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BINDING ENERGIES OF ON-AXIS HYDROGENIC AND NONHYDROGENIC DONORS IN GaAs/$Ga_{1-x}Al_xAs$

P. CSAVINSZKY and H. OYOKO
Department of Physics and Astronomy, University of Maine, Orono, Maine 04469, USA

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Abstract

In a previous work [Phys. Rev. B43(1991)9262], the binding energies of hydrogenic and nonhydrogenic on-axis donors in GaAs/$Ga_{1-x}Al_xAs$ quantum-well wires of circular cross section have been calculated as functions of the radius of the quantum-well wire. In both the hydrogenic and nonhydrogenic cases, a variational trial wave function was chosen that could be written as the product of an "envelope function", and a function containing the variational parameter. It was assumed in these calculations that the potential barrier that exists at the surface of the GaAs cylinder and the surrounding $Ga_{1-x}Al_xAs$ matrix is infinite. For the envelope function, an ordinary Bessel function of the first kind and of order zero was chosen. This envelope function satisfies the boundary condition, the vanishing of the trial function at the surface of the quantum-well wire. The question arises: how sensitive are the calculated binding energies to the choice of the envelope function? In the present work, we attempt to provide a partial answer to this question by choosing another envelope function, a spherical Bessel function of order zero. This function also satisfies the boundary condition and makes the trial wave function vanish at the interface between the GaAs cylinder and the $Ga_{1-x}Al_xAs$ matrix. Our calculations show that the binding energies of both the hydrogenic and the nonhydrogenic on-axis donors depend on the choice of the envelope function.

1. Introduction

In recent years, great advances were made in crystal-growth techniques, such as molecular-beam epitaxy [1] (MBE), liquid phase epitaxy [2] (LPE), and metal-organic chemical vapor deposition [3] (MOCVD). These advances made it possible to fabricate new semiconductor structures of lower dimensionality which are associated with exciting new properties. Among the new structures are the quasi two-dimensional quantum well (QW), the quasi one-dimensional quantum-well wire (QWW), and the quasi zero-dimensional quantum dot (QD). These hetero structures, exhibiting sharp interfaces, are associated with quantum confinement effects and have been the subject of extensive theoretical and experimental investigations.

An example of the quasi two-dimensional structure is a GaAs layer sandwiched between two thick slabs of $Ga_{1-x}Al_xAs$. This structure is called a quantum well

(QW), since the (x-dependent) discrepancy between the band gaps in the two semiconductors effectively confines a free electron to the GaAs layer. An example of the quasi one-dimensional structure is a GaAs wire of circular, rectangular, or triangular cross section, embedded in a $Ga_{1-x}Al_xAs$ matrix. This structure is called a quantum-well wire (QWW) and, for reasons mentioned above, in this structure, too, a free electron is effectively confined to the GaAs wire. An example of the quasi zero-dimensional structure is the quantum dot (QD), a GaAs sphere (or box) embedded in a $Ga_{1-x}Al_xAs$ matrix. It is this structure where quantum confinement effects are the most severe.

The nature of the energy levels of impurities in a QW, or in a QWW, is of interest. Bastard [4] has calculated, by a variational approach, the binding energy of a hydrogenic donor in a $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ QW of infinite depth and found that the binding energy of the donor increases as the width of the QW decreases. The assumption of infinite depth for the QW was relaxed later by Green and Bajaj [5], who considered a hydrogenic donor in a QW of finite depth, with the depth depending on the x-value of the surrounding $Ga_{1-x}Al_xAs$ slabs. These authors have found that, as the width of the QW is reduced, the binding energy of the donor at first increases then, at a certain QW width, it starts to decrease. A nonhydrogenic donor in a $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ QW has been considered by Csavinszky and Elabsy [6,7], both for infinite [6], and for finite [7] QW depths. In their calculations, the static dielectric constant of GaAs used in the hydrogenic model is replaced either by the spatial dielectric function of Resta [8], or that of Cornolti and Resta [9]. Their approach, leading to the spatial dielectric function in a numerical form, has been reformulated by Csavinszky and Brownstein [10,11], resulting in analytical expressions for the spatial dielectric function.

