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2002 J. Phys.: Condens. Matter 14 4543

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A fractional-dimensional space approach to the polaron effect in quantum wells

A Matos-Abiague

Max-Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

E-mail: amatos@mpi-halle.de

Received 28 August 2001, in final form 21 February 2002

Published 18 April 2002

Online at stacks.iop.org/JPhysCM/14/4543

Abstract

Polarons confined in rectangular and parabolic quantum wells are studied within the framework of the fractional-dimensional space approach. In this scheme, the real confined ‘polaron plus quantum well’ system is mapped into an effective fractional-dimensional bulk in which the polaron behaves in an unconfined fashion, and the fractional dimension is essentially related to the degree of confinement of the actual system. Analytical expressions allowing a very simple estimation of the corresponding polaron corrections are found. The fractional-dimensional theoretical results are shown to be in reasonable agreement with previous more detailed calculations.

1. Introduction

In the last decade, a considerable amount of work has been devoted to the study of artificial low-dimensional semiconductor systems, not only because of the physics underlying various properties of these systems but also due to their importance for 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 intensive investigations for a long time.

At earlier stages, polarons in bulk material were investigated and a wide variety of mathematical techniques were applied to the study of the polaron problem (see for instance [1] and [2]). The polaron effects in semiconductor heterostructures are, however, quite different from those in bulk materials. In GaAs–Al_xGa_{1-x}As quantum well (QW) systems, for instance, there are a variety of phonon modes (e.g. bulk-like phonon modes [3], slab modes [4], interface or surface modes [3], and coupled modes [5]) arising from the presence of the heterointerfaces. Consequently, a rigorous treatment of the electron–phonon interaction in such heterostructures

requires the consideration of all these modes. The polaron problem in QWs becomes then too complicated [6–11], and even the simplest models cannot be resolved analytically. The purpose of the present paper is to formulate a simplified model for estimating, analytically, the polaron corrections in QWs, with reasonable accuracy.

Of particular interest to the present work is the original approach proposed by He [12, 13]. In this approach the anisotropic (or confined) interactions in real three-dimensional space are treated as isotropic (or unconfined) ones in an effective fractional-dimensional environment whose 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 last few years, the fractional-dimensional space approach has been successfully used in modelling exciton [14–19], magnetoexciton [20, 21], biexciton [22, 23], and impurity states [18, 24, 25] in semiconductor heterostructures. The Stark shift of excitonic complexes [26] and the refractive index in QW structures [27] 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 rectangular and parabolic QWs. Thus, the real confined ‘polaron + QW’ system is mapped into an effective fractional-dimensional bulk in which the polaron behaves in an unconfined fashion, 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, the Fröhlich-like Hamiltonian describing the electron–LO-phonon interaction in a fractional-dimensional space is presented. 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 rectangular QW are obtained for varying well width. The results are compared with the results reported by other researchers. In section 5, the polaron problem in a parabolic QW is considered and a comparison of our results with calculations by other authors is shown. Finally, conclusions are summarized in section 6.

2. The Fröhlich-like Hamiltonian in fractional-dimensional spaces

The electron–phonon interactions in D dimensions have been considered by several authors [28–30]. Peeters *et al* proposed a Fröhlich-like Hamiltonian depending on the dimension of the space (see [28]). Although the procedure used by these authors in the derivation of the electron–phonon interaction Hamiltonian is valid only for integer values of the dimension¹, their results give correct expressions when we extend the dimension to non-integer values, as we will show in the present section. More recently, Thilagam has introduced an *a priori* definition of the Hamiltonian describing the exciton–phonon interaction in fractional-dimensional spaces (see [30]). This definition implies a Fröhlich-type Hamiltonian for the electron–phonon interaction whose coupling coefficient

$$C_q = -i\hbar\omega_{LO} \left(\frac{4\pi\alpha}{q^{D-1}V_D} \right)^{1/2} \left(\frac{\hbar}{2m\omega_{LO}} \right)^{1/4}, \quad V_D = \frac{\pi^{D/2}}{\Gamma[1 + D/2]} |r|^D, \quad (1)$$

¹ The authors used, basically, the properties of vectorial spaces in finding the coupling coefficient of the electron–phonon interaction. However, the fractional-dimensional space is not, in general, a vector space [31].

in spite of the statements of the author, cannot recover the well known two-dimensional limit [32]

$$C_q^{2D} = -\frac{i\hbar\omega_{LO}}{q^{1/2}} \left(\frac{2\pi\alpha}{S}\right)^{1/2} \left(\frac{\hbar}{2m\omega_{LO}}\right)^{1/4}, \quad S = \text{area}, \quad (2)$$

when $D = 2$. In the equations above and in what follows, m , α , and ω_{LO} represent the electron effective mass, the Fröhlich constant, and the bulk LO-phonon limiting frequency, respectively.

