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Polaron effects on excitons in parabolic quantum wells: fractional-dimension variational approach

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Abstract. Polaron effects on excitons in parabolic quantum wells are studied theoretically by using a variational approach with the so-called fractional dimension model. The numerical results for the exciton binding energies and longitudinal-optical phonon contributions in $GaAs/Al_{0.3}Ga_{0.7}As$ parabolic quantum well structures are obtained as functions of the well width. It is shown that the exciton binding energies are obviously reduced by the electron (hole)-phonon interaction and the polaron effects are un-negligible. The results demonstrate that the fractional-dimension variational theory is effectual in the investigations of excitonic polaron problems in parabolic quantum wells.

PACS. 71.35.-y Excitons and related phenomena – 71.38.-k Polarons and electron-phonon interactions

1 Introduction

With the development of semiconductor crystal growth techniques, quantum well (QW) structures can be successfully fabricated in different shapes, such as the square quantum well (SQW), triangular quantum well (TQW) and parabolic quantum well (PQW) [1–5]. Recently, optical and electric properties of PQW structures have attracted much attention because of their application potential. These properties are closely related to excitonic states and their coupling with optical phonon modes. There has been a considerable amount of experimental and theoretical works on the properties of excitons in different PQW structures [1,6–9]. The energies of exciton states in PQW structures have been calculated by using various technologies, such as the variational and perturbation-variational schemes [1,6], the functional integral technique [7] and also the fractional-dimensional space formalism [8,9].

As was well-known, the phonon modes and their interactions with electrons and holes in multi-layer structures become more complicated than that in bulk materials because of the break of the translational symmetry in the direction normal to interfaces. The electron-phonon (e-p) interaction in SQW structures has been investigated fully within the framework of continuous medium approximation [10–12]. However, these results cannot be immediately used to PQW systems. Some theoretical literatures have initially mentioned the e-p effects on the electron states in PQW structures by various approximations. Hai et al considered an electron interacting with bulk longitudinal optical (LO) phonons in a PQW and calculated the polaron energy and effective mass by a perturbation method [13]. The polaron problem in this kind of systems was also investigated by using the Lee-Low-Pines (LLP) like variational method, where the slab and half-spacing modes respectively for the confined well and barrier LO phonons are considered similar to that in a SQW [14]. As an approximation, the interface optical phonon modes were omitted in the above-mentioned papers because of the less difference between the well and barrier materials in the vicinity of the interfaces. The authors have recently discussed the e-p effect on polarons in PQW structures [15] and confirmed that the bulk-LO-phonon model is an acceptable approximation.

Many authors have calculated the binding energies of excitons in SQWs [16–25] by various variational methods. Generally speaking, the successful variational calculations need more complicated trial wave functions with many parameters, so that the computations are time-consuming. Ponomarev et al. introduced a self-consistent approach to study the characteristics of excitons in shallow QWs and obtained an analytical expression for the exciton binding energy and the ground state eigenfunction [26]. Some authors have used a fractional-dimensional space model to discuss the exciton states in low-dimension structures, and obtained a surprisingly accurate estimation for the binding energy [27–29]. The simpler and effective method was also used to treat polaron problems [9,30,31]. However, to our knowledge, the exciton-phonon interaction in PQW structures has rarely been discussed concretely.

In this paper a fractional-dimensional method in combination with a LLP-like transformation and a variational treatment is developed to investigate the polaron

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effects on excitons in PQWs. A characteristic potential confinement length and an effective space dimension for the exciton-phonon system in a PQW are introduced and evaluated. A trial wave function with a fractional-dimensional variational parameter is used to calculate the exciton energy. As an example, the numerical results for the GaAs/$Al_{0.3}Ga_{0.7}As$ PQW are given and discussed.

