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Fractional-dimensional space approach for parabolic-confined polarons

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Abstract

We study polarons confined in parabolic quantum wells and parabolic quantum well wires within the framework of the fractional-dimensional space approach. In this scheme, the real confined 'polaron plus parabolic confining potential' system is mapped into an effective fractional-dimensional bulk in which the polaron behaves in an unconfined way, and the fractional dimension is essentially related to the degree of confinement of the actual system. We find analytical expressions which allow a very simple estimation of the corresponding polaron corrections. The fractional-dimensional theoretical results are shown to be in overall agreement with previous, more detailed, calculations.

1. Introduction

Recent remarkable progress in device physics has made it possible to fabricate a wide variety of low-dimensional semiconductor systems. A great deal of research effort has been devoted to the study of these structures because of their potential applications in a wide range of electronic and optoelectronic devices. In particular, the electron–LO–phonon interaction leading to the polaron effect may be significantly modified by the confinement (e.g. it is well established that both the binding energy and the effective mass of the polaron increase as the confinement increases). These modifications in the polaron effect can strongly influence the optical and transport properties of the heterostructures. The polaron has therefore been the subject of intense investigations for a long time.

At earlier stages, polarons in bulk material have been investigated and a wide variety of mathematical techniques have been applied to the study of the polaron problem (see, for example [1, 2]). The polaron effects in heterostructures are, however, quite different from those in bulk materials. In the former case, a variety of phonon modes arises as a consequence of the presence of the heterointerfaces. The separation of optical phonons in a slab into confined and interfaces modes was, firstly, performed in [3, 4]. The studies of bulk-like phonon modes [5], slab modes [6], interface or surface modes [5], and coupled modes [7] in semiconductor quantum wells have also been the subject of intense research. In these low-dimensional systems, the phonon spectrum and the electron–phonon interaction were found to be strongly dependent on both the geometrical shape and the parameters of the constituent materials (see, for example [8, 9]). Consequently, a rigorous treatment of the electron–phonon interaction in such heterostructures requires the consideration of the different phonon modes as well as the geometrical configuration of the system. The polaron problem in quantum wells then becomes too complicated [8–15]. In systems with parabolic confinement, the situation becomes more simple, since the interaction with interface phonons can be ignored because of the absence of an abrupt interface [16]. This simplification makes it possible to obtain the polaron corrections in parabolic quantum dots within second-order perturbation theory in an analytical way [17]. Nevertheless, the polaronic corrections in parabolic quantum wells (PQWs) and parabolic quantum well wires (PQWWs) cannot be obtained in a simple analytical form [10, 18]. The purpose of this paper is to formulate a simplified model to estimate, analytically, the polaron corrections in PQWs and PQWWs, within a reasonable accuracy.

Of particular interest to this paper is the original approach proposed by He [19, 20]. In this approach the anisotropic (or confined) interactions in the real three-dimensional (3D) space are treated as isotropic (or unconfined) interactions in an effective fractional-dimensional environment, which dimension constitutes a measure of the degree of anisotropy (or confinement) of the actual physical system. The main advantage of this approach lies in the fact that all the information about a perturbation (confinement or anisotropy)

can be introduced in a single value—the dimensionality. Thus, given this simple value, the real system can be modelled in a simple analytical way. In the past few years, the fractional-dimensional space approach has been successfully used in modelling exciton [21–26], magnetoexciton [27–30], biexciton [31, 32] and impurity states [25, 33, 34] in semiconductor heterostructures. The Stark shift of excitonic complexes [35] and the refractive index in quantum well structures [36] have also been studied within the fractional-dimensional space approach.

