Front. Phys. 10, 107302 (2015)
DOI 10.1007/s11467-015-0472-2

RESEARCH ARTICLE

Novel method to determine effective length of quantum confinement using fractional-dimension space approach

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Received December 3, 2014; accepted March 23, 2015

The binding energy and effective mass of a polaron confined in a GaAs film deposited on an $Al_xGa_{1-x}As$ substrate are investigated, for different film thickness values and aluminum concentrations and within the framework of the fractional-dimensional space approach. Using this scheme, we propose a new method to define the effective length of the quantum confinement. The limitations of the definition of the original effective well width are discussed, and the binding energy and effective mass of a polaron confined in a GaAs film are obtained. The fractional-dimensional theoretical results are shown to be in good agreement with previous, more detailed calculations based on second-order perturbation theory.

Keywords fractional-dimensional approach, effective length of quantum confinement, polaron effect, GaAs film

PACS numbers 73.61.-r, 73.90.+f

1 Introduction

A considerable amount of research has been devoted to the study of the physical phenomena occurring in low-dimensional systems, such as quantum wells, core-shell structures, and quantum dots. One phenomenon that has attracted considerable research attention is the polaron effect. It is well known that the electron-longitudinal optical (LO) phonon interaction leading to the polaron effect may be modified significantly through confinement. Such modifications to the polaron effect can strongly influence the optical and transport properties of polar low-dimensional systems; this is particularly true for certain commonly used quantum wells (QW's), such as GaAs film deposited on an $Al_xGa_{1-x}As$ substrate. Consequently, polarons in bulk material have been investigated and a wide variety of theoretical models have been proposed by various researchers. However, the majority of these models involve tedious calculations with high computational cost [1–3]. We perform our present work using the fractional-dimensional space framework developed by Stillinger [4], He [5], Mathieu *et al.* [6], and Lefebvre *et al.* [7–9]. In the fractional-dimensional space approach, anisotropic interactions in the real three-dimensional (3D) space are treated as isotropic interactions in an effective fractional-dimensional system, the dimension of which constitutes a measure of the degree of anisotropy of the actual physical system. Thus, all anisotropy-related information can be introduced through a single value, i.e., the dimensionality. Through consideration of this simple value, the real system can be modeled in a simple analytical manner. In recent years, the fractional-dimensional space approach has been successfully applied to the modeling of excitons [7, 8, 10, 12], polarons [13, 17], and impurity states [18–21] in semiconductor hetero-structures.

In this study, we examine the application of the fractional-dimensional space approach to the polaron in a GaAs film deposited on an $Al_xGa_{1-x}As$ substrate [22, 23]. Hence, the polaron binding energy E, fractional dimension D, and the polaron effective mass m^* are calculated as functions of the film thickness L_w. However, we find that a problem arises as a result of the definition of the original effective well width L_w^* Specifically, a deformation divergence is exhibited for the GaAs film deposited on the $Al_xGa_{1-x}As$ substrate if the method proposed in previous literature is applied [22, 23]. When that approach is adopted, the E and D curves inevitably exhibit significant mutation. In this paper, we propose a new approach to defining the effective length of the quantum confinement L_w^*, because of the abovementioned limitations of the definition of the original effective a. The E, D, and m^* of a polaron confined in a GaAs film deposited on an $Al_xGa_{1-x}As$ substrate are then obtained. This paper is organized as follows. In Section 2, the theoretical basis of the fractional-dimensional model for polarons in symmetric [13-15] and asymmetric [16] quantum wells is extended to the case of polarons confined in our GaAs-$Al_xGa_{1-x}As$ system. The definition of$L_w^*$is discussed in Section 3, and numerical results and discussion are provided in Section 4.