2 LLP-like transformation and variational treatment

Let us consider a PQW structure with the well-width $2d$ generated by alternating multiple layers of GaAs and $Al_xGa_{1-x}As$ of varying thickness along z-direction [1]. The relative thickness of the GaAs layers in the well decreases quadratically with increasing the distance from the well center ($z = 0$). The barrier material $Al_xGa_{1-x}As$ is filled in the space of $|z| > 2d$. An exciton couples with a phonon field in the PQW system. The Hamiltonian of the exciton-phonon system then can be written as

$$H = H_{ex} + H_{ph} + H_{ex-ph}. \tag{1}$$

The first term in equation (1) is the Hamiltonian of a bare exciton without including the phonon influence and can be described within the framework of the isotropic effective mass approximation by

$$H_{ex} = -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 - \frac{e^2}{\varepsilon_\infty |\vec{r}_1 - \vec{r}_2|} + U_{well}, \tag{2}$$

where sub-labels "1" and "2" refer to the electron and hole respectively. ε_∞ is the high frequency dielectric constant and

$$U_{well} = \sum_j V_j(z_j), \tag{2a}$$

where $V_j(z_j)$ is the parabolic well potential for the electron ($j = 1$) or hole ($j = 2$) and given by

$$V_j(z_j) = \begin{cases} \frac{V_{0j}}{d^2} z_j^2, & |z_j| \leqslant d; \\ V_{0j}, & |z_j| > d. \end{cases} \quad (j = 1,\ 2). \tag{2b}$$

Here V_{0j} is the well-depth for the electron (hole) and depends on the composition x of $Al_xGa_{1-x}As$ [14]. Using the mass-center coordinate system, the bare exciton Hamiltonian (2) can be rewritten as

$$H_{ex} = -\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{e^2}{\varepsilon_\infty r} + U_{well}. \tag{3}$$

The excitonic mass-center and relative coordinates in equation (3) are given respectively by

$$\vec{R} = \beta_1\vec{r}_1 + \beta_2\vec{r}_2, \quad \vec{r} = \vec{r}_1 - \vec{r}_2,$$

where $\beta_1 = m_1/M$ and $\beta_2 = m_2/M$. $M = m_1 + m_2$ and $\mu = m_1m_2/M$ stand for the mass-center and reduced masses, respectively.

The second term in equation (1) is the free-phonon-field Hamiltonian

$$H_{ph} = \sum_q \hbar\omega a_q^\dagger a_q, \tag{4}$$

where $a_q^\dagger$ and a_q are respectively the creation and annihilation operators of the LO-phonon with the frequency ω and wave-vector $\boldsymbol{q}$.

The last term in equation (1) stands for the exciton-phonon interaction Hamiltonian and has the following form in the bulk-LO-phonons approximation [13,15]:

$$H_{ex-ph} = \sum_q [V_q a_q e^{i\vec{q}\cdot\vec{R}}(e^{i\beta_2\vec{q}\cdot\vec{r}} - e^{-i\beta_1\vec{q}\cdot\vec{r}}) + h.c.], \tag{5}$$

where

$$V_q = i\left[\frac{2\pi e^2}{V}\frac{\hbar\omega}{q^2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\right]^{1/2}. \tag{6}$$

Carrying out two LLP-like unitary transformations

$$U_1 = \exp\left[i\left(\vec{K} - \sum_q a_q^\dagger a_q\vec{q}\right)\cdot\vec{R}\right] \tag{7}$$

and

$$U_2 = \exp\left[\sum_q \left(a_q^\dagger f_q - a_q f_q^*\right)\right], \tag{8}$$

the exciton-phonon system Hamiltonian becomes

$$\begin{aligned} H^* &= U_2^{-1}U_1^{-1}HU_1U_2 \\ &= H_{ex} + \sum_q\left(\hbar\omega + \frac{\hbar^2q^2}{2M}\right)(a_q^\dagger + f_q^*)(a_q + f_q) \\ &\quad + \sum_q [V_q(a_q + f_q)(e^{i\beta_2\vec{q}\cdot\vec{r}} - e^{-i\beta_1\vec{q}\cdot\vec{r}}) + h.c.], \end{aligned} \tag{9}$$

where the multi-phonon processes have been neglected in the mono-phonon approximation. The displacement amplitudes f_q and f_q^* will be variationally determined later.

We now start with a variational method to calculate the ground state energy of the exciton. The ground state wave function of the exciton-phonon system is chosen as

$$|\psi\rangle = |\phi(\vec{r})\rangle\,|0\rangle\,, \tag{10}$$

where $|0\rangle$ is the zero-phonon state, and $|\phi(\vec{r})\rangle$ is a trial wave function for the excitonic ground state and will be determined by a fractional-dimensional variational treatment. Then the variational energy of the excitonic ground-state can be calculated as

$$\begin{aligned} E &= \langle 0|\,\langle\phi(\vec{r})|\,H^*\,|\phi(\vec{r})\rangle\,|0\rangle \\ &= E_0 + \frac{\hbar^2}{2M}\sum_q f_q^* f_q(u^2 + q^2) + \sum_q V(q)(V_q f_q + V_q^* f_q^*), \end{aligned} \tag{11}$$

