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Exciton *s* states in semiconductor quantum wells in a magnetic field

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We present a method to calculate the binding energy of exciton *s* states in any kind of layered structure potential including the case of zero valence- or conduction-band offsets. Furthermore, our numerical resolution of an effective Schrödinger equation allows one to take into account the effects of a magnetic field, of arbitrary intensity, perpendicular to the layers. This paper extends the Leavitt and Little method [Phys. Rev. B **42**, 11 774 (1990)], which deals only with the 1*s* state of the exciton in the absence of a magnetic field. Excellent agreement is obtained with experimental results.

INTRODUCTION

Semiconductor heterostructures have been of great interest for the past twenty years. The majority of the experimental and theoretical investigations has been carried out on the III-V semiconductor heterostructures, such as the GaAs/$\mathrm{Al}_x\mathrm{Ga}_{1-x}$As system for example. Comparatively, the II-VI semiconductor heterostructures represent a relatively recent innovation and extend the field of application for the confined quantum systems. We have previously reported on various CdTe/$\mathrm{Cd}_x\mathrm{Zn}_{1-x}$Te and CdTe/$\mathrm{Cd}_x\mathrm{Mn}_{1-x}$Te heterostructures.[1,2]

As the band gap depends on the layer composition, the heterostructures can be considered as having a spatially dependent gap acting as an additional potential for the carriers (we call it the heterostructure potential). This is the main idea behind the envelope function theory of heterostructures, which constitutes the basic theoretical tool used in this paper.

The heterostructure potential can localize the electron and the hole in the same or in different semiconductor layers. Therefore, these two particles form an exciton, whose binding energy can be very different from its bulk value. Considering the very large variety of heterostructures, it is convenient to have a calculation method of the exciton binding energy, whatever the characteristics of the quantum potential and the materials, which the heterostructure is made of.

Leavitt and Little[3] have developed a simple, rapid, and accurate method that allows us to estimate the binding energy of a 1*s* exciton confined in an arbitrary heterostructure potential (except for flat band offsets). They solved the problem with an adiabatic treatment of the in-plane motion, with respect to the one along the growth axis. This enabled them to simply write the binding energy as a double integral (over the electron and hole coordinates perpendicular to the layers) of a prescribed function weighted by the squares of the electron and hole subband envelope functions. They took into account both the relative electron-hole motion in the plane and along the growth axis. Therefore, they were able to express in a better way the intermediate dimensionality of the system [between two dimensional (2D) and 3D]. However, their one-parameter variational resolution of the effective Schrödinger equation limits their field of investigation to the exciton 1*s* state in the absence of a magnetic field.

The aim of this paper is to describe a method, which allows one to calculate the evolution of excited excitonic *ns* ($n \geq 1$) states, with a magnetic field (applied perpendicular to the layers) of arbitrary intensity. The magnetic field is a powerful tool for investigating the matter properties, particularly in the semiconductor systems, where it allows many studies. Among them we can mention important information about effective masses,[4,5] gyro magnetic factors, and exchange interaction.[6] Extensive magnetoexciton calculations in quantum well and in superlattices have been done by Bauer and Ando[7] and by Yang and Sham.[8] But these methods are usually used in the low- or high-field limits, and are not really satisfactory for intermediate-field values. Some of them are easily and quickly computed, but they only treat the extreme 2D (Ref. 9) or 3D (Ref. 10) limits, and do not reflect the intermediate dimension of the layered systems.

The outline of this paper is as follows. In Sec. I, we show the results that we have obtained with a numerical resolution (based on the finite difference method) of the effective Schrödinger equation. We show that our method is suitable in order to obtain the binding energy of the exciton excited *s* states. We test the method in a simple and specific case. We calculate the binding energy for a heavy exciton in a rectangular GaAs/$\mathrm{Al}_{0.3}\mathrm{Ga}_{0.7}$As quantum well as a function of the well width for different values of the magnetic field. A very good agreement is obtained with previously published results (for 1*s* and 2*s* states). In Sec. II, we extend the method to the case of an exciton in the presence of a magnetic-field applied perpendicular to the layers. In these first two sections, we consider that each exciton supported by the system can be associated with a specific pair of electron and hole subbands. It means that the Coulomb interaction does not mix the subbands states. Leavitt and Little show that, due to the electron-hole correlation along the quantization axis, a single term for the envelope function is sufficient in order to give reasonably accurate exciton binding energies for a wide range of quantum well widths.

