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Fractional-dimensional polaron corrections in asymmetric GaAs-$Ga_{1-x}Al_xAs$ quantum wells

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Abstract

Polaron effects in asymmetric GaAs-$Ga_{1-x}Al_xAs$ quantum wells (QWs) are investigated within the framework of the fractional-dimensional space approach and by using second-order perturbation theory. A well-width dependence of the polaron corrections with a dip and a peak is obtained for both symmetric and asymmetric QWs. The dip and the peak occur in the case of asymmetric QWs for larger well widths than in the case of symmetric QWs. An enhancement of the contrast between the dip and the peak of the polaron energy shift is found for the case of asymmetric QWs. These results show the convenience of using asymmetric QWs instead of symmetric ones in any experimental attempt of detecting the dip and the peak of the polaron energy shift.

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Keywords: Polaron effect; Electron–phonon interaction; Fractional-dimensional approach; Quantum wells

1. Introduction

In the last few decades a variety of low-dimensional systems as quantum wells (QWs), superlattices, quantum wires and quantum dots has been extensively studied from both theoretical and experimental points of view. The main interest in these heterostructured systems lies in their unique physical properties and applications in electronic and optoelectronic devices. In particular, one of the most commonly used low-dimensional heterostructures are the GaAs-$Ga_{1-x}Al_xAs$ QWs. It is well known that the electron–phonon interaction, leading to the polaron effect, influences the optical and transport properties of such weak polar low-dimensional systems. Consequently, a wide variety of theoretical models has been proposed by different researchers (see for instance, Refs. [1–9]). However, most of the previous theoretical studies concerning polarons confined in QWs have been devoted to symmetric structures and only a few works [10,11] deal with the case of asymmetric QWs. Unfortunately, these studies reported on the polaron effect in asymmetric QWs [10,11] appear to have some inconsistencies (probably caused during the numerical processing of the model). On the other hand, the set of material parameters used in these studies has recently been shown to be inappropriate [9].

In the present paper, we use a consistent set of material parameters in the theoretical study of polarons

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confined in asymmetric GaAs-$Ga_{1-x}Al_xAs$ QWs. As within the standard models this problem becomes rather complicated (see Refs. [10,11]), we alternatively perform our study within a very simple model recently introduced by Matos-Abiague [12,13] and based on the fractional-dimensional space approach (FDSA). Since its introduction by He [14,15] the FDSA has been successfully used in modelling various low-dimensional systems (see for instance, Ref. [13] and references therein). The main advantage in applying the FDSA to the study of the polaron problem is that the real confined system, in which a variety of phonon modes arises as a consequence of the presence of the heterointerfaces, is mapped into an effective fractional-dimensional bulk in which the polaron behaves in an unconfined fashion. Thus, while in the real "polaron + QW" system the electron interaction with the different phonon modes turns the problem complicated, in the effective fractional-dimensional environment that maps the real system, however, the electron interacts only with bulk-like phonons and analytical expressions for the fractional-dimensional polaron corrections can be easily obtained within second-order perturbation theory [12,13]. The FDSA constitutes then a suitable tool for an easy estimation of the polaron corrections with a good accuracy [12,13]. In addition, the FDSA provides a simple and comprehensive picture of the behaviour of the real physical system and can be easily generalized to different kind of heterostructures.

The paper is organized as follows. In Section 2 the theoretical basis of the fractional-dimensional model introduced by Matos-Abiague [13] for polarons in symmetric QWs, is extended to the case of polarons confined in asymmetric GaAs-$Ga_{1-x}Al_xAs$ QWs. Results and discussion are in Section 3, and conclusions in Section 4.

2. Theoretical framework

We consider the problem of a polaron confined in an asymmetric GaAs-$Ga_{1-x}Al_xAs$ QW characterized by the potential

$$V(z)=\begin{cases} V_{\rm l} & \text{if } z<0,\\ V_{\rm w}(=0) & \text{if } 0\leqslant z\leqslant L_{\rm w},\\ V_{\rm r} & \text{if } z>0, \end{cases} \tag{1}$$

where $L_{\rm w}$ represents the well width and the subscripts l, w, and r label the left, well, and right regions, respectively. This system possesses a small electron–phonon coupling constant ($\alpha \ll 1$), consequently, we restrict our study to the weak-coupling case.