In this paper we extend the fractional-dimensional space formalism to the case of polarons confined in PQWs and PQWWs. Thus, the real confined 'polaron plus parabolic confining potential' system is mapped into an effective fractional-dimensional bulk in which the polaron behaves in an unconfined way, and the fractional dimension is essentially related to the degree of confinement of the actual system. The paper is organized as follows. In section 2, we present the Fröhlich-like Hamiltonian describing the electron–LO–phonon interaction in a fractional-dimensional space. The corresponding fractional-dimensional polaronic corrections in the weak-coupling limit are obtained in section 3, within second-order perturbation theory. In section 4, the polaron binding energy and effective mass in a PQW are obtained for varying the inverse parabolic well confinement frequency. The results are compared with the results reported by other researchers. In section 5, we consider the polaron problem in a PQWW, and we compare our results with calculations by other authors. Finally, conclusions are summarized in section 6.

2. The electron–phonon Hamiltonian in fractional-dimensional spaces

A Fröhlich-like Hamiltonian describing the electron–phonon interaction in a D-dimensional space was proposed years ago by Peeters *et al* [37]. Basically, the authors used the properties of vector spaces in funding the coupling coefficient of the electron–phonon interaction. However, the fractional-dimensional space is not, in general, a vector space [38]. This fact, at first sight, makes us question the validity of the procedures used in [37] when extending the dimensional parameter to non-integer values. Nevertheless, one can straightforwardly demonstrate that the use of vector properties in obtaining the coupling coefficient of the electron–phonon interaction can be avoided by introducing the definition of fractional-dimensional Fourier transform [38]. Thus, the results obtained by Peeters *et al* [37] can actually be extended to fractional values of the dimension, as will be shown.

It is worth remarking that, although the fractional-dimensional space is not, in general, a vector space, one can trace a certain number of mutually perpendicular lines. A remarkable fact is that, for non-integer values of the dimension D of the space, the maximal number s of mutually perpendicular lines can even be greater than D (see [38]). Of course, when D is an integer we have $D = s$. The set of s mutually perpendicular lines can then be regarded as a set of orthogonal axes along which we can define certain *pseudocoordinates*. Thus, it is possible to describe the position of the electron by introducing an s-component *pseudovector* $\boldsymbol{r}$. In the same way we can define the wave *pseudovectors* $\boldsymbol{q}$ and $\boldsymbol{k}$ corresponding to the phonons and the electron, respectively. The Hamiltonian of the electron–phonon interaction in a fractional-dimensional space can then be written as

$$\hat{H}_{\mathrm{e-ph}} = \sum_{q} \left[C_q(D)\hat{b}_q \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}) + C_q^*(D)\hat{b}_q^\dagger \exp(-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}) \right] \tag{1}$$

where $b_q^\dagger(b_q)$ is the creation (annihilation) operator for a phonon with wave *pseudovector* $\boldsymbol{q}$, and $C_q(D)$ is the fractional-dimensional coupling coefficient of the electron–phonon interaction.

By considering now that the basic interaction characterizing the electron motion in D dimensions remains Coulomb-like ($\sim 1/r$) [37] we obtain

$$C_q(D) = -\mathrm{i}\hbar\omega_{\mathrm{LO}} \left(\frac{F_D(q)\alpha}{V_D} \right)^{1/2} \left(\frac{\hbar}{2m\omega_{\mathrm{LO}}} \right)^{1/4} \tag{2}$$

where

$$F_D(q) = (2\pi)^{D/2} \int_0^\infty \mathrm{d}r\, r^{D-1} (qr)^{1-D/2} J_{D/2-1}(qr) \frac{1}{r} \tag{3}$$

is the fractional-dimensional Fourier transform [38] of the Coulomb-like potential. In the above equations, m represents the electron effective mass, α is the Fröhlich constant, ω_{LO} denotes the bulk LO-phonon limiting frequency, V_D is the fractional-dimensional volume of the crystal to which Born–von Karman periodicity conditions are applied, and $J_\nu(x)$ represent the Bessel functions. Note that by introducing the fractional-dimensional transform we avoid the use of any property concerning vector spaces.