The binding energy of an on-axis hydrogenic donor in a $GaAs/Ga_{1-x}Al_xAs$ QWW of circular cross section has been calculated by Lee and Spector [12], and by Brown and Spector [13], using a variational approach. In the first of these calculations [12], it was assumed that the potential barrier that confines a free electron to the QWW is infinite, while in the second of these calculations [13], both infinite and finite potential barriers have been considered. Lee and Spector [12] have found that, for an infinite potential barrier between the GaAs cylinder and the $Ga_{1-x}Al_xAs$ matrix, the binding energy increases as the radius of the QWW decreases. This finding is similar to that obtained by Bastard [4] for a hydrogenic donor in a $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ QW. Brown and Spector [13], and Bryant [14], who also discussed hydrogenic on-axis donor states in a $GaAs/Ga_{1-x}Al_xAs$ QWW of circular cross section by a variational approach, have found that, for a finite potential barrier, as the radius of the QWW is reduced, the binding energy of the donor at first increases then, at a certain QWW radius, it starts to decrease. In the work of Lee and Spector [12], a variational wave function was used that does not satisfy the boundary condition, namely the vanishing of the wave function at the surface of the QWW. Lee and Spector [12], however, have suggested a wave function that does satisfy the boundary condition at the surface of the QWW. This

is the function that has later been used by Brown and Spector [13]. In a previous work [15], we have used their suggested trial wave function in variational calculations of the binding energies of on-axis hydrogenic and nonhydrogenic donors as a function of the radius of a GaAs/$Ga_{1-x}Al_xAs$ QWW of circular cross section. Our calculations for hydrogenic donors confirm the results of Brown and Spector [13]. In our previous work [15], we have also discussed the screening of the donor ion by the valence electrons of GaAs and calculated [15], again by a variational approach, the binding energy of a nonhydrogenic on-axis donor as a function of the radius of the GaAs/$Ga_{1-x}Al_xAs$ QWW.

In the present work, we raise the question of just how sensitive are the calculated [15] hydrogenic and nonhydrogenic binding energies of on-axis donors to the choice of the envelope function. We attempt to provide a partial answer to this question by choosing another envelope function, a spherical Bessel function of order zero. This function, too, satisfies the boundary condition, the vanishing of the trial wave function at the surface of the QWW. Our calculations show that the binding energies of both hydrogenic and nonhydrogenic on-axis donors in a GaAs/$Ga_{1-x}Al_xAs$ QWW of circular cross section do depend on the choice of the envelope function.

In what follows, atomic units [16] will be used.

2. Theory

2.1. HYDROGENIC MODEL, WITH J_0 FOR THE ENVELOPE FUNCTION

For an on-axis hydrogenic donor, the Hamiltonian, in circular cylindrical coordinates, is given [15] by

$$H^{\mathrm{h}} = -\frac{1}{2m^*}\nabla^2 - \frac{1}{\varepsilon(0)[z^2+\rho^2]^{1/2}} + V_{\mathrm{B}}, \tag{1}$$

where $m^* = 0.0665m_0$ is the effective mass [17] of an electron (of mass m_0) at the bottom of the conduction band of GaAs, $\varepsilon(0) = 12.56$ is the static dielectric constant [17] of bulk GaAs, while V_{B} is the potential barrier which confines a free electron to the GaAs wire. In what follows, it will be assumed that V_{B} is such that it vanishes for $\rho < a$ and is infinite for $\rho > a$, where a is the radius of the QWW. In eq. (1), the coordinate ρ measures the distance perpendicular to the axis of the QWW, and the coordinate z measures the distance along the axis of the QWW. Both ρ and z have their origin at the (point) donor ion.

The trial wave function for an on-axis donor, suggested by Lee and Spector [12], is given by

$$\psi_1(\rho, z) = N_1 J_0(k_{10}\rho)\mathrm{e}^{-\beta_1[\rho^2+z^2]^{1/2}}, \tag{2}$$

where N_1 is the normalization constant and β_1 is a variational parameter. The quantity $J_0(k_{10}\,\rho)$ is a Bessel function [18] of the first kind of order zero, with argument $k_{10}\,\rho$. The quantity k_{10} is related to the first zero [19] of the Bessel function $J_0(k_{10}\,\rho)$. The numerical value of this quantity is [19] $k_{10} = 2.4048\ldots/a$.