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On the opposite, in Sec. III, we deal with the case where the valence-band discontinuities are small (even zero). For the electron the confinement energy remains large with respect to the Coulomb energy. In such a case, the hole envelope function is determined both by the quantum heterostructure potential and the Coulomb interaction.[11] In the limit case of a zero valence-band confinement, the hole envelope function is entirely fixed by the Coulomb interaction. We meet this special situation in semimagnetic systems, such as CdTe/$\mathrm{Cd}_x\mathrm{Mn}_{1-x}\mathrm{Te}$ quantum wells and superlattices[1,11] subjected to a magnetic field. The numerous results obtained with these calculations being already published,[1,2] the aim of this paper is to focus on the method itself.

I. EXCITON BINDING ENERGY

We consider a general multilayer semiconductor system grown in the [001] direction. The Hamiltonian of an exciton associated with either the heavy-hole or the light-hole band in an arbitrary heterostructure is expressed as follows (considering a zero center-of-mass momentum):

$$H = E_{\mathrm{gap}} - \frac{\hbar^2}{2}\frac{\partial}{\partial z_e}\frac{1}{m_e}\frac{\partial}{\partial z_e} - \frac{\hbar^2}{2}\frac{\partial}{\partial z_h}\frac{1}{m_{hz}}\frac{\partial}{\partial z_h} + V_e(z_e) + V_h(z_h) + H^{2\mathrm{D}} , \qquad (1\mathrm{a})$$

$$H^{2\mathrm{D}} = -\frac{\hbar^2\nabla_\parallel^2}{2\mu_\parallel} - \frac{e^2}{4\pi\varepsilon\sqrt{\rho^2+Z^2}}$$

and

$$[H^{2\mathrm{D}} - E_n^{2\mathrm{D}}(Z)]g_n(Z) = 0 . \qquad (1\mathrm{b})$$

The respective hole and electron vector position $\mathbf{r}_{\mathrm{e}}(\boldsymbol{\rho}_{\mathrm{e}}, z_e)$ and $\mathbf{r}_{\mathrm{h}}(\rho_{\mathrm{h}}, z_h)$ are described in cylindrical symmetry suitable for the description of a particle motion in a layered heterostructure grown in the z direction. ρ_{e} and ρ_{h} refer to the in-plane direction. $\rho = |\boldsymbol{\rho}_{\mathrm{e}} - \boldsymbol{\rho}_{\mathrm{h}}|$ and $Z = |z_e - z_h|$ are the relative electron-hole coordinates. $\nabla_\parallel$ is the component of the gradient with respect to ρ. $V_e(z_e)$ and $V_h(z_h)$ are the heterostructure potentials for the conduction and the valence band, respectively. m_e and m_h are the respective electron and hole effective masses. Unlike m_h, m_e is taken to be isotropic, in each material composing the heterostructure. Therefore, m_h has different values whether the considered direction is the growth axis (m_{hz}) or the plane of the layers ($m_{h\parallel}$). This results in an anisotropy of the exciton reduced effective mass: $\mu_\parallel^{-1} = m_e^{-1} + m_{h\parallel}^{-1}$ in the plane of the layers and $\mu_z^{-1} = m_e^{-1} + m_{hz}^{-1}$ along the growth axis. It is well known that the valence-band coupling results in a large nonparabolicity of the in-plane hole energy dispersion.[12] Therefore, it is very difficult to extract a value for the in-plane effective hole mass. In order to avoid the difficulty of considering the valence-band mixing, a lot of authors[3,13–16] have used the diagonal approximation, where $m_{h\parallel} = 1/(\gamma 1 + \gamma 2)$ (heavy hole) and $m_{l\parallel} = 1/(\gamma 1 - \gamma 2)$ (light hole), $\gamma 1$ and $\gamma 2$ are the Luttinger parameters.[17] As noticed by Eckenberg and Altarelli[12] this is a dubious approximation. Our approach is definitely different. We use $m_{h\parallel}$ as an adjustable parameter by fitting the experimental results. It will be shown that only one value of $m_{h\parallel}$ is sufficient to fit all the data of the same sample. The way to define such a mass is a real theoretical problem and should be of great interest. However, in order to compare our results with previously published ones, we use the diagonal approximation. We allow the possibility for effective masses to depend on z, even if this position dependence is not explicitly expressed.