After the corresponding integration in equation (3) we obtain from equation (2) the coupling coefficient

$$C_q(D) = -\mathrm{i}\hbar\omega_{\mathrm{LO}} \left[\frac{(4\pi)^{(D-1)/2}\Gamma[(D-1)/2]\alpha}{q^{D-1}V_D} \right]^{1/2} \times \left(\frac{\hbar}{2m\omega_{\mathrm{LO}}} \right)^{1/4} \tag{4}$$

characterizing the electron–phonon interaction in the fractional-dimensional bulk.

3. The fractional-dimensional polaronic corrections

In this paper, we consider that the Fröhlich constant is small ($\alpha \ll 1$) and, consequently, we deal only with the weak-coupling case.

The electron self-energy due to the electron–LO–phonon interaction in the weak-coupling approximation can be calculated within second-order perturbation theory. The energy of a fractional-dimensional polaron in the ground state is given by

$$E = E_k^{(0)} + \sum_{k'} \frac{|\langle 1_{k'}, 0_k, 1_q | \hat{H}_{\mathrm{e-ph}} | 0_{k'}, 1_k, 0_q \rangle|^2}{\bar{E}_k - \bar{E}_{k'}} \tag{5}$$

where

$$\bar{E}_k = \langle 0_q, 1_k, 0_{k'} | \hat{H}^{(0)} | 0_{k'}, 1_k, 0_q \rangle = E_k^{(0)} \tag{6}$$

and

$$\bar{E}_{k'} = \left\langle 1_{k'}, 0_k, 1_q \left| \hat{H}^{(0)} \right| 1_q, 0_k, 1_{k'} \right\rangle = E^{(0)}_{k'} + \hbar\omega_{\mathrm{LO}} \qquad (7)$$

are the unperturbed electron energies corresponding to the initial and intermediate states, respectively.

In the above equations, $|0_{k'}, 1_k, 0_q\rangle$ denotes the initial state with one electron in the state $\boldsymbol{k}$, zero electrons in $\boldsymbol{k}'$ and zero phonons. The assumption of the absence of phonons in the initial state is usually fulfilled for low temperatures. The interpretation of the intermediate states $|1_q, 0_k, 1_{k'}\rangle$ is analogous to that of the initial states.

Taking into account the fact that the free electron motion in a fractional-dimensional space can be described by a plane wave [38], and after the corresponding integration over the volume V_D in the matrix elements present in equation (5), we obtain

$$E - E^{(0)}_{\boldsymbol{k}} = \frac{2m}{\hbar^2} \sum_{\boldsymbol{k}',\boldsymbol{q}} \frac{|C_q(D)|^2 |\Delta[\boldsymbol{k}' - \boldsymbol{k} + \boldsymbol{q}]|^2}{k^2 - k'^2 - R_{\mathrm{p}}^{-2}} \qquad (8)$$

where $R_{\mathrm{p}} = \sqrt{\frac{2m\omega_{\mathrm{LO}}}{\hbar}}$ is the polaron radius and $\Delta(x)$ represents the Kronecker delta function ($\Delta(x) = 1$ if $x = 0$, and $\Delta(x) = 0$ if $x \neq 0$). This function, as in the integer-dimensional bulk case, is an expression of the momentum conservation law.

Now, by approximating the summation over $\boldsymbol{q}$ in equation (8) by an integral

$$\sum_{\boldsymbol{q}} \cdots \approx \frac{V_D}{(2\pi)^D} \frac{2\pi^{(D-1)/2}}{\Gamma[(D-1)/2]} \times \int_0^{\infty} \int_0^{\pi} \cdots q^{D-1} (\sin\theta)^{D-2} \, \mathrm{d}q \, \mathrm{d}\theta \qquad (9)$$

and after the standard procedures, we obtain from equation (8) the following expression for the polaron energy

$$E = -g_1(D)\alpha\hbar\omega_{\mathrm{LO}} + \frac{\hbar^2 k^2}{2m^*} \qquad (10)$$

where

$$m^* = \frac{m}{1 - g_2(D)\alpha} \qquad (11)$$

is the polaron effective mass.