where

$$E_0 = \langle\phi(\vec{r})|H_{ex}|\phi(\vec{r})\rangle, \tag{12}$$

$$V(q) = \langle\phi(\vec{r})\left|e^{i\beta_2\bar{q}\cdot\vec{r}} - e^{-i\beta_1\bar{q}\cdot\vec{r}}\right|\phi(\vec{r})\rangle, \tag{13}$$

and

$$u^2 = (2M\omega/\hbar)^{1/2}. \tag{14}$$

Solving the minimum equation

$$\frac{\partial E}{\partial f_q} = \frac{\partial E}{\partial f_q^*} = 0, \tag{15}$$

one can obtain the displacement amplitudes f_q and f_q^* as follows

$$f_q = \frac{-V^*(q)V_q^*}{\hbar^2(u^2+q^2)/2M} \tag{16a}$$

and

$$f_q^* = \frac{-V(q)V_q}{\hbar^2(u^2+q^2)/2M}. \tag{16b}$$

Substituting equations (16a) and (16b) into equation (11), we obtain the variational energy as

$$E = E_0 - \sum_q \frac{|V(q)|^2|V_q|^2}{\hbar^2(u^2+q^2)/2M}. \tag{17}$$

The ground state energy of the exciton is then determined by minimizing equation (17).

3 Fractional-dimensional space approach

Now we consider a fractional dimension space description for the excitonic ground state in a PQW. The so-called fractional dimension model has been proposed to calculate the exciton binding energy in a SQW by previous authors [27,28]. In this approach, an effective dimension D of the system is simply introduced instead of the complicated calculations for the quantum well. The binding energy of the confined exciton in the well is written as [27]

$$E_n = \frac{R_y^*}{[n+(D-3)/2]^2}, \tag{18}$$

where n=1, 2, 3,... corresponds to the hydrogen-like bound state. R_y^* is the effective three dimensional (3D) Rydberg and the dimensionality D is determined by [28]

$$D = 3 - \exp\left(-L/a_B^*\right). \tag{19}$$

Here a_B^* is the 3D effective Bohr radius and L the characteristic potential confinement length in the z-direction. For a QW structure the dimension D can be determined as a value between 2 and 3 by different methods [9,27–32]. Kyrychenko et al have determined L by solving a differential equation for polarons in an "infinite" PQW [32]. Here we consider a "finite" PQW and determine L and D for excitons by a variational calculation.

The Hamiltonian of an electron (hole) moving in the finite PQW can be written as

$$H_j = -(1-\beta_j)\frac{\partial^2}{\partial z_j^2} + V_j(z_j), \ (j=1,2) \tag{20}$$

where $V_j(z_j)$ is determined by equation (2b). Choosing the trial wave function for the ground state of the electron (hole) in the system as

$$\psi(z_j) = \left(\sqrt{\frac{2}{\pi}}\frac{1}{\lambda_j}\right)^{1/2}\exp(-z_j^2/\lambda_j^2), \tag{21}$$

the corresponding variational energy is given by

$$E_j(\lambda_j) = \langle\psi(z_j)|\,H_j\,|\psi(z_j)\rangle. \tag{22}$$

Here λ_j is the variational parameter characterizing the localization range of the electron (hole) in the PQW, and can be determined by the following equation:

$$\left.\frac{\partial E_j(\lambda_j)}{\partial\lambda_j}\right|_{\lambda_j=\lambda_{j\,\min}} = 0.$$

The characteristic potential confinement length of excitons in the PQW is then chosen as the larger one in the localization ranges of the electron and hole, namely

$$L = \max(\lambda_{1\,\min}, \lambda_{2\,\min}). \tag{23}$$

As an example, we have performed the numerical calculation for the confinement length L and the dimensionality D in the finite GaAs/$Al_{0.3}Ga_{0.7}As$ PQW, and the results as functions of the half well-width are shown in Figure 1. It is found from Figure 1a that the calculated results for the confinement length L in this work are in coincidence with reference [32] in the case of larger well width, where L increases monotonously with increasing the well-width. Otherwise, when the well-width is getting narrower, L decreases monotonously for the infinite well in reference [32], but appears a minimum and then increases rapidly for the finite PQW in our results. The results are physically reasonable and will be used to calculate the excitonic energy in the finite PQW.