When, for a given QWW radius a, the expectation value of H^h is calculated with ψ_1, the z-integration can be done analytically but the ρ-integration can only be done numerically. The expectation value can be expressed by

$$\langle H^h\rangle_1 = \langle T\rangle_1 + \langle V^h\rangle_1, \tag{3}$$

where $\langle T\rangle_1$ and $\langle V^h\rangle_1$ are the expectation values of the kinetic and potential energies, defined in eq. (1). Detailed expressions for these expectation values are given below:

$$\langle T\rangle_1 = \frac{\beta_1^2}{2m^*} + \frac{\alpha^2}{2m^*}; \quad \alpha \equiv k_{10} \tag{4a}$$

and

$$\langle V^h\rangle_1 = -\frac{1}{\varepsilon(0)}\,\frac{\int_0^a \rho J_0(\alpha\rho)^2 K_0(2\beta_1\rho)\,\mathrm{d}\rho}{\int_0^a \rho^2 J_0(\alpha\rho)^2 K_1(2\beta_1\rho)\,\mathrm{d}\rho}. \tag{4b}$$

The normalization constant N_1 is given by

$$N_1 = \left[4\pi\int_0^a \rho^2 J_0(\alpha\rho)^2 K_1(2\beta_1\rho)\,\mathrm{d}\rho\right]^{-1/2}, \tag{5}$$

where K_1 is a modified Bessel function [17] of order one, with argument $2\beta_1\,\rho$.

The binding energy of an on-axis hydrogenic donor is obtained [12] from the expression

$$E_{b1}^h = \frac{\alpha^2}{2m^*} - \langle H^h\rangle_{1,\min} \tag{6}$$

Our values for the binding energy E_{b1}^h, as a function of the radius a of the GaAs/$Ga_{1-x}Al_xAs$ QWW, are shown in the third column of table 1, while the second column of table 1 displays the values of the variational parameter β_1 at which $\langle H^h\rangle_1$ attains its minimum. It is the finding of $\langle H^h\rangle_{1,\min}$ that requires extensive numerical integrations.

Table 1

Binding energy E_{b1}^{h} of an on-axis hydrogenic donor, and binding energy E_{b1}^{nh} of an on-axis nonhydrogenic donor, as functions of the radius a of the QWW. Values of the optimal values of the variational parameters β and β_1' for the hydrogenic and nonhydrogenic cases, respectively, are also listed.

	Hydrogenic donor		Nonhydrogenic donor	
a [a.u.]	$\beta_1 \times 10^{-2}$ $[\text{a.u.}]^{-1}$	$E_{b1}^{h}(a, \beta_1)$ [meV]	$\beta_1' \times 10^{-2}$ $[\text{a.u.}]^{-1}$	$E_{b1}^{nh}(a, \beta_1')$ [meV]
5.0	1.963	158.51	3.219	343.73
10.0	1.556	118.55	1.918	147.44
20.0	1.207	73.63	1.306	81.07
30.0	1.035	57.48	1.080	60.38
40.0	0.926	47.96	0.953	49.45
50.0	0.852	41.55	0.868	42.45
60.0	0.792	36.91	0.806	37.50
70.0	0.747	33.35	0.757	33.77
80.0	0.710	30.53	0.719	30.84
90.0	0.680	28.22	0.687	28.46
100.0	0.654	26.30	0.660	26.49
120.0	0.613	23.27	0.618	23.40
140.0	0.582	20.98	0.585	21.08
160.0	0.557	19.18	0.560	19.25
180.0	0.537	17.73	0.539	17.76
200.0	0.521	16.52	0.523	16.55
300.0	0.474	12.67	0.574	12.68
400.0	0.456	10.59	0.456	10.59
500.0	0.452	9.30	0.452	9.31
600.0	0.456	8.45	0.456	8.45
700.0	0.463	7.85	0.464	7.86
800.0	0.472	7.43	0.473	7.43

2.2. NONHYDROGENIC MODEL, WITH J_0 FOR THE ENVELOPE FUNCTION

In the nonhydrogenic model, eq. (1) is replaced by

$$H^{nh} = -\frac{1}{2m^*}\nabla^2 - \frac{1}{\varepsilon(r)[z^2+\rho^2]^{1/2}} + V_B, \tag{7}$$

where

$$\frac{1}{\varepsilon(r)} = \frac{1}{\varepsilon(0)} + \left(1 - \frac{1}{\varepsilon(0)}\right) e^{-r/c}, \tag{8}$$

is an expression suggested by Hermanson [20], and recently used by Oliveira and Falicov [21]. It is seen from eq. (8) that, as $r \to 0$, $\varepsilon(r) \to 1$. It is also seen from eq. (8) that, as $r \to \infty$, $\varepsilon(r) \to \varepsilon(0)$. This limiting behavior of $\varepsilon(r)$ is expected on the basis of general physical considerations.