In equations (10) and (11) the D-dependent functions $g_1(D)$ and $g_2(D)$ are given, respectively, by

$$g_1(D) = \frac{\sqrt{\pi}}{2} \frac{\Gamma[(D-1)/2]}{\Gamma[D/2]} \qquad (12)$$

and

$$g_2(D) = \frac{\sqrt{\pi}}{4} \frac{\Gamma[(D-1)/2]}{D\Gamma[D/2]}. \qquad (13)$$

In equations (9), (12) and (13) $\Gamma(x)$ represents the gamma function.

The set of equations (10)–(13) determines the polaronic corrections in a fractional-dimensional bulk. It is straightforward to check that these equations recover the well-known forms in both the exact two-dimensional (2D) and three-dimensional (3D) limits [39].

4. Polaron in a parabolic quantum well

In this section, we study the behaviour of a polaron confined in a PQW, within the framework of the fractional-dimensional space approach. In this approach, the actual 3D 'polaron plus PQW' system is considered as a polaron in an effective fractional-dimensional bulk, which dimension constitutes a measure of the degree of confinement of the real system. The question which arises is then how to calculate the appropriate value of the dimensional parameter, i.e. the effective dimension that would model the real system. At earlier stages, Mathieu and co-workers introduced a heuristic model for calculating the appropriate dimensionality in the case of confined excitons. Although their method is physically not strictly substantiated, it provides an accurate parametrization of the exciton binding energy in rectangular quantum wells [21, 22], quantum well wires [23] and superlattices [24]. More recently, de Dios-Leyva and co-workers [25] have developed a systematic procedure for determining the dimensionality of the effective medium in modelling exciton and impurity states in quantum wells [25, 26], multiple quantum wells [30, 33] and superlattices [34]. However, for the sake of simplicity, in this paper we consider a procedure analogous to that in [21–24].

Following Christol *et al* [23], since the dimensional parameter is a measure of the degree of confinement of the real system embedded in a 3D Euclidean space, it can be determined by

$$D = \beta_x + \beta_y + \beta_z \qquad (14)$$

where β_x, β_y and β_z are the ratios of the homothetic reduction of the unit length for the directions x, y and z in the real physical space, respectively.

In the case of a PQW extended along the z-direction, the motion in the (x, y)-plane is free and we get $\beta_x = \beta_y = 1$. The ratio of the homothetic reduction of the unit length in the z-direction produced by the confinement effects can be calculated through the relation

$$\beta_z = 1 - \exp[-\xi] \qquad (15)$$

where

$$\xi = \frac{\text{length of confinement}}{\text{effective characteristic length of interaction}}. \qquad (16)$$

Equations (14)–(16) have been successfully used in modelling exciton states in semiconductor quantum wells [21–24]. In the case of an exciton confined in an infinitely deep quantum well we have, for instance, $\xi = L_{\mathrm{w}}/(2a_0)$ [21], where L_{w} represents the well width and a_0 is the effective Bohr radius of the 3D exciton. The dimensionality is then given by $D = 3 - \exp[-\xi]$.

Now we consider a polaron confined in a PQW determined by a parabolic potential extending from $z = -\infty$ to $z = \infty$. The confining potential can be written as

$$V(z) = \frac{m}{2}\Omega^2 z^2 \qquad (17)$$

where Ω represents the confinement frequency. In this case, the effective characteristic length of the electron–phonon interaction is the polaron radius

$$R_{\mathrm{p}} = \sqrt{\frac{\hbar}{2m\omega_{\mathrm{LO}}}}. \qquad (18)$$

On the other hand, the confinement length l_z can be defined, as the root mean square position of the electron resulting from the harmonic confinement alone, i.e.

$$l_z = \langle z^2 \rangle^{1/2} = \sqrt{\frac{\hbar}{m\Omega}}. \tag{19}$$

There is, however, another convenient possibility in defining the confinement length, as pointed out by Kyrychenko and Kossut [40]. These authors have shown that the first zero of the third derivative of the oscillator wavefunction can be successfully used as the confinement length characterizing the problem of an exciton confined in a PQW. From this point of view we have

$$l_z = \sqrt{\frac{3\hbar}{m\Omega}} \tag{20}$$

for the ground state.