Now let us calculate variationally the excitonic ground-state energy by linking the LLP-like transformations with the fractional dimension model for the finite PQW. The trail wave function in equation (10) is chosen similarly to the 3D form:

$$\phi(r) = \sqrt{\frac{1}{\pi\lambda^3}}\exp\left(-\frac{r}{\lambda}\right), \tag{24}$$

but the variational parameterλ is related to the space fractional dimension D. The variational calculation will be performed in the D-dimensional space.

As we well-known, the variational energy of the exciton ground state in a 3D system is written as

$$E_0^{(3)} = \langle\phi(r)|-\nabla^2 - 2/r|\phi(r)\rangle = \frac{1}{\lambda^2} - \frac{2}{\lambda}. \tag{25}$$

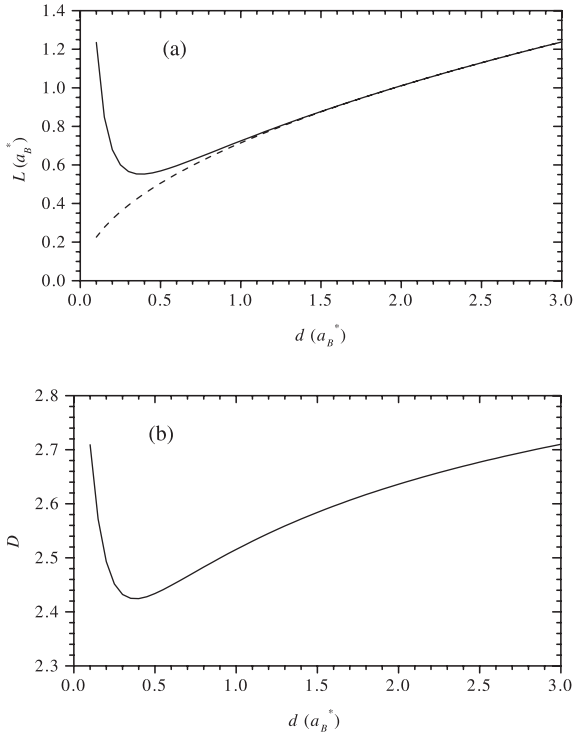

Fig. 1. Characteristic potential confinement length (a) and the fractional dimension (b) as functions of the half well-width in the GaAs/$Al_{0.3}Ga_{0.7}$As PQW. The dashed line in (a) is the result of reference [32] in the infinite PQW approximation.

Here the energy is measured in the 3D Rydberg and the length in 3D Bohr radius. Extending this expression into the fractional dimension model, the excitonic ground-state energy in the PQW can be written as the D-dimensional space form:

$$E_0^{(D)} = \frac{1}{\lambda^2} - \frac{2}{\lambda\,(1 - e^{-L}/2)}. \tag{26}$$

Minimizing (26), the variational parameter and the upper-limit energy of the exctionic ground state without the phonon influence can be easily determined as

$$\lambda = \left(1 - e^{-L}/2\right) \tag{27a}$$

and

$$E_0^{\min} = -\frac{1}{\left(1 - e^{-L}/2\right)^2}. \tag{27b}$$

It is expected that the variational parameter λ reduces to 1 and equation (26) degenerates to the 3D form ($E_0^{(3)} = -1$) when $L \to \infty$, otherwise λ reduces to 1/2 and the 2D result ($E_0^{(2)} = -4$) is obtained at the limit of $L \to 0$.

Substituting (24) into (12) and (13) and then (17), we obtain finally the variational energy of the exciton including the LO-phonon effect in the fractional dimensional model:

$$E(\lambda) = \frac{1}{\lambda^2} - \frac{2}{\lambda\,(1 - e^{-L}/2)} - \alpha\hbar\omega\frac{2}{\pi}\int_0^\infty dx \frac{1}{1 + \beta_1\beta_2 x^2}\left[\frac{16}{[4 + (\beta_1\lambda u x)^2]^2} - \frac{16}{[4 + (\beta_2\lambda u x)^2]^2}\right]^2, \tag{28}$$

where $\alpha = (Me^2/\hbar^2 u)(1/\varepsilon_\infty - 1/\varepsilon_0)$ is the exciton-phonon coupling constant. The above-obtained numerical results of the confinement length L will be used in the computation for the excitonic energy.