In eq. (8), c denotes a screening constant that we have determined by requiring that, in the screening region of Resta [8], $\varepsilon(r)$ should agree as well as possible with the spatial dielectric function of Resta [8]. We have found that this requirement is well satisfied with $c = 0.8$.

After some calculations, we find that the expectation value of the potential energy is

$$\langle V^{\mathrm{nh}} \rangle_1 = -\frac{1}{\varepsilon(0)} \frac{\int_0^a \rho J_0(\alpha\rho)^2 K_0(2\beta_1'\rho)\,\mathrm{d}\rho}{\int_0^a \rho^2 J_0(\alpha\rho)^2 K_1(2\beta_1'\rho)\,\mathrm{d}\rho} - \frac{\varepsilon(0)-1}{\varepsilon(0)} \frac{\int_0^a \rho J_0(\alpha\rho)^2 K_0[(2\beta_1' + 1/c)\rho]\,\mathrm{d}\rho}{\int_0^a \rho^2 J_0(\alpha\rho)^2 K_1(2\beta_1'\rho)\,\mathrm{d}\rho}, \tag{9}$$

where β_1' is the variational parameter that replaces β_1 in eq. (2). In eq. (9), K_0 and K_1 are modified Bessel functions [17] of orders zero and one, with argument $(2\beta_1' + 1/c)\rho$ and $2\beta_1'\rho$, respectively. The normalization constant N_1' is given by eq. (5) with β_1 replaced by β_1'.

The binding energies $E_{\mathrm{b}1}^{\mathrm{nh}}$ obtained from

$$E_{\mathrm{b}1}^{\mathrm{nh}} = \frac{\alpha^2}{2m^*} - \langle H^{\mathrm{nh}} \rangle_{1,\min}, \tag{10}$$

and the minimizing values of the variational parameter β_1', as functions of the radius a of the QWW, are presented in the fifth and fourth columns of table 1.

2.3. HYDROGENIC MODEL, WITH j_0 FOR THE ENVELOPE FUNCTION

For this case, the trial wave function, for an on-axis donor, is chosen as

$$\psi_2(\rho, z) = N_2 j_0(\mu\rho) \mathrm{e}^{-\beta_2[\rho^2 + z^2]^{1/2}}, \tag{11}$$

where N_2 is a normalization constant and β_2 is a variational parameter. The quantity $j_0(\mu\rho)$ is a spherical Bessel function of order zero [17] with argument $\mu\rho$ and $\mu = n\pi/a$, $n = 1, 2, 3, \ldots$. For the present case, $n = 1$.

When, for a given QWW radius a, the expectation value of H^h is calculated with eq. (11), the result can be expressed by

$$\langle H^h\rangle_2 = \langle T\rangle_2 + \langle V^h\rangle_2, \tag{12}$$

where $\langle T\rangle_2$ and $\langle V^h\rangle_2$ are the expectation values of the kinetic and potential energies, defined in eq. (1). Detailed expressions for the expectation values are given below:

$$\begin{aligned}\langle T\rangle_2 = &-\frac{2\pi\beta_2^2 N_2^2}{m^*}\int_0^a \rho\, j_0(\mu\rho)^2 K_1(2\beta_2\rho)\,\mathrm{d}\rho \\ &-\frac{2\pi N_2^2}{m^*}\int_0^a j_0(\mu\rho)^2 K_1(2\beta_2\rho)\,\mathrm{d}\rho \\ &-\frac{2\pi\mu N_2^2}{m^*}\int_0^a \rho\, j_0(\mu\rho) n_0(\mu\rho) K_1(2\beta_2\rho)\,\mathrm{d}\rho \\ &-\frac{4\pi\beta_2\mu N_2^2}{m^*}\int_0^a \rho^2 j_0(\mu\rho) n_0(\mu\rho) K_0(2\beta_2\rho)\,\mathrm{d}\rho \\ &+\frac{2\pi\mu^2 N_2^2}{m^*}\int_0^a \rho\, j_0(\mu\rho)^2 K_1(2\beta_2\rho)\,\mathrm{d}\rho\end{aligned} \tag{13}$$

and

$$\langle V^h\rangle_2 = -\frac{4\pi N_2^2}{\varepsilon(0)}\int_0^a \rho\, j_0(\mu\rho)^2 K_0(2\beta_2\rho)\,\mathrm{d}\rho, \tag{14}$$

where

$$n_0(\mu\rho) = -\frac{\cos(\mu\rho)}{\mu\rho} \tag{15}$$

is a spherical Neumann function [17] of order zero with argument $\mu\rho$.

