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Exciton and donor binding energies in quantum-well wires and quantum dots a fractional-dimensional space approach*

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A simple method for calculating the free-exciton binding energies in the fractional-dimensional-space model for single-quantum-well structure has been extended to quantum-well wires and quantum dots, in which the real anisotropic system is modelled through an effective isotropic environment with a fractional dimension. In this scheme, the fractional-dimensional parameter is chosen via an analytical procedure and involves no *ansatz*. We calculated the ground-state binding energies of excitons and donors in quantum-well wires with rectangular cross sections. Our results are found to be in good agreement with previous variational calculations and available experimental measurements. We also discussed the ground-state exciton binding energy changing with different shapes of quantum-well wires.

Keywords: binding energy, fractional-dimensional
PACC: 7850G, 7135

1. Introduction

With the recent advances in the technique of molecular-beam epitaxy, it is possible to confine electrons in extremely thin semiconducting wires, namely, quantum-well wires. In these quasi-one-dimensional structures the electron motion along the length of the wire is free but is quantized in the two dimensions perpendicular to the wire. In particular, due to their large binding energies, oscillator strengths, and confinement effects, excitons may have a large influence on a variety of physical phenomena observed in such heterostructures, and have attracted considerable attention from the experimental, theoretical, and technological points of view.[1−22]

Several authors have calculated binding energies of excitons in both infinite and finite quantum wires (QWs). All these calculations are variational,[9,10] which do or do not include different phenomena such as valence-band mixing, nonparabolicity of dispersion relations, effective-mass, and/or dielectric-constant mismatch between the well and barrier materials, Coulomb coupling between excitons belonging to different subbands, etc. These calculations require significant computation time and the accuracy of the result depends to a large extent on the form of the trial wavefunction. In the last few years, the concept of fractional-dimensional space has been successfully used in the study of the optical spectra and excitonic properties of anisotropic systems.[11−13]

Although the space of the real world is 3D Euclidean, the motion of material objects is not always in three dimensions. The dimensionality depends on restraint conditions. Some people adopt the fractional-dimensional approach to calculating exciton binding energies.[11,14−18] The excitons in an anisotropic solid are treated as being in an isotropic fractional-dimensional space, where the dimension is determined by the degree of anisotropy. Such a space, termed dynamic space, differs from the one that embeds geometric bodies in that its dimensionality is determined by the physical interactions. Thus the Schrödinger equation is solved in a noninteger-dimensional space, where the interactions are assumed to occur in an effectively isotropic environment. The Schrödinger

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equation is in fact that of an αD hydrogen atom problem, for which the discrete bound-state energies and orbital radii are[19] $E_n = E_g - \frac{\frac{1}{1+\sigma}\mathrm{Ry}^*}{\left(n+\frac{\alpha-3}{2}\right)^2}$, $a_n = (1+\sigma)a^*\left(n+\frac{\alpha-3}{2}\right)^2$, where $n = 1, 2, 3\ldots$, is the principal quantum number, $\sigma = \frac{m_e^*}{m_h^*}$, Ry^* and a^* are, respectively, the Rydberg and Bohr radius, either for excitons or for donors. The binding energy of 1s exciton is given by

$$E_b = \left(\frac{2}{\alpha-1}\right)^2\left(\frac{1}{1+\sigma}\right)\mathrm{Ry}^*. \quad (1)$$

For the determination of the fractional-dimensional parameter α, there are roughly speaking two approaches. One of them is the MLC[15,16,18] approach in particular. A systematic study has been done in the area of excitonic states and absorption spectra in semiconductor QW,[15] quantum-well wires, and double QWs,[16] in which one assumes an *ansatz* for the choice of the fractional dimension, and the other adopts a systematic procedure to determine the α parameter to avoid an *ansatz* for the choice of the fractional dimension,[11–13,17] and it was successfully used in the study of some excitonic and shallow impurity properties confined in QW, in which $2 < \alpha < 3$. The Hamiltonian corresponding to the hydrogen atom in a fractional α-dimensional space is

$$H_\alpha = -\frac{\hbar^2}{2\mu_w}\left[\frac{1}{r^{\alpha-1}}\frac{\partial}{\partial r}\left(r^{\alpha-1}\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin^{\alpha-2}\theta}\frac{\partial}{\partial\theta}\left(\sin^{\alpha-2}\theta\frac{\partial}{\partial\theta}\right)\right] - \frac{e^2}{\epsilon r}, \quad (2)$$

where $\alpha = 3$ and $\alpha = 2$ are respectively identical to the 3-dimensional and 2-dimensional hydrogen atom Hamiltonian. When $\alpha < 2$, the situation is unfamiliar and it is necessary to examine its applicability to lower-dimensional physics such as the excitonic and impurity properties in quantum-well wires and quantum dots, etc.