Within the fractional-dimensional space approach, the actual confined polaron is modelled through an unconfined effective fractional-dimensional polaron. The fractional-dimensional polaronic corrections were calculated, within second-order perturbation theory, in Refs. [12,13], where the polaron energy shift was found to be given by

$$\Delta E=-\frac{\sqrt{\pi}}{2}\,\frac{\Gamma[(D-1)/2]}{\Gamma[D/2]}\,\alpha\hbar\omega_{\rm LO} \tag{2}$$

and the polaron effective mass by

$$m^*=\frac{4D\Gamma[D/2]m}{4D\Gamma[D/2]-\sqrt{\pi}\Gamma[(D-1)/2]\alpha}. \tag{3}$$

In Eqs. (2) and (3) D represents the dimensionality, α the Fröhlich constant, $\omega_{\rm LO}$ the LO-phonon limit frequency in the non-dispersive approximation, and m is the electron effective mass.

The dimensional parameter D that guarantees the mapping of the actual system into the fractional-dimensional environment can be calculated through the relation [13]

$$D=3-\exp[-\xi], \tag{4}$$

where ξ represents the ratio of the length of confinement to the effective characteristic length of interaction. The effective length that characterizes the electron–phonon interaction is the polaron diameter $2R_{\rm p}$ (with $R_{\rm p}=\sqrt{\hbar/2m\omega_{\rm LO}}$ being the polaron radius), while the length of confinement is characterized by an effective well width $L_{\rm w}^*$ that takes account of the carrier penetration into the barriers [13]. In the case of an asymmetric QW we have

$$L_{\rm w}^*=\frac{1}{k_{\rm l}}+L_{\rm w}+\frac{1}{k_{\rm r}} \tag{5}$$

and Eq. (4) reduces to

$$D=3-\exp\left[-\frac{L_{\rm w}^*}{2R_{\rm p}}\right]. \tag{6}$$

In Eq. (5) $k_{\rm l}$ and $k_{\rm r}$ represent the electron wave vectors in the left and right barriers, respectively.

After solving the Schrödinger equation

$$\left[-\frac{\hbar^2}{2}\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{m(z)}\frac{\mathrm{d}}{\mathrm{d}z}\right)+V(z)\right]\Psi=E\Psi \tag{7}$$

that describes the motion of the single electron confined in the QW potential [Eq. (1)], the values of k_l and k_r can be obtained from the relations

$$k_i=\frac{\sqrt{2m_i(V_i-E)}}{\hbar},\quad i=\mathrm{l},\mathrm{r}. \tag{8}$$

In Eq. (8) $m(z)$ represent the electron z-dependent effective mass

$$m(z)=\begin{cases} m_\mathrm{l} & \text{if } z<0,\\ m_\mathrm{w} & \text{if } 0\leqslant z\leqslant L_\mathrm{w},\\ m_\mathrm{r} & \text{if } z>0. \end{cases} \tag{9}$$

In an asymmetric GaAs-$Ga_{1-x}Al_xAs$ QW, the material parameters that characterize the polaron properties differ when passing from one region to other. In order to take account of this fact, we assign to the effective fractional-dimensional bulk an average of the material parameters over the polaron positions. If one consider the polaron as a phonon cloud around the electron, the polaron position will be determined, essentially, by the electron position. The mean values of the material parameters that characterize the fractional-dimensional electron–phonon interaction can therefore be calculated as [13]

$$m^{-1}=\sum_{i=\mathrm{l,w,r}}\frac{P_i}{m_i}, \tag{10}$$

$$\omega_\mathrm{LO}=\sum_{i=\mathrm{l,w,r}}\omega_i P_i, \tag{11}$$

$$\alpha=\left[\sum_{i=\mathrm{l,w,r}}\left(P_i\frac{\omega_i}{\omega_\mathrm{LO}}\sqrt{\alpha_i\sqrt{\frac{m\omega_\mathrm{LO}}{m_i\omega_i}}}\right)\right]^2 \tag{12}$$