The ground state energy of the exciton-phonon system is given by

$$E_g = \min_\lambda E(\lambda). \tag{29}$$

The exciton binding energy E_b can be defined by

$$E_b = E_{free} - E_g. \tag{30}$$

In equation (30) E_{free} is the sum of the energies of the free electron and hole polarons, which can be calculated by the method used in reference [15], and here we use the results directly but omit the detail for short.

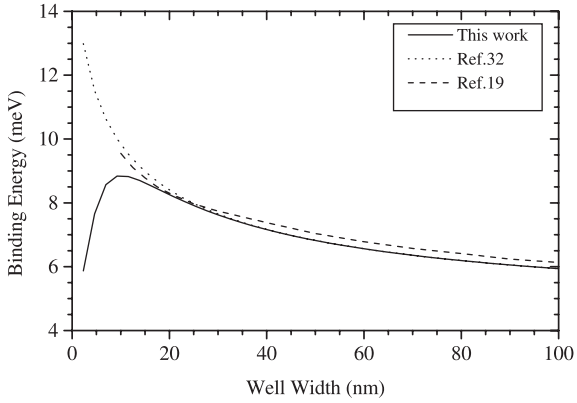

Fig. 2. Binding energies of the exciton without phonon influence as functions of the well-width for the GaAs/$Al_{0.3}Ga_{0.7}$As PQW. The solid line is given by this work and "dotted" and "dashed" lines by the methods of references [32] and [19] respectively.

4 Numerical results and discussions

The binding energy of the exciton in the GaAs/$Al_{0.3}Ga_{0.7}$As PQW have been computed numerically by the fractional-dimension variational approach and the results are illustrated in Figures 2–5.

Our results for the excitonic binding energy without including the phonon influence in the finite-barrier GaAs/$Al_{0.3}Ga_{0.7}$As PQW are plotted as a function of the well-width in Figure 2 (solid line). Kyrychenko et al has

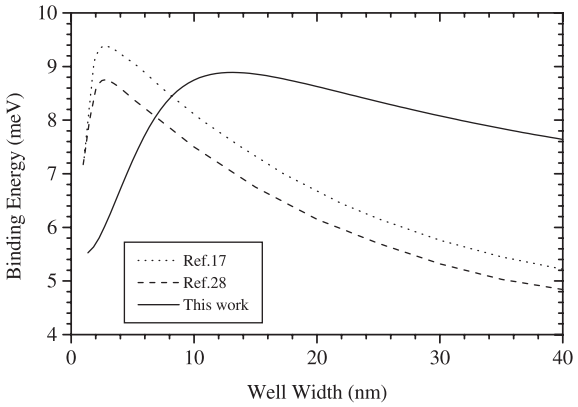

Fig. 3. Binding energies of the exciton without phonon influence as functions of the well-width for the GaAs/$Al_{0.3}Ga_{0.7}$As PQW given by this work (solid line), and for the SQW from reference [17] (dotted) and reference [28] (dashed line) respectively.

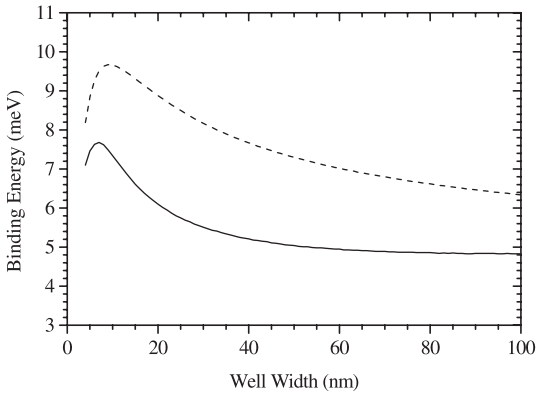

Fig. 4. Exciton binding energies with (solid line) and without phonon contributions (dashed line) as functions of the well-width in the finite GaAs/$Al_{0.3}Ga_{0.7}$As PQW.