In Sec.2 we present the theoretical framework of fractional-dimensional scheme used in the calculations of excitons and donors confined in quantum-well wires and quantum dots, together with a systematic procedure for the determination of the fractional dimension for ground states. Theoretical results, discussions and conclusions are given in Sec.3.

2. Theory

We consider the problem of an exciton confined in a quantum-well wire with rectangular cross section. The Hamiltonian for the exciton is given by

$$\left[-\frac{\hbar^2}{2m_e^*}\nabla_e^2 - \frac{\hbar^2}{2m_h^*}\nabla_h^2 + V_e + V_h\right] \times f_e(x_e, y_e)f_h(x_h, y_h)\psi(\boldsymbol{R}, \boldsymbol{r}) = E' f_e(x_e, y_e)f_h(x_h, y_h)\psi(\boldsymbol{R}, \boldsymbol{r}), \quad (3)$$

where the z-direction is the free axis, $m_e{}^*$ and $m_h{}^*$ are the effective masses of the electron and hole, respectively, and V_e and V_h are the corresponding confining potentials. $\psi(\boldsymbol{R}, \boldsymbol{r}) = \exp(\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{R})\phi_E(\boldsymbol{r})/\sqrt{V}$, where $\boldsymbol{K}$ is the exciton z-part wavevector, $\boldsymbol{R}$ is the z-part coordinate of the exciton centre of mass, $\boldsymbol{r}$ is the relative coordinate. $f_e(x_e, y_e) = f_e(x_e)f_e(y_e)$, $f_h(x_h, y_h) = f_h(x_h)f_h(y_h)$, where $f_e(x_e)$(or $f_e(y_e)$) and $f_h(x_h)$(or $f_h(y_h)$) are the x (or y) part of the electron and hole envelope wavefunctions, respectively, in the absence of the Coulomb potential. After using Eq.(3) and assuming the relative motion of the carriers and that of the centre of mass are independent, we have

$$\left(-\frac{\hbar^2}{2\mu_w h(x,y)}\nabla\cdot[h(x,y)\nabla] - \frac{e^2}{\varepsilon r}\right)\phi_E(\boldsymbol{r}) = E\phi_E(\boldsymbol{r}), \quad (4)$$

with

$$h(x,y) = \int\int f_e^2(\xi)f_h^2(\xi - x)f_e^2(\eta)f_h^2(\eta - y)\mathrm{d}\xi\mathrm{d}\eta,$$

$$E = E' - E_e - E_h,$$

where μ_w is the reduced mass of the exciton in the well. One may write Eq.(4)in spherical coordinates as

$$(H_\alpha + W)\phi_E = E\phi_E, \quad (5)$$

where H_α and W are given by Eq.(2), and

$$W = -\frac{\hbar^2}{2\mu_w h(x,y)}\nabla\cdot[h(x,y)\nabla] + \frac{\hbar^2}{2\mu_w}\left[\frac{1}{r^{\alpha-1}}\frac{\partial}{\partial r}\left(r^{\alpha-1}\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin^{\alpha-2}\theta}\frac{\partial}{\partial\theta}\left(\sin^{\alpha-2}\theta\frac{\partial}{\partial\theta}\right)\right], \quad (6)$$

where H_α is the Hamiltonian corresponding to the hydrogen atom Hamiltonian in a fractional α-dimensional space. If one denotes as ϕ_j and E_j the eigenfunctions and eigenvalues of Eq.(2), i.e.

$$H_\alpha\phi_j = E_j\phi_j, \quad (7)$$

the exciton binding energy may be written, after some straightforward algebraic manipulations of Eqs.(5) and (7), as

$$E = E_j + \frac{\int h\phi_E^* W \phi_j \mathrm{d}V}{\int h\phi_E^* \phi_j \mathrm{d}V}. \tag{8}$$