and

$$R_\mathrm{p}=\left[\sum_{i=\mathrm{l,w,r}}\left(P_i\frac{\omega_i}{\omega_\mathrm{LO}}\sqrt{\frac{\alpha_i R_{\mathrm{p}i}}{\alpha}}\right)\right]^2,$$

$$R_{\mathrm{p}i}=\sqrt{\frac{\hbar}{2m_i\omega_i}}. \tag{13}$$

In Eqs. (10)–(13) α_i and ω_i represent the Fröhlich constants and the phonon frequencies in the different regions, and

$$P_\mathrm{l}=\int_{-\infty}^{0}|\Psi(z)|^2\,\mathrm{d}z,$$

$$P_\mathrm{w}=\int_{0}^{L_\mathrm{w}}|\Psi(z)|^2\,\mathrm{d}z,\quad P_\mathrm{r}=1-P_\mathrm{l}-P_\mathrm{w} \tag{14}$$

denote the probabilities of finding the single electron in the left barrier, well, and right barrier regions, respectively. The energy shift and the effective mass of a polaron confined in an asymmetric GaAs-$Ga_{1-x}Al_xAs$ QW can then be computed in a very simple way from Eqs. (2), (3) and (6) and assuming the material parameter main values defined in Eqs. (10)–(13). The results are discussed in Section 3.

3. Results and discussion

In order to compare our calculations with those reported in Refs. [10,11], we have used the same set of material parameters as in Refs. [10,11]. However, it has recently been shown that such a set of parameters is inconsistent [9]. For this reason we also have performed our calculations by using the correct set of material parameters as discussed by Smondyrev et al. [9]. In all the figures, dashed lines correspond to our calculations with the correct set of material parameters [9], while other curves represent calculations performed by using the inconsistent set of parameters used in Refs. [10,11].

The well-width dependence of the fractional-dimensional polaron binding energy (dashed line) in a symmetric GaAs-$Ga_{0.75}Al_{0.25}As$ QW compared with the corresponding results reported by Shi et al. [10] (dash-dot-dot line) and Smondyrev et al. [9] (dash-dotted line) is displayed in Fig. 1(a). A dashed line corresponding to our calculations with the correct set of material parameters is also shown in the figure. As for symmetric QWs the material parameters have the same values in the left and right barriers, we refer to the left and right barrier regions in Fig. 1 indistinctly with the subscript *out*. One can observe that our calculations agree reasonably well with those reported in Ref. [9], and that the agreement of both results with the calculations by Shi et al. [10] is quite poor. In fact, one can see that the results by Shi et al. [10] for very small and very large well widths have