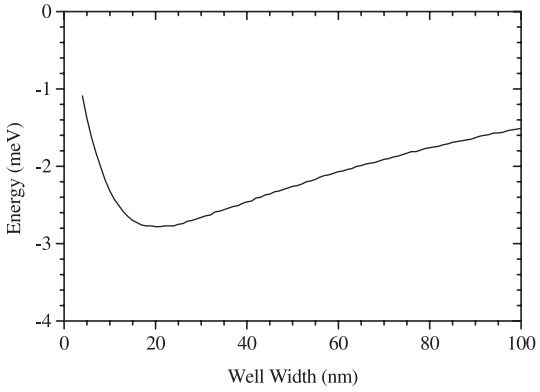

Fig. 5. Contribution of LO-phonons to the binding energy of the exciton as a function of the well-width in the finite GaAs/$Al_{0.3}Ga_{0.7}$As PQW.

calculated the excitonic binding energies in the infinite CdTe/$Cd_{0.8}Mn_{0.2}$Te PQW by using fractional dimension model [32]. We have calculated the corresponding energies in the infinite GaAs/$Al_{0.3}Ga_{0.7}$As PQW by using their model and plot the curve (dotted line) in Figure 2 for comparison. In the meantime, we also illustrate the general variational results (dashed line) for the infinite GaAs/$Al_{0.3}Ga_{0.7}$As PQW given by Yang et al. [19] in the same figure. For ease of comparison, the material parameters in the calculations have been chosen as those used by the previous authors [19].

It is seen that the binding energy increase monotonously with decreasing the well-width and our result is excellently in agreement with those given by the previous methods [19,32] for the wide-well case. Otherwise, in the narrower well region the binding energy curve of this work for the finite-depth PQW system gets a knee point qualitatively different from those in infinite-depth well approximation, where the binding energies increase monotonously to the 2D values as the well-width tends to zero. It is easily understood that the binding energy first increases with decreasing the well-width for the wider-well case, since the exciton wave function remains mainly confined in the well. Once the well-width is reduced and less than the exciton size, the excitonic wave function will penetrates into the barriers so that the binding energy decreases suddenly. It follows that the fractional-dimension variational approach gives the reasonable results and is simpler and useable for finite PQW systems.

In Figure 3 we compare our result for the GaAs/$Al_{0.3}Ga_{0.7}$As PQW with those for the SQW obtained by a variational approach [17] and the fractional dimension model [28]. It can be seen that the exciton binding energies in the PQW are smaller than those in the SQW at small well-widths, but larger than those at larger well-widths. This is due to the fact that the wave functions in the PQW penetrate more easily into the barriers than that in the SQW for the narrow wells, but the confinement is stronger than the latter in the wider well case.

Figure 4 plots the curves of the binding energies of the exciton with and without phonon contributions respectively as functions of the well-width in the finite GaAs/$Al_{0.3}Ga_{0.7}$As PQW. It is found that the binding energies of the exciton, either with or without the phonon contributions, increase rapidly at beginning with increasing the well-width and get the maxima at a well-width of around 10nm, then decrease and finally approach to their 3D values when the well-width is large enough. Moreover, it is also seen that the binding energy is reduced by the exciton-phonon interaction because of the phonon screening on the Coulomb potential. The contribution of the exciton-phonon coupling to the binding energies is around 15–30% for the calculated system and cannot be neglected.

To understand the polaron effect clearly, we have also illustrated the contribution of LO-phonons to the binding energy of the exciton in the same system as a function of the well-width in Figure 5. It is shown that the contribution of LO-phonons varies non-monotonously because of the non-monotony of the dimension D with the well-width. When the well-width decreases, the exciton-phonon coupling effect increases firstly with the reduction of the system dimension D and then gets a maximum at a well-width slightly over the exciton size, where the exciton

localization is almost strongest and the fractional dimension of the system is smallest. Once the well-width is less than the above-mentioned width, the e-p contribution to the binding energy is reduced with the penetration of the exciton wave function.

5 Conclusions

In summary, we have introduced a fractional-dimensional variational approach to calculate the binding energy of an exciton interacting with bulk longitudinal optical phonons in finite-barrier parabolic quantum wells. The confinement length and the space dimension for an exciton-phonon system in a parabolic quantum well have been determined and used in the variational calculation. As an example, the numerical results for the $GaAs/Al_{0.3}Ga_{0.7}As$ parabolic quantum well are given. It is found that the binding energies of excitons are reduced by the exciton-phonon interaction and the corresponding polaronic effects are un-negligible. The exciton binding energies and the phonon contributions as functions of the well-width have their maxima because of the penetration of the exciton wave function, different from those in infinite quantum well approximation. It is demonstrated that the fractional-dimension variational approach developed here is useable in the investigations of excitonic polaron problems in parabolic quantum wells.

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