2 Fractional-dimensional space approach

We consider the problem of a polaron confined in a GaAs film deposited on an $Al_xGa_{1-x}As$ substrate, and assume that no electron can escape from the system. The system potential is characterized by

$$V(z)=\begin{cases} V_w(=0), & \text{if } 0\leqslant z\leqslant L_w,\\ V_b, & \text{if } L_w<z\leqslant L_w+L_b,\\ \infty, & \text{otherwise}\end{cases} \tag{1}$$

where L_b represents the substrate thickness. The subscripts w and b indicate the film (GaAs, the quantum well material) and substrate ($Al_xGa_{1-x}As$, barrier material) regions, respectively. This system possesses a small electron-phonon coupling constant ($\alpha \ll 1$); consequently, we restrict our study to the weak-coupling case. The potentials of the electrons as functions of the structure are shown in Fig. 1.

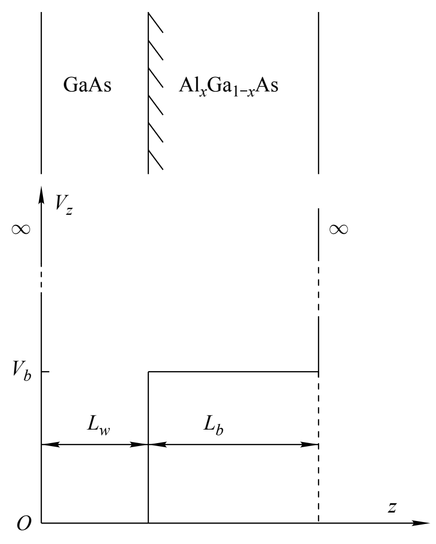

Fig. 1 The potential energy function in GaAs film deposited on $Al_xGa_{1-x}As$ substrate.

Within the fractional-dimensional space approach, the actual confined polaron is modeled through an unconfined effective fractional-dimensional polaron. The fractional-dimensional polaronic corrections were previously calculated in Refs. [8, 11], using second-order perturbation theory, and the polaron energy shift was found to be given by

$$\Delta E=\alpha\hbar\omega_{\mathrm{LO}}G_1(D), \tag{2}$$

with

$$m^*=\frac{m}{1-\alpha G_2(D)}. \tag{3}$$

In Eqs. (2) and (3), α is the Fröhlich constant, ω_{LO} is the LO-phonon limit frequency in the non-dispersive approximation, and m is the electron effective mass. The D-dependent functions, $G_1(D)$ and $G_2(D)$, are given by

$$G_1(D)=\frac{\sqrt{\pi}}{2}\frac{\Gamma\left[(D-1)/2\right]}{\Gamma\left[D/2\right]}, \tag{4a}$$

$$G_2(D)=\frac{\sqrt{\pi}}{4}\frac{\Gamma\left[(D-1)/2\right]}{D\Gamma\left[D/2\right]}, \tag{4b}$$

respectively. In Eqs. (4), $\Gamma(x)$ represents the Gamma function. D, which guarantees the mapping of the actual system into the fractional-dimensional environment, can be calculated through the relation [8, 11–13]

$$D=3-\exp\left[-\frac{L_w^*}{2R_p}\right], \tag{5}$$

where $2R_P$ (polaron radius $R_P=\sqrt{\hbar/(2m)\omega_{\mathrm{LO}}}$) is the polaron diameter.

The Schrödinger equation

$$\left[-\frac{\hbar^2}{2}\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{m\left(z\right)}\frac{\mathrm{d}}{\mathrm{d}z}\right)+V_z\right]\Psi(z)=E\Psi(z), \tag{6}$$

which describes the motion of the single electron confined in $V(z)$ [Eq. (1)] can be solved, where$E$ represents the electron ground-state energy in the GaAs-$Al_xGa_{1-x}As$ system and $m(z)$ represents the electron z-dependent effective mass. Note that

$$m_z=\begin{cases} m_w, & \text{if } 0\leqslant z\leqslant L_w,\\ m_b, & \text{if } L_w<z<L_w+L_b.\end{cases} \tag{7}$$