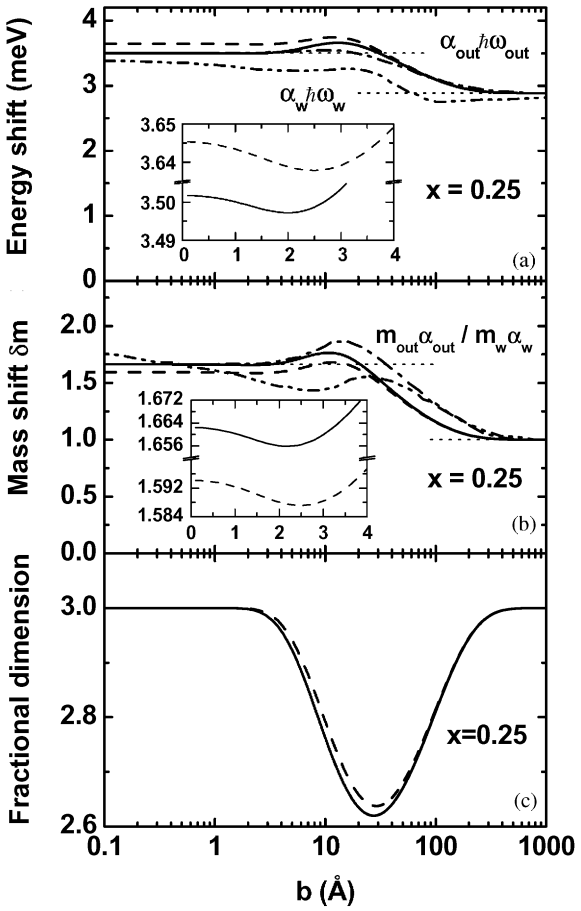

Fig. 1. Well-width dependence of the polaron energy shift (a), the polaron mass shift (b), and the corresponding fractional dimension (c) for a polaron confined in a symmetric GaAs-$Ga_{0.75}Al_{0.25}As$ QW. Solid, dash-dotted, and dash-dot-dot curves were obtained by using the same material parameters as in Ref. [10] and correspond to the present fractional-dimensional results, calculations by Smondyrev et al. [9] and by Shi et al. [10], respectively. The dashed lines represent our fractional-dimensional results by using the correct set of material parameters [9].

a quite different asymptotic behaviour from those of our calculations and the calculations in Refs. [8,9]. It is surprising, for instance, that for well widths of about 0.3 Å the corresponding asymptotic 3D limit value is not still reached in the calculations by Shi et al. [10]. On the other hand, for very large well widths, the curve by Shi et al. [10] approaches the asymptotic value from below, something that is physically unclear. One may think then that there is something wrong in the results of Ref. [10]. For a more detailed discussion of the inconsistencies of the results in Ref. [10], the reader can consult Ref. [9].

It is worth noting that although our calculations agree, in general, with those reported by Smondyrev et al. [9], a qualitative difference between both calculations appears for narrow QWs. While the curve by Smondyrev et al. (dash-dotted line) posses only a peak, our calculations [both, with the inconsistent set of parameters (solid line) and with the correct parameterization (dashed line)] exhibit a more complicated structure with a dip and a peak [cf. Fig. 1(a) and the corresponding inset]. Such a behaviour with a dip and a peak is also supported by more sophisticated calculations [8], and its origin has been explained in Ref. [13] within the fractional-dimensional space approach.

In Fig. 1(b) we compare our fractional-dimensional results (solid line) corresponding to the well-width dependence of the polaron mass shift $\delta m = \Delta m/\Delta m_w$ in a symmetric GaAs-$Ga_{0.75}Al_{0.25}As$ QW with the results by Smondyrev et al. [9] (dash-dotted line) and by Shi et al. [10] (dash-dot-dot line). Notice that, actually, δm represents the ratio of the mass shift (Δm) to that in the well material (Δm_w). For brevity, however, from now on we will refer to δm just as the polaron mass shift. An overall agreement between our results and those in Ref. [9] can be appreciated although our calculations exhibit again a dip and a peak [see also the inset in Fig. 1(b)] in the well-width dependence of the mass shift in contrast with the only peak appearing in the results by Smondyrev et al. [9]. As in the case of the polaron binding energy, the mass shift calculations by Shi et al. [10] also exhibit a wrong asymptotical behaviour. We have also included in Fig. 1(b) the results of our calculations with the correct set of material parameters (dashed line). One can appreciate from Figs. 1(a) and (b) that the use of an appropriate set of material parameters becomes important for narrow wells. This behaviour is quite normal because the inconsistencies in defining the material parameters refer to the $Ga_{1-x}Al_xAs$ regions (i.e., the barrier regions) [9]. Therefore, as for small well widths the tunnelling process becomes important, it is precisely for narrow QWs that the polaron is appreciably influenced by the parameters of the barrier materials.

The fractional-dimensional parameter corresponding to Figs. 1(a) and (b) is displayed as a function of the well width in Fig. 1(c). Dashed and solid lines

correspond to calculations performed by using the correct and the inconsistent set of material parameters, respectively. For large well widths the system behaves as a GaAs bulk and, consequently, the dimensional parameter has the limit value $D=3$. When the well-width decreases, the system becomes more and more confined, the polaron turns more and more *compressed*, and the effective dimension decreases, reaching a minimum for $b \approx 25$ Å. If we continue decreasing the well width, the tunnelling through the barriers becomes important and the degree of confinement of the system decreases. Consequently, the corresponding fractional dimension increases and recovers the value 3 for very narrow QWs.