In this paper we will reconsider the model proposed in [28] for the electron–phonon interaction in an n -dimensional space. This model gives the well known results in both the exact two-dimensional and three-dimensional limits, and can be straightforwardly generalized to the case of non-integer values of the dimension of the space.

We recall that the fractional-dimensional space is not, in general, a vector space [31]. However, 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 [31]). 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* r . In the same way we can define the wave *pseudovectors* q and 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

$$\hat{H}_{e-ph} = \sum_q [C_q(D)\hat{b}_q \exp(iq \cdot r) + C_q^*(D)\hat{b}_q^\dagger \exp(-iq \cdot r)], \quad (3)$$

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

By now considering that the basic interaction characterizing the electron motion in D dimensions remains Coulomb-like ($\sim 1/r$) [28] we get

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

where

$$F_D(q) = (2\pi)^{D/2} \int_0^\infty dr r^{D-1} (qr)^{1-D/2} J_{D/2-1}(qr) \frac{1}{r} \quad (5)$$

is the fractional-dimensional Fourier transform [31] of the Coulomb-like potential. In the equations above, V_D is the fractional-dimensional volume of the crystal to which Born–Von Karman periodicity conditions are applied and the $J_\nu(x)$ represent the Bessel functions. Notice that by introducing the fractional-dimensional transform we avoid the use of any property concerning vector spaces.

After the corresponding integration in equation (5) we obtain from equation (4) the coupling coefficient

$$C_q(D) = -i\hbar\omega_{LO} \left[\frac{(4\pi)^{(D-1)/2} \Gamma[(D-1)/2] \alpha}{q^{D-1} V_D} \right]^{1/2} \left(\frac{\hbar}{2m\omega_{LO}}\right)^{1/4}, \quad (6)$$

characterizing the electron–phonon interaction in the fractional-dimensional bulk. It is worth remarking that, although the treatment used by the authors in [28] is valid only for integer values of the dimension, if we extend the values of the dimensional parameter in their results to non-integer values, we obtain an expression for the coupling coefficient that coincides precisely with equation (6).

3. The fractional-dimensional polaronic corrections

We recall that the purpose of the present work is to model the polaron effect in real systems such as semiconductor QWs. Often heterostructures of this kind are made out of weak polar semiconductors (e.g. GaAs–Al_xGa_{1-x}As). Therefore we will consider in our study that the Fröhlich constant is small ($\alpha \ll 1$) and, consequently, we will 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

$$E = E_k^{(0)} + \sum_{k'} \frac{|\langle 1_{k'}, 0_k, 1_q | \hat{H}_{e-ph} | 0_{k'}, 1_k, 0_q \rangle|^2}{\bar{E}_k - \bar{E}_{k'}}, \quad (7)$$

where

$$\bar{E}_k = \langle 0_q, 1_k, 0_{k'} | \hat{H}^{(0)} | 0_{k'}, 1_k, 0_q \rangle = E_k^{(0)}, \quad (8)$$

and

$$\bar{E}_{k'} = \langle 1_{k'}, 0_k, 1_q | \hat{H}^{(0)} | 1_{k'}, 0_k, 1_q \rangle = E_{k'}^{(0)} + \hbar\omega_{LO} \quad (9)$$