If one now is interested in evaluating the exciton binding energy, one may choose the α parameter such that the second term in the right-hand side of Eq.(8) is zero for ϕ_j chosen as the ground state associated with Eq.(7), so that both ground states coincide. The condition for α is, therefore,

$$\frac{\int h\phi_E^* W \phi_j \mathrm{d}V}{\int h\phi_E^* \phi_j \mathrm{d}V} = 0. \tag{9}$$

One should notice that the above equation provides an exact expression for determining the dimension of the α fractional-dimensional space that would model the actual system for obtaining the exciton ground-state solution. Of course, the solutions ϕ_E of Eq.(5) are not known, and one simple choice is to take $\phi_E = \phi_{j=0}$ where $\phi_{j=0}$ is the ground-state solution of the α-dimensional Hamiltonian in Eq.(7), use Eq.(9) to find α, and obtain the ground state exciton energy of the problem at hand by solving the α-dimensional equivalent Hamiltonian. One would expect that this simple choice would give an appropriate physical solution for the ground-state exciton energy, provided that the actual system is not strongly anisotropic.

Similarly, we attack the problem of a shallow hydrogenic donor confined in an infinite quantum-well wire with rectangular cross section by using the effective-mass and non-degenerate-parabolic band approximations, and the relative motion of a donor can then be described by the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\varepsilon r}\right)\phi_E(\boldsymbol{r}) - \frac{\hbar^2}{2m^* h'(x,y)} \times \left[\frac{\mathrm{d}h'(x,y)}{\mathrm{d}x}\frac{\partial}{\partial x} + \frac{\mathrm{d}h'(x,y)}{\mathrm{d}y}\frac{\partial}{\partial y}\right]\phi_E(\boldsymbol{r}) = E\phi_E(\boldsymbol{r}), \tag{10}$$

where the z-direction is the free axis, $h'(x,y) = f^2(x+x_i, y+y_i)$, ε is the dielectric constant, $r = \sqrt{(x-x_i)^2 + (y-y_i)^2 + z^2}$, and the donor is located at the position (x_i, y_i). We can notice that the first term in the right-hand side of Eq.(10) is the Hamiltonian of a hydrogen atom in a fractional α-dimensional space satisfying $H_\alpha \phi_j = E_j \phi_j$, thus Eq.(10) can be written as

$$(H_\alpha + W')\phi_E = E_j \phi_E. \tag{11}$$

The exciton binding energy may be written as

$$E = E_j + \frac{\int h'\phi_E^* W' \phi_j \mathrm{d}V}{\int h'\phi_E^* \phi_j \mathrm{d}V}. \tag{12}$$

We can determine the α parameter through

$$\frac{\int h'\phi_E^* W' \phi_j \mathrm{d}V}{\int h'\phi_E^* \phi_j \mathrm{d}V} = 0,$$

and then the donor binding energy $E = E_j$.

Finally, we consider the problem of an exciton confined in a quantum dot of cubic shape. By using the effective-mass and nondegenerate-band approximations, the relative motion of a free exciton can be described by the Schrödinger equation

$$\left(-\frac{\hbar^2}{2\mu_w h''(x,y,z)}\nabla \cdot [h''(x,y,z)\nabla] - \frac{e^2}{\varepsilon r}\right)\phi_E(\boldsymbol{r}) = E\phi_E(\boldsymbol{r}) \tag{13}$$

with

$$h''(x,y,z) = \int\int f_{\mathrm{e}}^2(\xi) f_{\mathrm{h}}^2(\xi - x) f_{\mathrm{e}}^2(\eta) f_{\mathrm{h}}^2(\eta - y) \times f_{\mathrm{e}}^2(\gamma) f_{\mathrm{h}}^2(\gamma - z)\mathrm{d}\xi\mathrm{d}\eta\mathrm{d}\gamma.$$

Similarly, we split the Hamiltonian of Eq.(13) into two parts, H_α and W'', thus the α parameter can be determined through $\dfrac{\int h''\phi_E^* W'' \phi_j \mathrm{d}V}{\int h''\phi_E^* \phi_j \mathrm{d}V} = 0$, and then the donor binding energy $E = E_j$.