The polaron corrections and the dimensional parameter as functions of the well width for an asymmetric $Ga_{0.82}Al_{0.18}$-GaAs-$Ga_{0.58}Al_{0.42}As$ QW are shown in Fig. 2. Dashed and solid lines represent our results by using the correct [9] and the inconsistent [10,11] set of material parameters, respectively. The results by Shi et al. [10] (dash-dot-dot line) are also included in the figure just for a formal comparison, since, as was previously discussed, these results appear to have inconsistencies. On the other hand, unfortunately, no other results concerning polarons in asymmetric QWs have been reported.

As for the case of symmetric QWs (cf. Fig. 1), a structure with a dip and a peak is also obtained in the behaviours of the energy shift [Fig. 2(a)] and the mass shift [Fig. 1(b)] for the asymmetric-QW case. In the case of asymmetric QWs, however, the contrast between the dip and the peak of the polaron corrections is appreciably stronger than in the case of symmetric QWs, as can be seen from the comparison of Figs. 1 and 2. A comparison between Figs. 1 and 2 also reveals that although the general behaviours of the well-width dependence of the polaron corrections in symmetric and asymmetric QWs are more or less similar, in the region of narrow QWs, in the case of asymmetric QWs the curves are shifted with respect to the symmetric-QW case. Thus, one can clearly appreciate that while for the symmetric case (cf. Fig. 1) the 3D limit is approached for very narrow QWs ($b \approx 2$ Å), this limit is approached for larger values of the well width ($b \approx 15$ Å) in the case of asymmetric QWs (cf. Fig. 2). This fact is not surprising. It is well known that for a single electron in a given rectangular symmetric QW there exists always at least one discrete energy level [16]. The discrete energy levels in the well are a direct consequence of the confinement effects. Consequently, in the symmetric QW, the polaron in its ground state *feels* the confinement effects even for very small values of the well width. As the dimensional parameter constitutes a measure of the degree of confinement of the real system, it appears that, in the region of narrow QWs, the asymptotic unconfined 3D limit is only approached for very small values of the well width, as can be appreciated in Fig. 1(c). In the case of rectangular asymmetric QWs the situation