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

In the equations above, $|0_{k'}, 1_k, 0_q\rangle$ denotes the initial state with one electron in the state k , zero electrons in the state k' , and zero phonons. The assumption of 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 that the free-electron motion in a fractional-dimensional space can be described by a plane wave [31], after the corresponding integration over the volume V_D in the matrix elements present in equation (7) we get

$$E - E_k^{(0)} = \frac{2m}{\hbar^2} \sum_{k',q} \frac{|C_q(D)|^2 |\Delta[\mathbf{k}' - \mathbf{k} + \mathbf{q}]|^2}{k^2 - k'^2 - R_p^{-2}}, \quad (10)$$

where $R_p = \sqrt{2m\omega_{LO}/\hbar}$ 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 approximating the summation over \mathbf{q} in equation (10) by an integral

$$\sum_{\mathbf{q}} \dots \approx \frac{V_D}{(2\pi)^D} \frac{2\pi^{(D-1)/2}}{\Gamma[(D-1)/2]} \int_0^\infty \int_0^\pi \dots q^{D-1} (\sin \theta)^{D-2} dq d\theta, \quad (11)$$

and following the standard procedures, we obtain from equation (10) the following expression for the polaron energy:

$$E = -\Delta E + \frac{\hbar^2 k^2}{2m^*}, \quad (12)$$

where

$$\Delta E = g_1(D)\alpha\hbar\omega_{LO} \quad (13)$$

is the polaron binding energy, and

$$m^* = \frac{m}{1 - g_2(D)\alpha} \quad (14)$$

is the polaron effective mass.

In equations (13) and (14) the D -dependent functions $g_1(D)$ and $g_2(D)$ are given by

$$g_1(D) = \frac{\sqrt{\pi}}{2} \frac{\Gamma[(D-1)/2]}{\Gamma[D/2]}, \quad (15)$$

and

$$g_2(D) = \frac{\sqrt{\pi}}{4} \frac{\Gamma[(D-1)/2]}{D\Gamma[D/2]}, \quad (16)$$

respectively. In equations (11), (15), and (16) $\Gamma(x)$ represents the Gamma function.

The set of equations (12)–(16) 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- and three-dimensional limits.

4. Polaron in a rectangular quantum well

In the present section we will study the behaviour of the polaron confined in a rectangular QW, within the framework of the fractional-dimensional space approach. In this approach the real three-dimensional ‘polaron + QW’ system will be treated as a polaron in an effective fractional-dimensional bulk, whose dimension constitutes a measure of the degree of confinement of the real system. Thus, given this simple value—the dimensionality—we can obtain the polaron corrections from equations (12) and (14) in a very simple way. The question arising is then that of how to calculate the appropriate value of the dimensional parameter. At earlier stages, Mathieu and co-workers introduced a heuristical model for calculating the appropriate dimensionality in the case of confined excitons. Although their method has no strict physical substantiation it does provide a surprisingly accurate parametrization of the exciton binding energy in rectangular QWs [14, 15], QW wires [16], and superlattices [17]. More recently de Dios-Leyva and co-workers [18] have developed a systematic procedure for determining the dimensionality of the effective medium in modelling exciton and impurity states in QWs [18, 19], multiple QWs [21, 24], and superlattices [25]. For the sake of simplicity, however, we will consider in the present paper a procedure analogous to that in [14–17].

Following Christol *et al* [16], since the dimensional parameter is a measure of the degree of confinement of the real system embedded in a three-dimensional Euclidean space, it can be determined by

$$D = \beta_x + \beta_y + \beta_z, \quad (17)$$

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 rectangular QW grown 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

$$\beta_z = 1 - \exp[-\xi], \quad (18)$$

where

$$\xi = \frac{\text{length of confinement}}{\text{effective characteristic length of interaction}}. \quad (19)$$

Equations (17)–(19) have been successfully used in modelling exciton states in semiconductor QWs [14–17]. In the case of an exciton confined in an infinitely deep QW we have, for instance, $\xi = L_w/d$ [14], where L_w represents the well width and $d = 2a_0$ is the effective Bohr diameter of the three-dimensional exciton. The dimensionality is then given by $D = 3 - \exp[-\xi]$.

Consider now a polaron confined in an infinitely deep rectangular QW. In this case, the effective characteristic length of the electron–phonon interaction is the polaron diameter

$$d = 2R_p = 2\sqrt{\frac{\hbar}{2m\omega_{LO}}}. \quad (20)$$

Therefore, the dimensional parameter can be calculated through the simple relation

$$D = 3 - \exp\left[-\frac{L_w}{2R_p}\right], \quad (21)$$

where R_p is the polaron radius.