In a GaAs film deposited on an $Al_xGa_{1-x}As$ substrate system, the material parameters that characterize the polaron properties differ when passing from the film to the substrate region. To take this fact into consideration, we assign average values of the material parameters over all the polaron positions to the effective fractional-dimensional bulk. If one considers the polaron as a phonon cloud around the electron, the polaron position is determined, essentially, by the electron position. The mean values of the material parameters that characterize the fractional-dimensional electron-phonon interaction can therefore be expressed as [15]

$$m^{-1} = \sum_{i=w,b} \frac{P_i}{m_i}, \tag{8}$$

$$\omega_{\rm LO} = \sum_{i=w,b} \omega_i P_i, \tag{9}$$

and

$$\alpha = \left[\sum_{i=w,b} \left(P_i \frac{\omega_i}{\omega_{\rm LO}} \sqrt{\alpha_i \sqrt{\frac{m\omega_{\rm LO}}{m_i \omega_i}}} \right) \right]^2, \tag{10}$$

$$R_p = \left[\sum_{i=w,b} \left(P_i \frac{\omega_i}{\omega_{\rm LO}} \sqrt{\frac{\alpha_i R_{pi}}{\alpha}} \right) \right]^2, \tag{11a}$$

$$R_{pi} = \sqrt{\frac{\hbar}{2m_i\omega_i}}. \tag{11b}$$

In Eqs. (8)–(11), α_i and ω_i represent the Fröhlich constants and the phonon frequencies in the different regions, respectively, and

$$P_w = \int_0^{L_w} |\Psi(z)|^2 {\rm d}z, \tag{12a}$$

$$P_b = 1 - P_w, \tag{12b}$$

denote the probabilities of finding the single electron in the film (GaAs, the well material) and substrate ($Al_xGa_{1-x}As$, the barrier material) regions, respectively. The E and m^* of a polaron confined in a GaAs film deposited on an $Al_xGa_{1-x}As$ substrate can then be computed in a very simple manner from Eqs. (2), (3), and (5), assuming the material parameter mean values defined in Eqs. (8)–(12). E and m^* can also be calculated as functions of L_w. The numerical results and discussion related to this case have already been given [22, 23].

3 Discussion of the effective length of the quantum confinement

Note that D in Eq. (5) is significantly influenced by the definition of the electron L_w^*. A large number of studies [6, 13–16] present the following definition

$$L_w^* = L_w + \frac{1}{k_b}, \tag{13}$$

where k_b represents the electron wave vector in the substrate. By solving the Schrödinger equation (6), the values of k_b can be obtained from the relation

$$k_b = \frac{\sqrt{2m_b(V_b - E)}}{\hbar}, \tag{14}$$

where $\hbar$ is the reduced Planck constant. Because E is a function of the L_w of the GaAs film deposited on the $Al_xGa_{1-x}As$ substrate, E varies in response to changing L_w. We note that k_b in the substrate tends to zero if $E = V_b$ when L_w has a certain value. Then, L_w^* tends to infinity and D appears to have an outburst value. After solving Eqs. (13) and (5), the values of L_w^* and D, respectively, are obtained for our system. However, these results are unphysical because of the outburst value. This is the problem affecting the application of the traditional fractional-dimensional space approach to the case of a GaAs film deposited on an $Al_xGa_{1-x}As$ substrate.

As we know, E and a in a one-dimensional infinite potential are related by

$$E = \frac{\pi^2\hbar^2}{2m_e a^2}. \tag{15}$$

By solving the Schrödinger equation (6), the eigenenergy E in our system can be found, and we obtain a from Eq. (15). Then, we can define $L_w^* \equiv a$. Through this new approach to determining L_w^*, the outburst value problem is solved directly, and the L_w^* and D values of our system can also be obtained. To summarize the motivation and justification for the new method presented here, we propose to use the equivalent width of the structure as the electron L_w^*. The equivalent width is defined as the width at which the E of the electrons in the actual structure are equal to an energy level of a of the infinite-depth potential well; thus, a is the electron L_w^*, as given by Eq. (15).