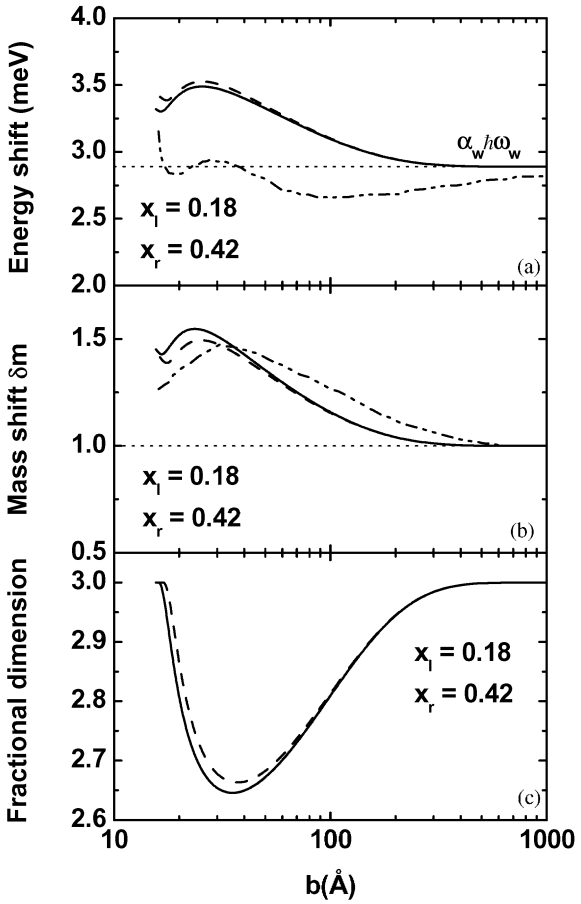

Fig. 2. Same as in Fig. 1, but now for an asymmetric $Ga_{0.82}Al_{0.18}As$-GaAs-$Ga_{0.58}Al_{0.42}As$ QW. Solid and dash-dot-dot curves were obtained by using the same material parameters as in Ref. [10] and correspond to the present fractional-dimensional results and calculations by Shi et al. [10], respectively. The dashed lines represent our fractional-dimensional results by using the correct set of material parameters [9].

is quite different because one cannot guarantee the existence of at least one discrete energy level of the single electron for arbitrary values of the well parameters [16]. In fact, for the asymmetric QW defined by the potential in Eq. (1) there exists a critical value of the well width b_c such that for well widths $b < b_c$ no discrete energy level of the single electron exists [16]. One then has that, basically, in the asymmetric-QW case the polaron does not *feel* the confinement effects for well width values below b_c. Consequently, the unconfined 3D limit is approached, in this case, once b approaches the critical well width b_c (notice that b_c is not, necessarily, a small value). This behaviour can be clearly appreciated in Fig. 2(c), where the dimensional parameter approaches the value 3 for a well width of about 15 Å.

The well-width dependence of the polaron corrections and the dimensional parameter is displayed in Fig. 3 for an asymmetric $Ga_{0.8}Al_{0.2}As$-GaAs -$Ga_{0.6}Al_{0.4}As$ QW. Dashed and solid lines represent our results by using the correct [9] and the inconsistent [10,11] set of material parameters, respectively. Dash-dot-dot lines representing the calculations by Zhu et al. [11] are also included for a formal comparison. Notice that the calculations performed by Zhu et al. [11] are quite similar to those in Ref. [10] and present, consequently, the same inconsistencies. The general trend of the curves in Fig. 3 is similar to that of the curves in Fig. 2. One can notice, however, that in the present case, there is an increase in the energy shift [Fig. 3(a)] and in the mass shift [Fig. 3(b)] with respect to their corresponding values in the case of the asymmetric QW considered in Fig. 2. The heterostructure considered in Fig. 3 can be obtained from that considered in Fig. 2 by increasing the height of the left barrier (i.e., by increasing the Al concentration from 0.18 to 0.2) and decreasing the height of the right barrier (i.e., by decreasing the Al concentration from 0.42 to 0.4). This procedure tends to make more symmetric the QW increasing the confinement effects [notice, for instance, that the minimum value of the dimensional parameter in Fig. 2(c) is greater that its minimum value in Fig. 3(c)] and leading to an increase in the polaron corrections. In fact, one can expect that when the symmetrization of the QW is reached (i.e., when the Al concentration in the left barrier is increased from 0.18 to 0.3 and the Al concentration in the right barrier is decreased from