In the real system the polaron ground state can be written as [6, 10]

$$E = -\Delta E + E_{pol}^{KE} + E_z \quad (22)$$

where ΔE , E_{pol}^{KE} , and $E_z = \hbar^2\pi^2/(2mL_w^2)$ represent the polaron contribution to the binding energy, the polaron kinetic energy, and the first energy level for the electron motion in the z -direction, respectively. Now, we note that if we take the zero of the energy scale at the bottom of the first conduction subband in the well, we can rewrite equation (22) in a form quite similar to equation (12):

$$E = -\Delta E + E_{pol}^{KE}. \quad (23)$$

Thus, by defining the energy band gap in the effective fractional-dimensional system (E_g^D) as

$$E_g^D = E_g + E_z \quad (24)$$

where E_g represents the energy band gap of the actual system, and by comparing equations (12) and (23), the polaron binding energy due to the electron–phonon interaction (ΔE) and the polaron effective mass (m^*) can be estimated through the set of equations (13)–(16) and (21). We note that, in fact, the quantity ΔE can also be interpreted as a shift in the band-gap energy. That is why sometimes in the literature authors refer to ΔE as the energy gap shift due to the electron–phonon interaction. In order to be consistent with the terminology used by different authors when comparing our results with their calculations, in what follows we will refer to the polaron contribution to the binding energy (ΔE) as the polaron energy (gap) shift or, simply, the polaron binding energy, generally. The numerical results are displayed in figures 1 and 2. In obtaining figures 1 and 2 we have used the same material parameters as Thilagam and Singh in [10] and Hai *et al* in [6], respectively.

The well width dependence of the fractional-dimensional polaron energy shift (ΔE) compared with the corresponding calculations by Thilagam and Singh (TS model) [10] is displayed in figure 1(a). In both cases the polaron energy shift decreases as the well width increases. The same monotonic behaviour can be observed in figure 1(b) for the well width dependence of the increase in polaron effective mass. From figure 1, one may notice the existence of a qualitative and a reasonably quantitative agreement between the present fractional-dimensional results and the calculations within the TS model. The discrepancy in the energy shift results between the two calculations is less than 0.2 meV for the whole well width range. On the other hand, the maximal discrepancy for the increase of the polaron effective mass is about 0.5% at $L_w \approx 25$ Å. In the wide well width region ($L_w \geq 150$ Å) our results practically coincide with those of the TS approach.

The fractional-dimensional parameter as a function of the well width is plotted in figure 1(c). A transition between the two-dimensional limit (for an infinitely narrow QW) and the three-dimensional limit (for wide QWs) is clearly shown.

In figure 2(a) we present a comparison between the well width dependence of the fractional-dimensional polaron binding energy and the corresponding results obtained from

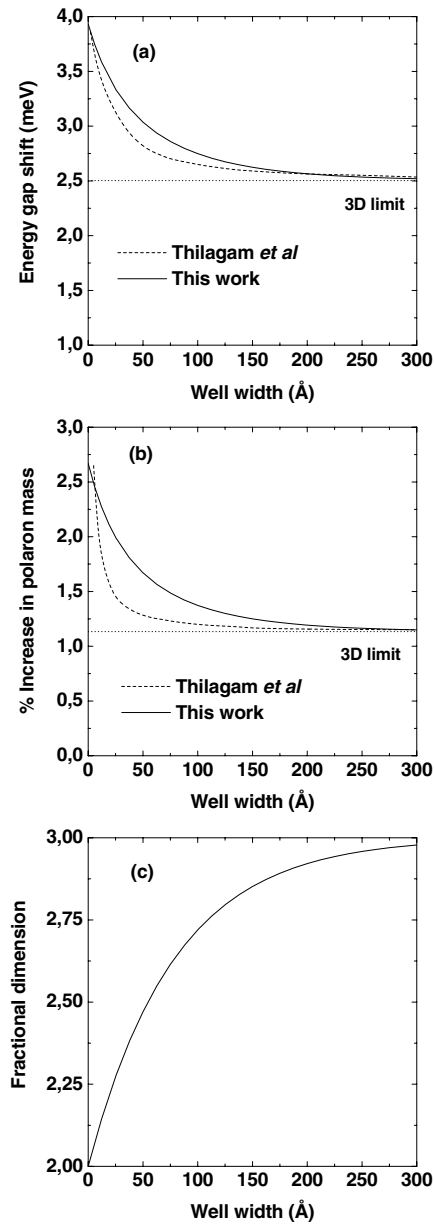


Figure 1. Well width dependence of the polaron energy shift (a), the increase in polaron mass (b), and the corresponding fractional dimension (c), for a polaron confined in an infinite rectangular QW. Full curves correspond to the present fractional-dimensional results and the dashed curves to calculations by Thilagam and Singh [10].