3. Results and discussion

The fractional-dimensional approach is used to discuss the exciton and donor binding energies confined in the quantum-well wires. Our results are just the conclusions for the exciton confined in QW with the $l_x = 20a^*$, compared with the conclusion in Ref.[20], and obviously compares with it very well (cf. Fig.1). Figure 2 shows the donor binding energies in infinite quantum-well wires, and our results fit very well with the conclusions in Refs.[21,22] adopting theoretical variational calculations. Figure 3 shows the exciton binding energies in infinite quantum-well wires with rectangular cross section and one finds that the results are in good agreement with the values of Ref.[10]. All these prove that our results and conclusions are reasonable and reliable.

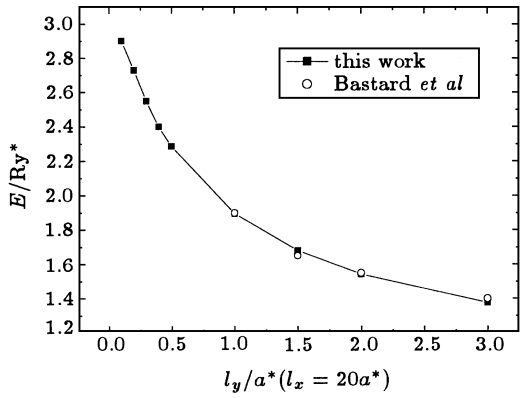


Fig.1. Exciton binding energy in infinite QW as a function of well thickness.

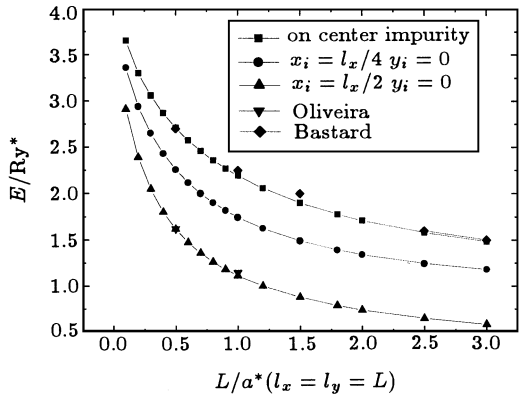


Fig.2. Donor binding energies in infinite quantum-well wires as functions of well thickness.

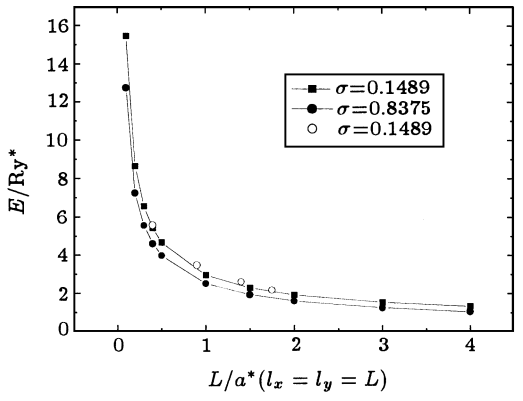


Fig.3. Exciton binding energies in infinite quantum-well wires as functions of well thickness.

It is clear from the four curves in Fig.4 that the effective dimension of the exciton obviously changes from one-dimensional to three-dimensional for extremely narrow to large well widths of quantum-well wires. We can even see from Figs.4 and 5 that both the effective dimension and binding energies decrease with the increase of the σ value. The reason is that the electron–hole's ability to 'move' is higher since the quantities of electron and hole are similar due to the bigger σ value and the fact that the 'space' they 'sense' is smaller, resulting in lower effective dimension. From Eq.(1), the exciton binding energy depends on both α and σ, and we can see that the effective dimensions and binding energies are both decreasing with increasing σ value in Figs.4 and 5.

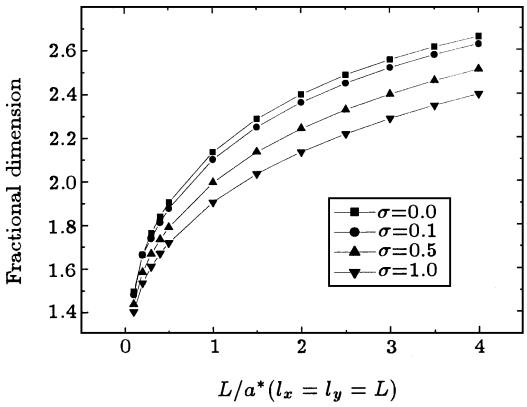


Fig.4. Change of excitonic effective dimensions in infinite quantum-well wires with the well width.