The normalization constant N_2 is given by

$$N_2 = \left[4\pi\int_0^a \rho^2 j_0(\mu\rho)^2 K_1(2\beta_2\rho)\,\mathrm{d}\rho\right]^{-1/2}. \tag{16}$$

The binding energies E^{h}_{b2} obtained from

$$E^{h}_{b2} = \frac{\alpha^2}{2m^*} - \langle H^{h} \rangle_{2,\min}, \tag{17}$$

and the minimizing values of the variational parameter β_2, as functions of the radius a of the QWW, are presented in the third and second columns of table 2.

Table 2

Binding energy E^{h}_{b2} of an on-axis hydrogenic donor, and binding energy E^{nh}_{b2} of an on-axis nonhydrogenic donor, as functions of the radius a of the QWW. Values of the optimal values of the variational parameters β_2 and β'_2 for the hydrogenic and nonhydrogenic cases, respectively, are also listed.

	Hydrogenic donor		Nonhydrogenic donor	
a [a.u.]	$\beta_2 \times 10^{-2}$ [a.u.]$^{-1}$	$E^{h}_{b2}(a, \beta_2)$ [meV]	$\beta'_2 \times 10^{-2}$ [a.u.]$^{-1}$	$E^{nh}_{b2}(a, \beta'_2)$ [meV]
20.0	6.026	1911.55	6.356	1969.64
30.0	5.602	1015.40	5.754	1016.61
40.0	5.217	618.37	5.306	619.17
50.0	4.910	418.02	4.970	418.43
60.0	4.656	302.99	4.697	303.26
70.0	4.446	230.89	4.473	231.09
80.0	4.257	182.68	4.277	182.82
90.0	4.091	148.80	4.116	148.91
100.0	3.957	121.04	3.975	124.16
120.0	3.728	90.95	3.740	91.01
140.0	3.539	70.35	3.550	70.39
160.0	3.386	56.60	3.90	56.63
180.0	3.252	46.93	3.260	46.96
200.0	3.144	39.84	3.150	39.86
300.0	2.767	22.03	2.770	22.04
400.0	2.551	15.08	2.555	15.08
500.0	2.423	11.53	2.425	11.53
600.0	2.341	9.52	2.340	9.41
700.0	2.288	7.90	2.290	8.03
800.0	2.257	7.06	2.260	7.06

2.4. NONHYDROGENIC MODEL, j_0 FOR THE ENVELOPE FUNCTION

Using eq. (11) to evaluate the expectation value of eq. (7), with the consideration of eq. (8), the result may be expressed by

$$\langle H^{nh}\rangle_2 = \langle T\rangle_2 + \langle V^{nh}\rangle_2, \tag{18}$$

where $\langle T\rangle_2$ and $\langle V^{nh}\rangle_2$ are expectation values of the kinetic and potential energies, defined in eqs. (7) and (8). The detailed expression for the expectation value $\langle V^{nh}\rangle_2$ is given by

$$\langle V^{nh}\rangle_2 = -\frac{4\pi N_2'^2[\varepsilon(0)-1]}{\varepsilon(0)} \int_0^a \rho j_0(\mu\rho)^2 K_0[(2\beta_2' + 1/c)\rho]\,d\rho. \tag{19}$$

The normalization constant N_2' is given by replacing β_2 by β_2' in eq. (16).

The binding energies E_{b2}^{nh} obtained from

$$E_{b2}^{nh} = \frac{\alpha^2}{2m^*} - \langle H^{nh}\rangle_{2,min}, \tag{20}$$

and the minimizing values of the variational parameter β_2', as functions of the radius a of the QWW, are presented in the fifth and fourth columns of table 2.

3. Discussion

It is seen from table 1 that both the hydrogenic and the nonhydrogenic binding energies of on-axis donors are sensitive functions of the QWW radius a and, for infinite barrier height, increase without limit as the wire radius a decreases. This is in agreement with the hydrogenic results of Lee and Spector [12], and of Brown and Spector [13], who have also used a trial wave function with one variational parameter. It should be mentioned, however, that Brown and Spector [13] and Bryant [14] have found that, for finite barrier height, the hydrogenic binding energy first increases and then decreases as the radius a of the QWW decreases.