the Hai, Peeters and Devreese (HPD) model [6]. An excellent agreement between our results and those of the HPD model for three-dimensional bulk LO-phonon modes can be clearly appreciated. Notice that in figure 2(a) the polaron binding energy is given in units of the two-dimensional polaron binding energy limit ($\Delta E_{2D} = \alpha\pi\hbar\omega_{LO}/2$), i.e. $\Delta E_r = \Delta E/\Delta E_{2D}$. The overall agreement between our results and the calculations within the HPD model can also be

appreciated in figure 2(b) for the well width dependence of the polaron effective mass. Here the polaron effective mass has also been referred to its two-dimensional value ($\Delta m_{2D} = \alpha\pi m/8$), i.e. $\Delta m_r = \Delta m/\Delta m_{2D}$.

The fractional dimension corresponding to the results shown in figures 2(a) and (b) is displayed in figure 2(c) as a function of the well width. Again the transition between the two-dimensional limit and the three-dimensional limit when the well width increases is quite apparent. In fact, for $L_w \geq 400 \text{ \AA}$ the effective system becomes practically three dimensional.

It is worth noting that our results for the polaron corrections are, in general, greater than those from the TS model (see figure 1), but smaller than the results obtained within the HPD approach (see figure 2). Consequently, the discrepancies between the TS and the HPD approaches are greater than those between our fractional-dimensional model and the TS (or the HPD) approach.

5. Polaron in a parabolic quantum well

Consider now a polaron confined in a parabolic QW determined by a parabolic potential extending from $z = -\infty$ to $+\infty$. The confining potential can be written as

$$V(z) = \frac{m}{2}\Omega^2 z^2, \quad (25)$$

where Ω represents the confinement frequency.

In order to describe the real system ‘polaron + parabolic QW’ via the effective fractional-dimensional space approach, we have to calculate the appropriate value of the dimension of the effective environment in which the confined polaron is treated as an unconfined polaron. The dimensional parameter can be now calculated through a straightforward extension of the results obtained in the previous section. While the effective characteristic length of interaction remains the polaron diameter ($2R_p$), the obvious length of confinement in the present case is the width l corresponding to the range of classical motion in the parabolic potential, i.e.

$$l = 2\sqrt{\frac{\hbar}{m\Omega}}. \quad (26)$$

The dimension can be then calculated as

$$D = 3 - \exp\left[-\frac{l}{2R_p}\right]. \quad (27)$$

Following the same procedures as in the previous section, the polaronic corrections can be calculated. We remark, however, that in the present case the conduction subbands are determined by the Landau levels $E_{zn} = \hbar\Omega(n + 1/2)$. Thus, for the ground state we have to take $E_z = \hbar\Omega/2$ in equation (24).

The polaron binding energy as a function of the inverse parabolic well confinement frequency ω_{LO}/Ω is displayed in figure 3(a), where we compare our results with the calculations by Hai *et al* [6]. One notices that the fractional-dimensional polaron binding energy is in reasonable agreement with the results in [6]. The maximal discrepancy for the polaron binding energy is about 6.2% (0.23 meV).

Figure 3(b) compares the fractional-dimensional polaron effective mass, for varying inverse parabolic well confinement frequency, with the corresponding calculations by Hai *et al* [6]. One may notice that the agreement of our results and those obtained in [6] is quite good.

Notice that both the polaron binding energy and the polaron effective mass plotted in figure 3 are referred to their two-dimensional corresponding values, as in figure 2.

The dependence of the dimensional parameter on ω_{LO}/Ω is shown in figure 3(c). The fractional dimension starts from the value $D = 2$ for an infinite parabolic well confinement