In what follows, we refer to equations (19) and (20) as the approximations 1 and 2, respectively.

The dimensional parameter can be calculated through the simple relation

$$D = 3 - \exp\left[-\frac{l_z}{R_p}\right]. \tag{21}$$

By now substituting the above equation into equations (10)–(13) we can estimate in a very simple way the energy and the effective mass of the confined polaron.

The polaron binding energy as a function of the inverse parabolic well confinement frequency ω_{LO}/Ω is displayed in figure 1(*a*), where we compare our results with the calculations by Hai *et al* [10]. One can see that the fractional-dimensional polaron binding energy calculated within approximation 1 is in reasonable agreement with the results in [10]. The maximal discrepancy between both results is about 6.2% (0.23 meV). On the other hand, the agreement is excellent for approximation 2.

Figure 1(*b*) shows a comparison between the fractional-dimensional polaron effective mass, for varying ω_{LO}/Ω, and the corresponding calculations by Hai *et al* [10]. One can see that the agreement between our results and those obtained in [10] is quite good (especially for approximation 1).

It is worth noting that both the polaron binding energy and the polaron effective mass plotted in figure 1 refer to their 2D corresponding values, i.e. $\Delta E_r = \Delta E/\Delta E_{2D}$ and $\Delta m_r = \Delta m/\Delta m_{2D}$.

The dependence of the dimensional parameter, calculated within approximations 1 and 2, on ω_{LO}/Ω is shown in figure 1(*c*). A similar trend can be appreciated for both approximations. The fractional dimension starts from the value $D = 2$ for an infinite parabolic well confinement frequency ($\Omega \to \infty$, $(\omega_{LO}/\Omega) \to 0$). As Ω increases, the confinement becomes weaker and weaker leading to an increase in the dimensionality that reaches the value $D = 3$ at $\Omega \to 0$. However, the increase in the dimension as the confinement decreases is faster for approximation 2.

A comparison between our results and those reported by Yildirim and Erçelebi [18] for a polaron confined in a PQW is displayed in figure 2. There is clearly a good agreement between our results and the corresponding calculations performed in [18]. Note that in figure 2 we have used the same notation as in [18].