We can verify the rationality of Eq. (15) as follows. Taking V_b= 0 in the system shown in Fig. 1, the $E$of our system is equal to the energy level of the well width $L_w + L_b$ of the infinite-depth potential well. Then, the electron L_w^* is also $L_w + L_b$. If $V_b = \infty$ in the setup shown in Fig. 1, the E of our system is equal to the energy level of the well width L_w of the infinite-depth potential well, and the electron L_w^* is also L_w. Finally, if V_b is between 0 and infinity, the electron L_w^* is between L_w and $L_w + L_b$. So, it is appropriate to replace Eq. (13) with Eq. (15) when calculating D and E. Therefore, the calculated results of L_w^*, D, and $E$for our system should change monotonously within the range of the potential well width.

In order to compare results calculated using the method proposed in this paper with those reported in Refs. [16, 22, 23], we have used the same set of material parameters as in Ref. [16]. Further, we consider L_w^*, D, and E as functions of the L_w of the GaAs film deposited on the $Al_xGa_{1-x}As$ substrate, for L_b = 2 nm and $x = 0.3$. The calculated results for these functions are presented in Figs. 2, 3, and 4, respectively. In these figures, the dashed lines correspond to the results of our calculations using the traditional fractional-dimensional space approach [16], while the solid lines represent the results of calculations performed using the proposed new method. It is obvious from the dashed line in Fig. 2 that L_w^* decreases as L_w decreases from a wide well width. With a continued decrease in L_w, L_w^* exhibits a sudden increase near $L_w = 4.0$ nm according to the dashed lines, and then decreases suddenly near $L_w = 3.6$ nm. That is to say, the entire curve exhibits a significant mutation as L_w decreases from a wide well width to zero. This exemplifies the problem that renders the traditional fractional-dimensional space approach unsuitable for our actual physical system. In contrast, the solid line indicating the results calculated using our new method decreases monotonously as L_w decreases, for the entire range of L_w values. One can observe that L_w^* is always slightly larger than L_w, at any position on the graph. It is easily understood that, as L_w decreases, the system becomes increasingly confined, and the polaron in turn becomes increasingly compressed. Thus, L_w^* also decreases monotonously. However, at the critical interface between the film and the substrate, the polaron wave function penetrates the substrate so that L_w^* varies more quickly than L_w.

Within the range of the potential well width, the solid line in Fig. 4, which represents the values of D calculated using the proposed approach, increases monotonously for continuously increasing L_w. However, the dashed line indicating the results obtained using the traditional method exhibits a significant mutation. In the same manner, the solid line in Fig. 5, which represents the E calculated using our approach, decreases monotonously for continuously increasing L_w, while the dashed line exhibits a corresponding significant mutation.

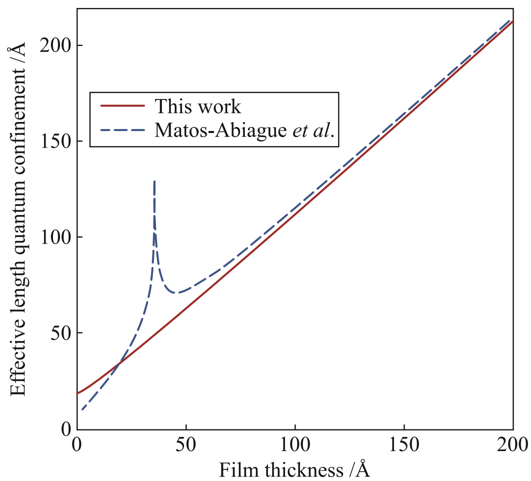

Fig. 2 The fractional-dimensional polaron effective length of quantum confinement as a function of the film thickness in the GaAs film deposited on the $Al_{0.3}Ga_{0.7}As$ substrate at the substrate thickness $L_b = 20$ Å. Solid curve correspond to our new method result and the dash curve to calculation by Matos-Abiague *et al.* [16].