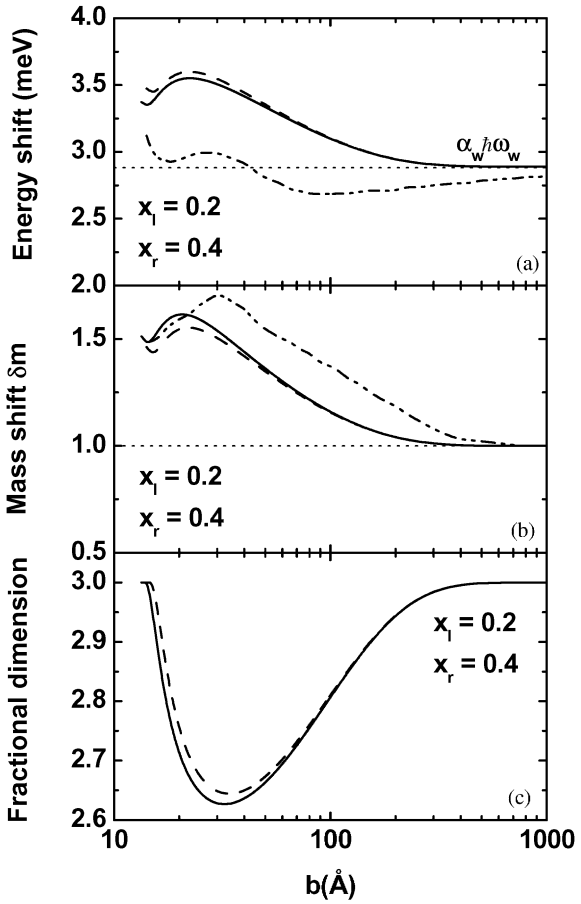

Fig. 3. Same as in Fig. 2, but for an asymmetric $Ga_{0.8}Al_{0.2}As$-GaAs-$Ga_{0.6}Al_{0.4}As$ QW. Solid and dash-dot-dot curves were obtained by using the same material parameters as in Refs. [10,11] and correspond to the present fractional-dimensional results and calculations by Zhu et al. [11], respectively. The dashed lines represent our fractional-dimensional results by using the correct set of material parameters [9].

0.42 to 0.3) the confinement effects will be increased and the minimum value of the dimensional parameter will be still smaller than in the case of Figs. 2(c) and 3(c). We do not show an explicit calculation for the symmetric GaAs-$Ga_{0.7}Al_{0.3}$ QW, but it is clear that for such a structure the minimum value of the dimensional parameter will be, actually, smaller than in the case of the asymmetric QWs considered in Figs. 2(c) and 3(c) because even for the case of the symmetric QW with Al concentration in the barriers of 0.25 this condition is already fulfilled, as can be observed from the comparison between Figs. 1(c), 2(c) and 3(c).

It is worth remarking that the FDSA leads to the existence of a dip and a peak in the well-width dependence of the polaron energy shift for both symmetric and asymmetric QWs [cf. Figs. 1(a), 2(a) and 3(a)]. This behaviour is also supported, in the case of symmetric QWs, by the more sophisticated calculations reported in Ref. [8]. Apart from the FDSA, the other available simple model for treating the polaron problem in layered heterostructures is the one proposed by Smondyrev et al. [9]. Within this model, however, no dip was found in the well-width dependence of the polaron energy shift. It would be desirable to experimentally detect whether the behaviour with the dip and the peak exist or no. It seems, however, very difficult to detect the existence of the peak and the dip of the polaron energy shift because of the smallness of the energy difference between them. Nevertheless, the results reported in the present work suggest that asymmetric QWs are better candidates than symmetric QWs for performing such an experiment. Indeed, based on our results, we can conclude that the use of asymmetric QWs has two fundamental advantages over the use of symmetric ones. The first one is that the contrast between the dip and the peak is enhanced in the case of asymmetric QWs. The second one is based on the fact that in asymmetric QWs the position of the dip and the peak is shifted to larger well widths and then no extremely narrow wells are, in principle, required for the experiment.

Finally, we would like to stress that it would be also desirable to compare our results with more sophisticated calculations and experimental results. However, to our knowledge, no theoretical (apart from Refs. [10,11], that, as was previously discussed, appear to have some inconsistencies) neither experimental results concerning polarons in asymmetric QWs have been reported until now.

4. Conclusions

In summary, we have extended the fractional-dimensional space approach to the study of polarons confined in a rectangular asymmetric GaAs-$Ga_{1-x}Al_xAs$ QW. The FDSA allows the estimation of the well-width dependence of the polaron energy shift and the mass shift in a very simple way, avoiding the tedious and complicated calculations arising in the standard treatments. A well-width dependence of the polaron corrections with a dip and a peak was obtained for both symmetric and asymmetric QWs. In the case of asymmetric QWs the dip and the peak occur for larger well widths than in the case of symmetric ones. It was also shown that the contrast between the dip and the peak of the energy shift is enhanced in the case of asymmetric QWs. Therefore, the use of asymmetric QWs instead of symmetric ones is recommended for any experimental attempt of detecting the dip and the peak of the polaron energy shift.

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