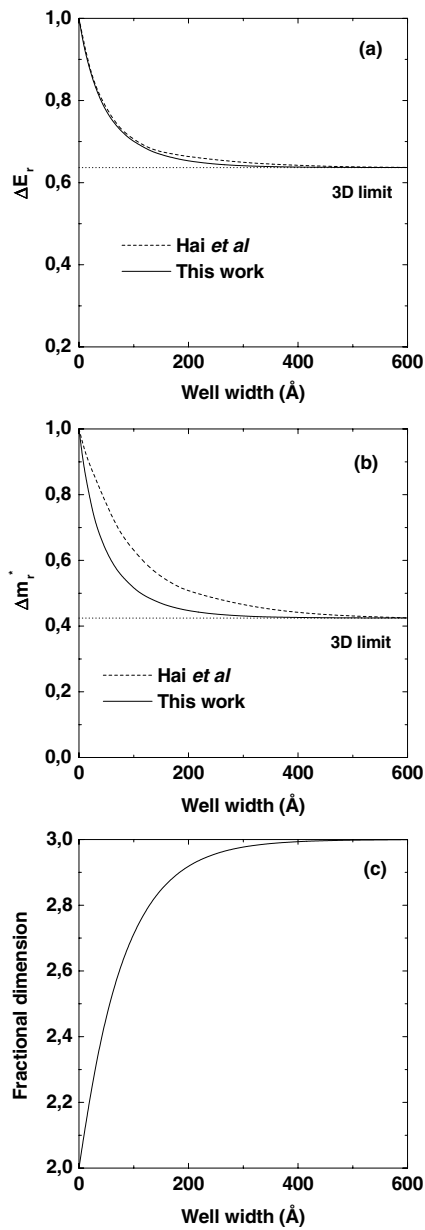


Figure 2. Well width dependence of the polaron binding energy (a), the polaron effective mass (b), and the corresponding fractional dimension (c), for a polaron confined in an infinite rectangular QW. Both the polaron binding energy and effective mass are referred to their corresponding two-dimensional values. Full curves correspond to the present fractional-dimensional results and the dashed curves to calculations by Hai *et al* [6].

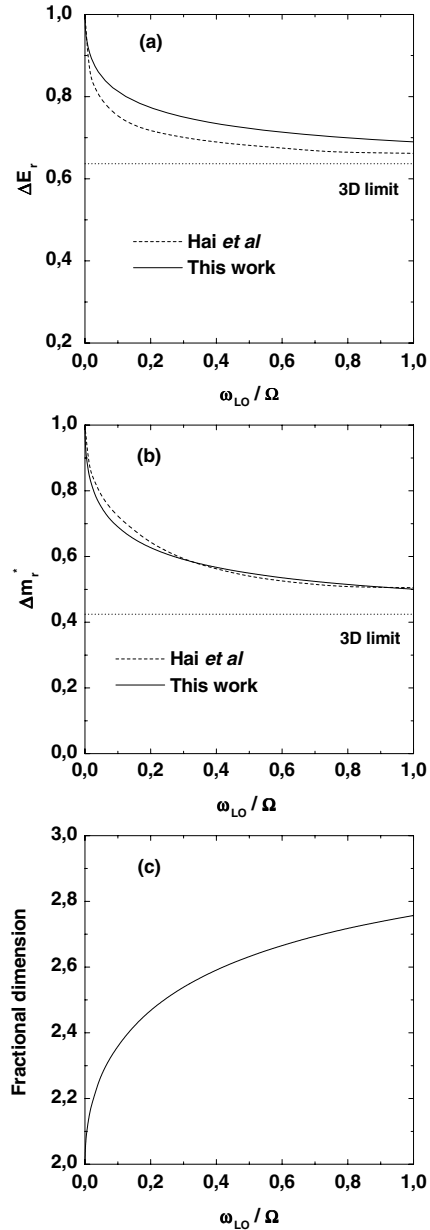


Figure 3. Inverse parabolic well confinement frequency dependence of the polaron binding energy (a), the polaron effective mass (b), and the corresponding fractional dimension (c), for a polaron confined in a parabolic QW. Both, the polaron binding energy and effective mass are referred to their corresponding two-dimensional values. Full curves correspond to the present fractional-dimensional results and the dashed curves to calculations by Hai *et al* [6].

frequency ($\Omega \rightarrow \infty$, $(\omega_{LO}/\Omega) \rightarrow 0$). As Ω decreases, the confinement becomes more and more weak, leading to an increase in the dimensionality that reaches the value $D = 3$ at $\Omega \rightarrow 0$.

6. Conclusions

In conclusion, the fractional-dimensional space approach was extended to the study of polarons confined in rectangular and parabolic QWs. In this approach, the real confined ‘polaron + QW’ system is modelled in 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 were found. These expressions allow us to estimate, with reasonable accuracy, the polaron binding energy and effective mass in a very simple way, avoiding the tedious and complicated calculations arising in the standard treatments.

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