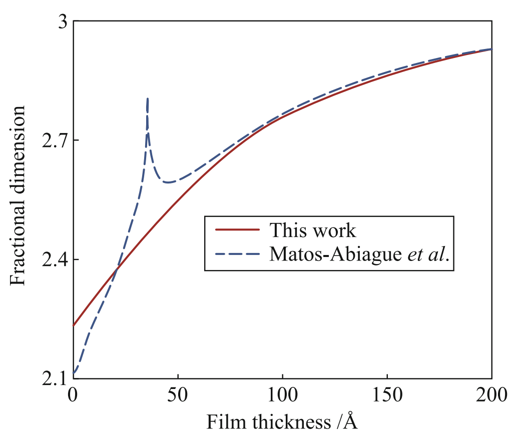

Fig. 3 The corresponding fractional dimension as a function of the film thickness for a polaron confined in the GaAs film deposited on the $Al_{0.3}Ga_{0.7}As$ substrate at the substrate thickness $L_b = 20$ Å . Solid curve correspond to our new method result and the dash curve to calculation by Matos-Abiague *et al.* [16].

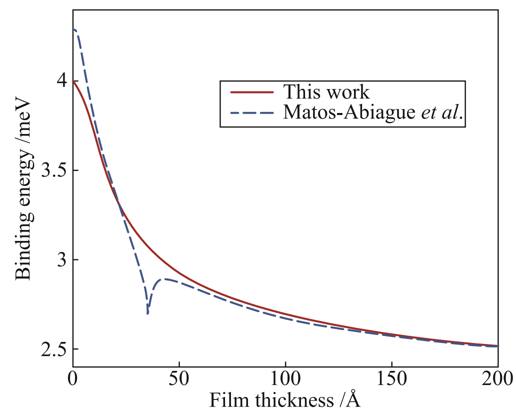

Fig. 4 The fractional-dimensional polaron binding energy as a function of the film thickness in the GaAs film deposited on the $Al_{0.3}Ga_{0.7}As$ substrate at the substrate thickness $L_b = 20$ Å. Solid curve correspond to our new method result and the dash curve to calculation by Matos-Abiague *et al.* [16].

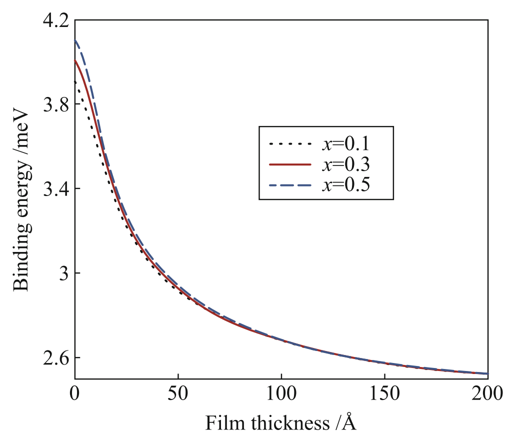

Fig. 5 The fractional-dimensional polaron binding energy as a function of the film thickness in the GaAs film deposited on the $Al_xGa_{1-x}As$ substrate for different aluminum concentration at the substrate thickness $L_b = 20$ Å.

4 Numerical results and discussion

Above, the value of D as a function of the L_w of the GaAs film deposited on the $Al_xGa_{1-x}As$ substrate was calculated using our new method, for $L_b = 20$ Å and $x = 0.3$. The results are displayed in Fig. 3 (solid line). It can be seen that, as L_w increases from zero to a wide well width, D increases monotonously for a given aluminum concentration.

In Figs. 5 and 6, E and m^* decrease in the GaAs film deposited on the $Al_xGa_{1-x}As$ substrate with increasing L_w and $L_b = 20$ Å. The results exhibit the same tendencies for different aluminum concentrations, as shown in these figures. It is remarkable that the different values of aluminum concentration obviously influence E and m^* for cases of narrow and medium L_w, but have no significant influence in cases of large L_w. To understand the E and m^* results more clearly, we consider the case of varying E. As the analysis of the variation in m^* is quite similar, we omit this discussion. In order to understand the origin of the changes in E, we first review Eq. (2), which indicates that E depends on the factor $\alpha\hbar\omega_{\mathrm{LO}}$, and also on $G_1(D)$. We know that $\alpha\hbar\omega_{\mathrm{LO}}$ depends on the material parameters only, and that it varies slowly and monotonously with L_w. In contrast, $G_1(D)$ depends on the dimensionality of the effective system and varies monotonously, but rapidly, if $L_w < 4.6$ nm. In other regions, $G_1(D)$ varies slowly. This behavior leads to the curved shape of $E$for different aluminum concentrations and narrow or medium L_w, as shown in Fig. 6.