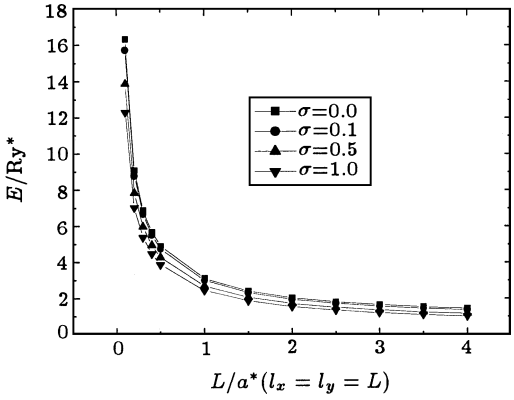


Fig.5. Change of exciton binding energies in infinite quantum-well wires with the well width.

It is seen from Fig.6 that the donor binding energies, confined in square sectional quantum-well wires, decrease with the donor position's excursion from the quantum-well wire center. The well has a tendency to 'push' the electron to move nearer the donor when the donor is located at the centre, which results in maximum binding energy, and in contrast, to 'push' the electron away from the donor when the donor is located on the edge, which results in minimum binding energy. It is also clear from Fig.6, that in the large-L limit and infinite barrier potentials, the exact binding energy of on-centre impurities is $\mathrm{Ry}^*(\alpha = 3)$ and on-edge impurities is $\mathrm{Ry}^*/4(\alpha = 5)$.

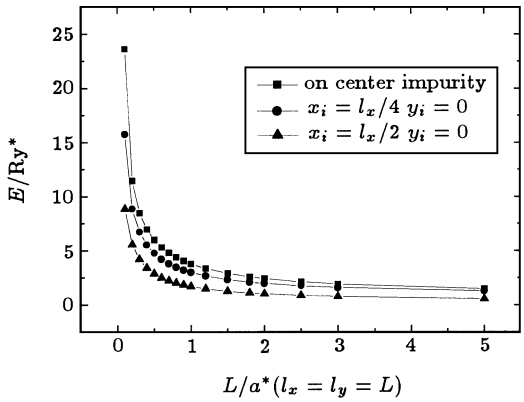


Fig.6. Change of the donor binding energies in infinite quantum-well wires with the well width.

In Figs.7 and 8 we give the effective dimensions of the exciton/impurity confined in quantum-well wires with the same cross section area for different shapes controlled by the values of the l_x/l_y. We can see obviously the effective dimension approaching 2 with the l_x/l_y value decreasing close to 0.

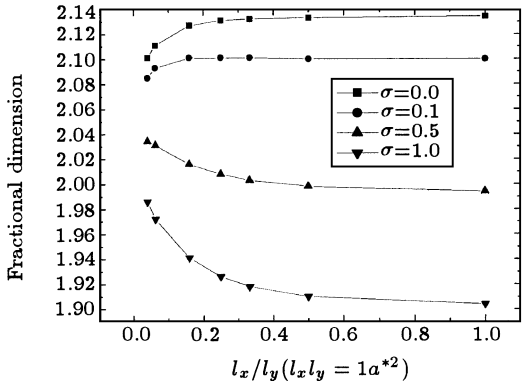


Fig.7. The shape effect on the exciton binding energies in infinite quantum-well wires.

Figure 8 shows in more detail the effective dimension change with the shape controlled by the values of the l_x/l_y for different cross section area (s) when the value of s is kept constant, and we find that for different value of s the effective dimension changes in different manners along with the values of l_x/l_y changing from 0 to 1, respectively, corresponding to the shape changing from that of the two-dimensional QW to square-sectional quantum-well wires ($l_x = l_y = a{=}\sqrt{s}$). We assume that $\alpha = \beta_x + \beta_y + \beta_z$, i.e. the fractional-dimensional parameter α can be taken as the sum of β_x, β_y, β_z which are the effective dimensions along different coordination axes directions with $\beta_z \equiv 1$. Along with the change of l_x/l_y from 0 to 1, the sides of the rectangular cross section change accordingly, and the form of the QW changes from the ideal two-dimensional to a wire with square cross section. In the course, the value of β_x increases and β_y reduces accordingly. The effective dimension is determined totally by the value of β_x and β_y ($\beta_z \equiv 1$). In Fig.8 we can find there is a special s denoting as critical area (s=1.44) in which the binding energy or effective dimension is almost keeping constant with different well shapes. This point is very useful in building an apparatus.