Table 1 also reveals that the screening of the donor ion by the spatial dielectric function, displayed in eq. (8), begins to be important only for $a \lesssim 80$ a.u. Finally, it is also seen from table 1 that the binding energies, in all cases considered, tend towards the bulk value (5.77 meV) as the radius of the QWW becomes "very large" (800 a.u.).

It is seen from table 2 that both the hydrogenic and the nonhydrogenic binding energies are sensitive functions of the QWW radius a and, for infinite barrier height, increase without limit as the wire radius a decreases. This finding, based on calculations with the envelope function j_0, parallels that obtained by calculations with the envelope function J_0.

A cross comparison of table 1 with table 2, however, shows that E_{b2}^{h} increases faster with decreasing wire radius a than E_{b1}^{h}. The cross comparison of table 1 with table 2 also shows that the same trend is valid when E_{b2}^{nh} is compared with E_{b1}^{nh}.

Here, it is also mentioned that, in the calculations of refs. [12–15] and in the present work, the nonparabolicity of the GaAs conduction band is not considered.

This effect, for an on-center hydrogenic donor in a $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ QW of finite depth has been considered by Chaudhuri and Bajaj [22]. The effect of nonparabolicity for an off-center hydrogenic donor in a $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ QW has been investigated by Csavinszky and Elabsy [23]. None of the calculations for donors in a QWW considers image charges. For a hydrogenic donor in a $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ QW, this effect has been considered by Mailhiot et al. [24].

Finally, it should be mentioned that binding energies of impurities have also been calculated for a QWW of noncircular cross section. The case of rectangular and square cross sections have been considered by Weber et al. [25], Brum [26], and Osório et al. [27].

References

[1] A.Y. Cho, Appl. Phys. Lett. 19(1971)467.
[2] M. Konagi, K. Katsukowa and K. Takahashi, J. Appl. Phys. 48(1977)4389.
[3] R.D. Dupuis and P.D. Dapkus, Appl. Phys. Lett. 31(1977)366.
[4] G. Bastard, Phys. Rev. B24(1981)4714.
[5] R.L. Green and K.K. Bajaj, Sol. Stat. Commun. 45(1983)825.
[6] P. Csavinszky and A.M. Elabsy, Phys. Rev. B32(1985)6498.
[7] P. Csavinszky and A.M. Elabsy, Int. J. Quant. Chem.: Quant. Chem. Symp. 20(1986)325.
[8] R. Resta, Phys. Rev. B16(1977)2727.
[9] F. Cornolti and R. Resta, Phys. Rev. B17(1978)3239.
[10] P. Csavinszky and K.R. Brownstein, Phys. Rev. B24(1981)4566.
[11] P. Csavinszky and K.R. Brownstein, Phys. Rev. B25(1982)1362.
[12] J. Lee and H.N. Spector, J. Vac. Sci. Tech. B2(1984)16.
[13] J.W. Brown and H.N. Spector, J. Appl. Phys. 59(1986)1179.
[14] G.W. Bryant, Phys. Rev. B29(1984)6632.
[15] P. Csavinszky and H. Oyoko, Phys. Rev. B43(1991)9262.
[16] The unit of length is the Bohr, the unit of energy is the Hartree.
[17] H.C. Casey, Jr. and M.B. Panish, *Heterostructure Lasers* (Academic Press, New York, 1978), Part A.
[18] G.A. Arfken, *Mathematical Methods for Physicists*, 3rd ed. (Academic Press, New York, 1985).
[19] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1964).
[20] J. Hermanson, Phys. Rev. 150(1966)660.
[21] L.E. Oliveira and L.M. Falicov, Phys. Rev. B34(1986)8676.
[22] S. Chaudhuri and J.J. Bajaj, Phys. Rev. B29(1984)1803.
[23] P. Csavinszky and A.M. Elasbsy, Int. J. Quant. Chem.: Quant. Chem. Symp. 22(1988)25.
[24] C. Mailhiot, Y.C. Chang and T.C. McGill, Phys. Rev. B26(1982)4449.
[25] G. Weber et al., Mater. Sci. Forum 38–41(1989)1415.
[26] J.A. Brum, Sol. Stat. Commun. 54(1985)179.
[27] F.A.P. Osório, M.H. Degani and O. Hipolito, Phys. Rev. B37(1988)1402.