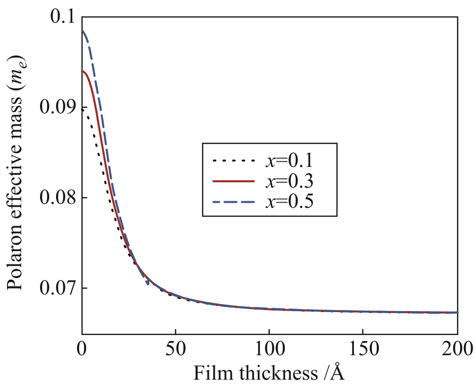

Fig. 6 The fractional-dimensional polaron effective mass as a function of the film thickness in the GaAs film deposited on the $Al_xGa_{1-x}As$ substrate for different aluminum concentration at the substrate thickness $L_b = 20$ Å.

In summary, we extended the fractional-dimensional space approach to the study of polarons confined in a GaAs film deposited on an $Al_xGa_{1-x}As$ substrate. We defined the effective length of the quantum confinement in order to solve the problem of the mutating polaron dimensional parameter reported in the literature. Because the electron ground-state energy and barrier height are approximately equal at certain film thicknesses, the electron wave vector becomes equal to zero and its reciprocal becomes infinite. Thus, the dimensional parameter exhibits significant mutation in response to changes in the film thickness. The definition of the effective length of the quantum confinement is based on the determination of the effective length of the quantum confinement of the sandwich structure. When the ground-state energy of our system is equivalent to the energy of the infinite-depth potential well, the width of the infinite-depth potential well is defined as the effective length of the quantum confinement. And furthermore, we find dimensional parameter D is different for different aluminum concentrations at a certain film thickness. That leads to the curves shape of the binding energy E and polaron effective mass m^* corresponding changes.

The fractional-dimensional space approach allows the well-width dependence of the polaron binding energy and the polaron effective mass to be estimated in a very simple manner, avoiding the tedious and complicated calculations arising in the standard treatments. However, the behavior of polarons in thin film differs from that in sandwich structures. In this article, through application of different definitions of the effective length of the quantum confinement, the characteristics of polarons in thin films were calculated, and their responses to changes in the film thickness were examined. This approach has reference value to the field of thin film electronics and to optoelectronic devices.

Acknowledgements The authors are grateful for the financial support received during the development of this work from the National Natural Science Foundation of China (Grant Nos. 10574011 and 10974017).

References

1. L. Wendler and R. Haupt, Electron-phonon interaction in semiconductor superlattices, *Phys. Status Solidi B* 143(2), 487 (1987)
2. N. Mori and T. Ando, Electron optical-phonon interaction in single and double heterostructures, *Phys. Rev. B* 40(9), 6175 (1989)
3. X. X. Lang, The interaction of interface optical phonons with an electron in an asymmetric quantum well, *J. Phys.: Condens. Matter* 4(49), 9769 (1992)
4. F. H. Stillinger, Axiomatic basis for spaces with non integer dimension, *J. Math. Phys.* 18(6), 1224 (1977)
5. X. F. He, Excitons in anisotropic solids: The model of fractional dimensional space, *Phys. Rev. B* 43(3), 2063 (1991)

6. H. Mathieu, P. Lefebvre, and P. Christol, Simple analytical method for calculating exciton binding energies in semiconductor quantum wells, *Phys. Rev. B* 46(7), 4092 (1992)

7. P. Lefebvre, P. Christol, and H. Mathieu, Excitons in semiconductor superlattices: Heuristic description of the transfer between Wannier-like and Frenkel-like regimes, *Phys. Rev. B* 46(20), 13603 (1992)