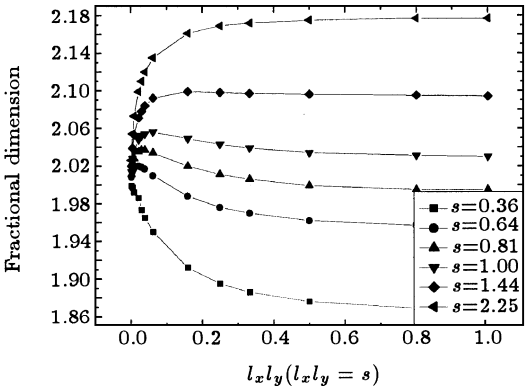


Fig.8. The shape effect on the impurity binding energies in infinite quantum-well wires.

It is clearly seen from Fig.9 that there is an obvious change from the low-dimensional to three-dimensional limits for narrow and large widths of quantum dots.

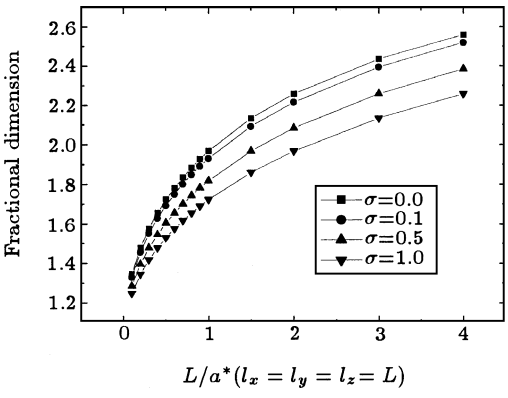


Fig.9. Change of exciton binding energies in infinite quantum dots with the well width.

In conclusion, we have developed a systematic mathematical procedure for determining the fractional dimensionality of the isotropic effective space which would model and give reliable values for the energies of the actual physical system under consideration. Our work introduces the fractional-dimensional space approach to deal with the binding energies in quantum-well wires and quantum dots for the first time and gives reasonable results.

References

[1] Jiang Z J and Mo D 2000 *Chin. Phys.* **9** 290

[2] Shi J J 2002 *Chin. Phys.* **11** 1286

[3] Kayanuma Y 1991 *Phys. Rev.* B **44** 13085

[4] Liu J J and Kong X J 1997 *Phys. Rev.* B **55** 1349

[5] Bryant G W 1988 *Phys. Rev.* B **37** 8763

[6] Liu J J, Zhang S F, Yang G C and Li S S 2002 *Chin. Phys. Lett.* **19** 114

[7] Liu W M, Wu B and Niu Q 2000 *Phys. Rev. Lett.* **84** 2294

[8] Liu W M, Fan W B, Zheng W M, Liang J Q and Chui S T 2002 *Phys. Rev. Lett.* **88** 170408

[9] Kodama T, Osaka Y and Yamanishi M 1985 *Japan. J. Appl. Phys.* **24** 1370

[10] Degani M H and Hipólitó O 1987 *Phys. Rev.* B **35** 9345

[11] Abiague A M, Oliveira L E and Leyva M D 1998 *Phys. Rev.* B **58** 4072

[12] Leyva M D, Alfonso A B, Abiague A M and Oliveira L E 1997 *J. Appl. Phys.* **82**(6) 3155

[13] Leyva M D, Alfonso A B, Abiague A M and Oliveira L E 1997 *J. Phys: Condens. Matter* **9** 8477

[14] He X F 1990 *Phys. Rev.* B **42** 11751

[15] Mathieu H, Lefebvre P and Christol P 1992 *Phys. Rev.* B **46** 4092

[16] Zhao Q X, Monemar B, Holtz P O, Willander M, Fimland B O and Johannessen K 1994 *Phys. Rev.* B **50** 4476

[17] Gómez E R, Oliveira L E and Leyva M D 1999 *J. Appl. Phys.* **85** 4045

[18] Christol P, Lefebvre P and Mathieu H 1993 *J. Appl. Phys.* **74** 5626

[19] He X F 1991 *Phys. Rev.* B **43** 2063

[20] Bastard G, Mendez E E, Chang L L and Esaki L 1982 *Phys. Rev.* B **26** 1974

[21] Oliveira L E 1988 *Phys. Rev.* B **38** 10641

[22] Bastard G 1981 *Phys. Rev.* B **24** 4714