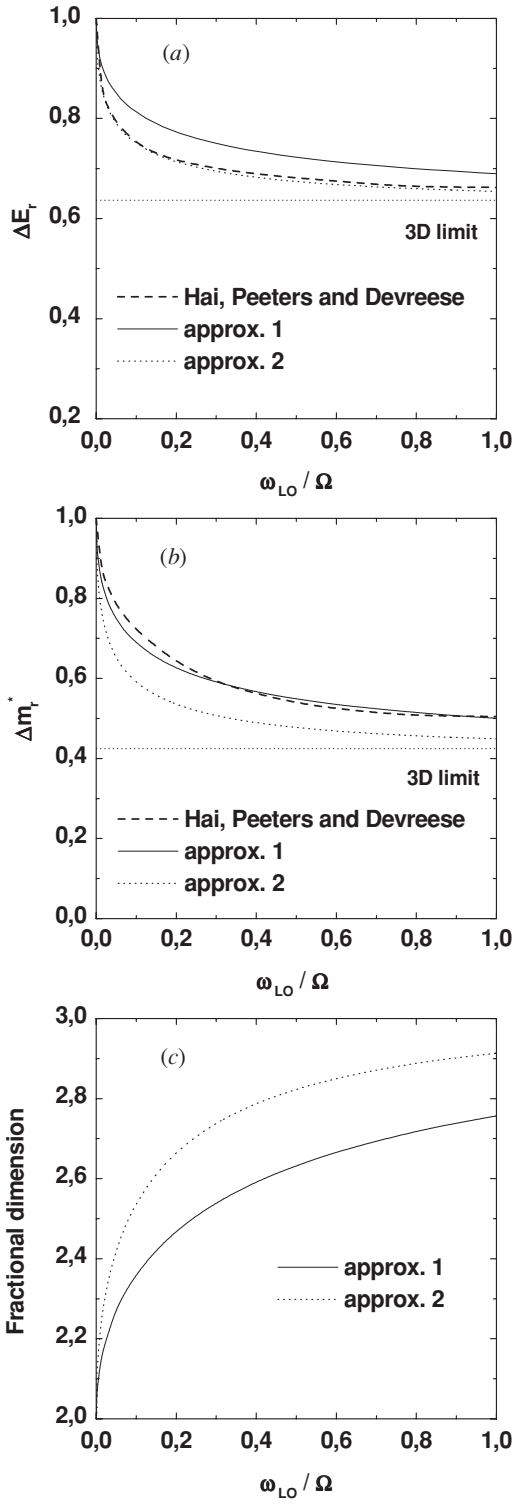

Figure 1. Inverse parabolic well confinement frequency dependence of: (*a*) the binding energy, (*b*) the polaron effective mass, and (*c*) the corresponding fractional dimension for a polaron confined in a PQW.

The fractional dimension corresponding to the results shown in figures 2(*a*) and (*b*) is displayed in (*c*) as a function of $\omega = \Omega/\omega_{LO}$. Again, the transition between the 2D and 3D limits when the confinement decreases is quite apparent.

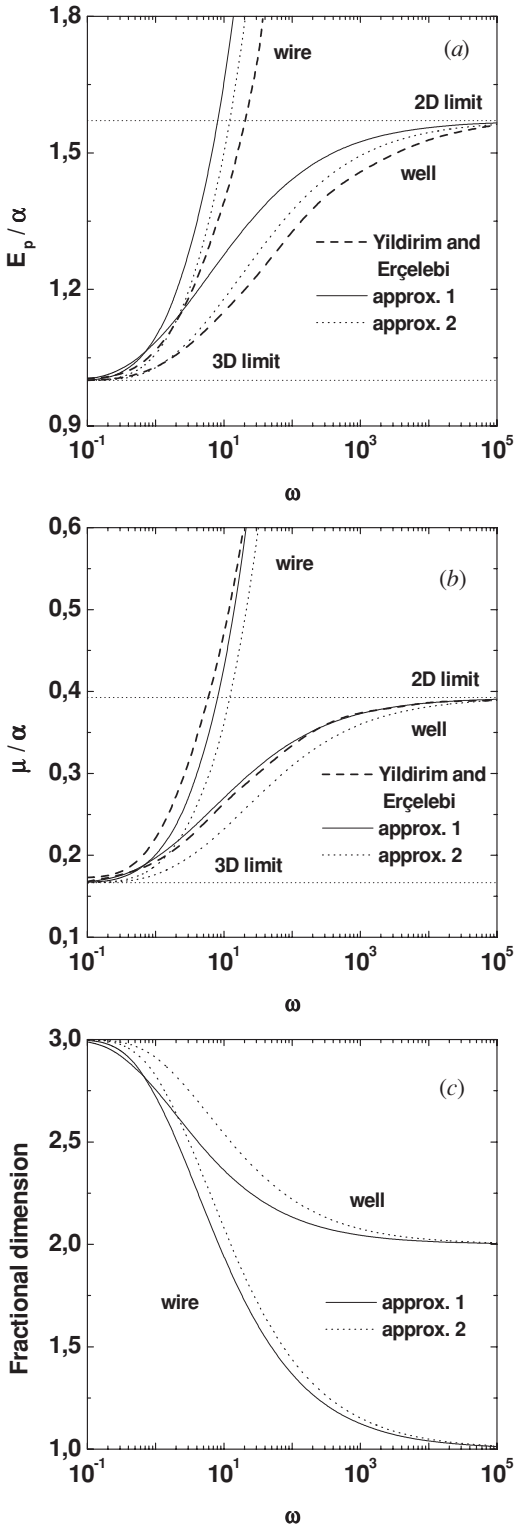

Figure 2. (*a*) The polaron binding energy, (*b*) the phonon correction to the effective mass and (*c*) the corresponding fractional dimension as functions of the parabolic confinement frequency for PQWs and PQWWs.

