2005)
11. R.A. Farrer, F.L. Butterfield, V.W. Chen, Fourkas J.YT., Nano Letters **5**, 1139 (2005)
12. Z.H. Zhong, Y. Fang, W. Lu, Lu W., Lieber C.M., Nano Letters **5**, 1143 (2005)
13. J.W. Haus, S.H. Zhou, I. Honma, H. Komiyama, Phys. Rev. B **47**, 1359 (1993)
14. K. Chang, J.B. Xia, Phys. Rev. B **57**, 9780 (1998)
15. Y. Takahashi, Y. Hayamizu, H. Itoh, M. Yoshida, H. Akiyama, N.L. Pfeiffer, K.W. West, Appl. Phys. Lett. **86**, 243101 (2005)
16. D. Ninno, G. Iadonisi, F. Buonocore, Sol. State Comm. **112**, 521 (1999)
17. Z.Y. Zeng, Y. Xiang, L.D. Zhang, Eur. Phys. J. B **17,** 699 (2000)
18. S.S.Z. Ashraf, A.C. Sharma, J. Phys.: Cond. Matt. **17**, 3043 (2005)
19. T. Enss, V. Meden, S. Andergassen, X. Barnabé-Theriault, W. Metzner, K. Schönhammer, Phys. Rev. B **71**, 155401 (2005)
20. Z. Jiang, S.Q. Duan, X.G. Zhao, Phys. Lett. A **340**, 309 (2005)
21. C. Ghosh, S. Pal, B. Goswami, P. Sarkar, Chem. Phys. Lett. **407**, 498 (2005)
22. G. Cantele, D. Ninno, G. Iadonisi, J. Phys.: Condens. Matter **12**, 9019 (2000); G. Cantele, D. Ninno, G. Iadonisi, Nano-Letters **1**, 121 (2001)
23. G. Cantele, G. Piacente, D. Ninno, G. Iadonisi, Phys. Rev. B **66**, 113308 (2002); G. Cantele, F. Trani, D.Ninno, G. Iadonisi, J. Phys.: Cond. Matt. **15**, 5715 (2003); F. Trani, G. Cantele, D.Ninno, G. Iadonisi, Physica E **22**, 808 (2004); G. Cantele, D. Ninno, G. Iadonisi, Phys. Rev. B **64**, 125325 (2001); G. Iadonisi, G. Cantele, V. Marigliano Ramaglia, D. Ninno, Phys. Status Solidi B **237**, 320 (2003)
24. H. Leon, J.L. Marin, R. Riera, Physica E **27**, 385 (2005)
25. D. Ninno, G. Iadonisi, F. Buonocore, G. Cantele, G. Di Francia, Sens. Actuators B **68**, 17 (2000); F. Buonocore, D. Ninno, G. Iadonisi, Phys. Status Solidi B **225**, 343 (2001); G. Cantele, D. Ninno, G. Iadonisi, Phys. Rev. B **61**, 13730 (2000)
26. R.C.T. da Costa, Phys. Rev. A **23**, 1982 (1981)
27. H. Aoki, M. Koshino, D. Takeda, H. Morise, K. Kuroki, Phys. Rev. B **65**, 35102 (2002)
28. G. Parascandolo, G. Cantele, D. Ninno, G. Iadonisi, Phys. Rev. B **68**, 245318 (2003)
29. H. Fröhlich, Adv. Phys. **3**, 325 (1954)
30. J. Licari, R. Evrard, Phys. Rev. B **15**, 2254 (1977)
31. L. Wendler, R. Haupt, Phys. Stat. Sol. (b) **143**, 487 (1987)
32. N. Mori, T. Ando, Phys. Rev. B **43**, 5155 (1991)
33. J.J. Shi, S. Ling-Xi, S. Pan, Phys. Rev. B **51**, 17681 (1995)
34. Z.W. Yan, X.X. Liang, Int. J. Mod. Phys. B **15**, 3539 (2001)
35. S. Yu, K. W. Kim., J. Appl. Phys. **82**, 3363 (1997)
36. K. Huang, B. Zhu, Phys, Rev. B **38**, 13377 (1988)
37. M.A. Stroscio, K.W. Kim, M.A. Littlejohn, H. Chuang, Phys. Rev. B **42**, 1488 (1990)
38. C.R. Bennett, N.C. Constantinou, M. Babiker, B.K. Ridley, J. Phys.: Cond. Matt. **7**, 9819 (1995)
39. P.A. Knipp, T.L. Reinecke, Phys. Rev. B **48**, 5700 (1993)
40. K.S. Klimin, E.P. Pokatilov, F.M. Fomin, Phys. Stat. Sol. (b) **184**, 373 (1994)
41. R. Fuchs, K.L. Kliever, Phys. Rev. **140**, A2076 (1985)
42. S.F. Ren, Y.C. Chang, Phys. Rev B **43**, 11857 (1991)
43. B. Zhu, Phys. Rev. B **44**, 1926 (1991)

44. F. Rossi, L. Rota, P. Lugli, E. Molinari, Phys. Rev. B **47**, 1695 (1993); H. Rucker, E. Molinari, P. Lugli, Phys. Rev. B **44**, 3463 (1991); H. Rucker, E. Molinari, P. Lugli, Phys. Rev. B **45**, 6747 (1992)
45. H.J. Xie, C.Y. Chen, B.K. Ma, Phys. Rev. B, **61**, 4827 (2000); H.J. Xie, C.Y. Chen, B.K. Ma, J. Phys.: Cond. Matt. **12**, 8623 (2000)
46. L. Zhang, X.J. Xie, C.Y. Chen, Phys. Rev. B **66**, 205326 (2002); Commun. Theor. Phys. **39**, 238 (2003); Li Zhang, H.J. Xie, Int. J. Mod. Phys. B **18**, 379 (2004)
47. F. Comas, C. Trallero-Giner, A. Cantarero, Phys. Rev. B **47**, 7602 (1993); F. Comas, C. Trallero-Giner, M. Moshinski, J. Phys. Cond. Matt. **7**, 1789 (1995)
48. J.M. Bergues, R. Betancourt-Riera, R. Riera, J.L. Marin, J. Phys.: Cond. Matt. **12**, 7983, (2000)
49. F. Buonocore, G. Iadonisi, D. Ninno, F. Ventriglia, Phys. Rev. B **65**, 205415 (2002)
50. A. Ercelebi, R.T. Senger, Phys. Rev. B **53**, 11008 (1996)
51. E.P. Pokatilov, V.M. Fomin, J.T. Devreese, S.N. Balaban, S.N. Klimin, Physica E **4**, 156 (1999)
52. M. Babiker, J. Phys. C **19,** 683 (1988)
53. N.C. Constantinou, B.K. Ridley, Phys. Rev. B **41**, 10622 (1990)
54. F. Trani, G. Cantele, D. Ninno, G. Iadonisi, Phys. Rev. B **72**, 75423 (2005)
55. T.D. Lee, F. Low, D. Pines, Phys. Rev. **90**, 297 (1953)
56. G. Iadonisi, F. Bassani, G. Strinati, Physica Status Solidi (b) **153** (611), 1989; F. Bassani, M. Geddo, G. Iadonisi, D. Ninno, Phys. Rev. B **43**, 5296 (1991)
57. M. Abramowitz, I.A. Stegun, *Hanbook of Mathematical Functions*, (Dover Publications, Inc., N.Y., 1972)
58. O. Sato, Y. Tanaka, M. Kobayashi, Phys. Rev. B **48**, 1947 (1993)
59. G.Q. Hai, F.M. Peeters, J.T. Devreese, Phys. Rev. B **48**, 4666 (1993)