8. P. Christol, P. Lefebvre, and H. Mathieu, Fractional-dimensional calculation of exciton binding energies in semiconductor quantum wells and quantum-well wires, *J. Appl. Phys.* 74(9), 5626 (1993)

9. P. Lefebvre, P. Christol, H. Mathieu, and S. Glutsch, Confined excitons in semiconductors: Correlation between binding energy and spectral absorption shape, *Phys. Rev. B* 52(8), 5756 (1995)

10. M. Dios-Leyva, A. Bruno Alfonso, A. Matos-Abiague, and L. E. Oliveira, Excitonic and shallow-donor states in semiconducting quantum wells: A fractional dimensional space approach, *J. Phys.: Condens. Matter* 9(40), 8477 (1997)

11. A. Matos-Abiague, L. E. Oliveira, and M. de Dios-Leyva, Fractional-dimensional approach for excitons in GaAs-$Ga_{1-x}Al_xAs$ quantum wells, *Phys. Rev. B* 58(7), 4072 (1998)

12. Z. P. Wang and X. X. Liang, Electron-phonon effects on Stark shifts of excitons in parabolic quantum wells: Fractional-dimension variational approach, *Phys. Lett. A* 373(30), 2596 (2009)

13. A. Matos-Abiague, A fractional-dimensional space approach to the polaron effect in quantum wells, *J. Phys.: Condens. Matter* 14(17), 4543 (2002)

14. A. Matos-Abiague, Fractional-dimensional space approach for parabolic-confined polarons, *Semicond. Sci. Technol.* 17(2), 150 (2002)

15. A. Matos-Abiague, Polaron effect in GaAs-$Ga_{1-x}Al_xAs$ quantum wells: A fractional-dimensional space approach, *Phys. Rev. B* 65, 165321 (2002)

16. R. L. R. Suárez and A. Matos-Abiague, Fractional-dimensional polaron corrections in asymmetric GaAs-$Ga_{1-x}Al_xAs$ quantum wells, *Physica E* 18(4), 485 (2003)

17. A. Thilagam and A. Matos-Abiague, Excitonic polarons in confined systems, *J. Phys.: Condens. Matter* 16(23), 3981 (2004)

18. E. R. Gómez, L. E. Oliveira, and M. de Dios Leyva, Shallow impurities in semiconductor superlattices: A fractional-dimensional space approach, *J. Appl. Phys.* 85(8), 4045 (1999)

19. I. D. Mikhailov, F. J. Betancur, R. A. Escorcia, and J. Sierra-Ortega, Shallow donors in semiconductor heterostructures: Fractal dimension approach and the variational principle, *Phys. Rev. B* 67(11), 115317 (2003)

20. J. Kundrotas, A. Cerškus, S. Ašmontas, Steponas Asmontas, G. Valusis, B. Sherlikerl and M. P. Harrison, Excitonic and impurity-related optical transitions in Be delta-doped GaAs/AlAs multiple quantum wells: Fractional-dimensional space approach *Phys. Rev. B* 72(23), 235322 (2005)

21. J. Kundrotas, A. Cerškus, S. Ašmontas, G. Valušis, M. P. Halsall, E. Johannessen, and P. Harrison, Impurity-induced Huang–Rhys factor in beryllium δ-doped GaAs/AlAs multiple quantum wells: Fractional-dimensional space approach, *Semicond. Sci. Technol.* 22(9), 1070 (2007)

22. Z. H. Wu, H. Li, L. Yan, B. Liu, and Q. Tian, The polaron in a GaAs film deposited on $Al_xGa_{1-x}As$ influenced by the thickness of the substrate, *Superlattices Microstruct.* 55, 16 (2013)

23. Z. H. Wu, H. Li, L. Yan, B. Liu, and Q. Tian, Polaron effect in a GaAs film: The fraction-dimensional space approach, *Acta Phys. Sin.* 62, 097302 (2013) (in Chinese)