5. Polaron in a parabolic quantum well wire

In this section we generalize the formulae of the previous section to the case of a polaron confined in a PQWW determined by an isotropic harmonic potential

$$V(z) = \frac{m}{2}\Omega^2\rho^2 \tag{22}$$

where $\rho = \sqrt{x^2 + y^2}$ is the radial polar coordinate of the electron.

In the present case, the motion in the z-direction is free and therefore $\beta_z = 1$. The confinement in the (x, y)-plane is characterized by β_x and $\beta_y (\beta_x = \beta_y = 1 - \exp[-\xi])$. Hence, the dimensional parameter can be now written as

$$D = 3 - 2\exp[-\xi]. \tag{23}$$

While the effective characteristic length of interaction remains the polaron radius (R_p), the confinement length l_ρ can be calculated through a straightforward extension of the results obtained in the previous section. Indeed, the analogue of approximation 1 (see equation (19)) is now

$$l_\rho = \langle\rho^2\rangle^{1/2} = \sqrt{\frac{2\hbar}{m\Omega}}. \tag{24}$$

On the other hand, it is not difficult to prove that the first zero of the third derivative of the 2D oscillator wavefunction coincides, precisely, with equation (20). Hence approximation 2 gives

$$l_\rho = \sqrt{\frac{3\hbar}{m\Omega}}. \tag{25}$$

In figure 2(*a*) we show the fractional-dimensional binding energy of a polaron confined in a PQWW as a function of the parabolic confinement frequency $\omega = \Omega/\omega_\mathrm{LO}$. Our results obtained through the approximations 1 (equation (24)) and 2 (equation (25)) are compared with the calculations reported by Yildirim and Erçebeli [18]. A qualitative agreement can clearly be seen. However, the increase in the polaron binding energy with ω becomes very fast and the discrepancy between our calculations and those in [18] becomes too large in the region of strong confinement. One can expect that, in this region, the present fractional-dimensional model cannot provide accurate values because the expressions for the polaron corrections (see equations (10) and (11)) diverge at $D = 1$. On the other hand, recent studies concerning polarons in cylindrical and planar quantum well wires with parabolic confinement potential for arbitrary electron–phonon coupling [41] has revealed that the weak and intermediate coupling regimes become shorter when the strength of confinement increases. Consequently, the perturbative treatment of the electron–phonon interaction becomes questionable in the region of strong confinement.

The confinement frequency dependence of the effective mass of a polaron in a PQWW is shown in figure 2(*b*), where an overall agreement between our results and those in [18] can be appreciated.

The behaviour of the fractional dimension for varying the parabolic well wire confinement frequency is displayed in figure 2(*c*). The dimension starts from the value $D = 3$ in the absence of confinement ($\omega \to 0$) and decreases as the confinement increases. The one-dimensional limit is then approached for a very strong confinement ($\omega \to \infty$).

6. Conclusions

In conclusion, the fractional-dimensional space approach has been extended to the study of polarons confined in PQWs and PQWWs. In this approach, the real confined 'polaron plus parabolic confining potential' system is modelled into an effective fractional-dimensional environment in which the polaron remains unconfined, and the fractional dimension is a measure of the degree of confinement of the real system. Analytical expressions for the corresponding polaron corrections have been found. In the region of weak confinement, these expressions allow us, within a good accuracy, to estimate the polaron binding energy and effective mass in a very simple way, avoiding the tedious and complicated calculations arising in the standard treatments. In the strong confinement region the fractional-dimensional polaron corrections are found to agree only qualitatively with previous, more detailed, theoretical results.

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