$H^{2\mathrm{D}}$ can be considered as a Hamiltonian describing the Coulomb interaction between an electron and a hole liable to move in the planes $z = z_e$ and $z = z_h$, respectively. $E_n^{2\mathrm{D}}(\rho;Z)$ and $g_n(\rho;Z)$ are the eigenvalue and eigenfunction of $H^{2\mathrm{D}}$. Z is considered as a parameter. We can use the same static dielectric constant $\varepsilon = \varepsilon(\omega = 0)$ for the whole structure or, as Leavitt and Little, we can also use an average value for ε taking into account the probability density of the carriers in the different layers. Image charge effects are neglected. Following Leavitt and Little, we choose the following form for the trial wave function of an electron-hole pair:

$$\Psi_n(\mathbf{r}_{\mathrm{e}}, \mathbf{r}_{\mathrm{h}}) = \Phi(z_e, z_h) g_n(\rho;Z) , \qquad (2)$$

where $n = 1, 2, \ldots$ labels the eigenstates in order of increasing energy (i.e., $n = 1$ is the excitonic ground 1*s* state). Φ depends on the absolute position of the two carriers along the growth axis, g_n depends on their relative motion. This approach was first used by Born and Oppenheimer[18] in order to describe a molecule by separating the electronic and nuclear coordinates: the electronic motion is fast and the nuclear motion is comparatively slow. Therefore, the ions are moving in an effective potential created by the average motion of the electrons. Here ρ, the in-plane relative motion, is associated to a fast motion and, on the contrary, Z is associated to a slow motion. In that way $g_n(\rho;Z)$ is normalized,[3] whatever the value of the Z distance between the electron and the hole along the growth axis. It is the classical hypothesis of the Born and Oppenheimer's theory. Since $\Phi(z_e, z_h)$ is normalized, it leads, after a straightforward calculation, to the main result of Leavitt and Little, which is the following simple expression for the exciton binding energy (defined as a positive value):

$$E_{n=1}^{B} = \int_{-\infty}^{+\infty} dz_e \int_{-\infty}^{+\infty} dz_h \, |\Phi(z_e, z_h)|^2 |E_{n=1}^{2\mathrm{D}}(Z)| . \qquad (3)$$

$E_{n=1}^{2\mathrm{D}}$ ($Z = |z_e - z_h|$) is the lower eigenenergy of $H^{2\mathrm{D}}$ and is, therefore, independent of the heterostructure potential shape. This energy is weighted by the presence probability of the electron and of the hole along this axis and integrated over all the space coordinates (z_e and z_h).

The main point is now to calculate $E_n^{2\mathrm{D}}(Z)$, i.e., to solve the Schrödinger equation [Eq. (1b)]. This equation is parametrically dependent on the Z coordinate through the Coulomb potential. Leavitt and Little use a one-parameter variational resolution restraining themselves to $n = 1$. With a finite difference numerical method, we propose to solve Eq. (1b), whatever the value of n. $E_n^{2\mathrm{D}}(Z)$ is plotted on Fig. 1 for $n = 1$, 2, 3, and 4.

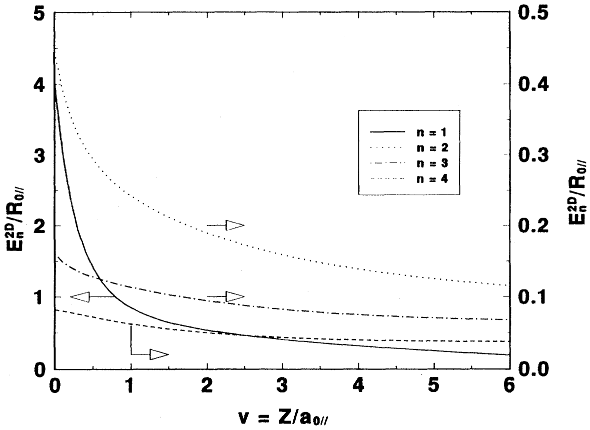

FIG. 1. The function E_n^{2D} is plotted versus $Z=|z_e-z_h|$, for $n=1$, 2, 3, 4. The energies are expressed in Rydberg unit: $R_{0\|}=\mu_\| e^4/[2(4\pi\varepsilon\varepsilon_0)^2\hbar^2]$. The lengths are expressed in Bohr radius unit: $a_{0\|}=4\pi\varepsilon\hbar^2/(\mu_\| e^4)$. We note $v=Z/a_{0\|}$. For $n=1$, our calculation give the same result than Leavitt and Little. $E_n^{2D}(Z)$ can be fitted by the functions given in Table I.

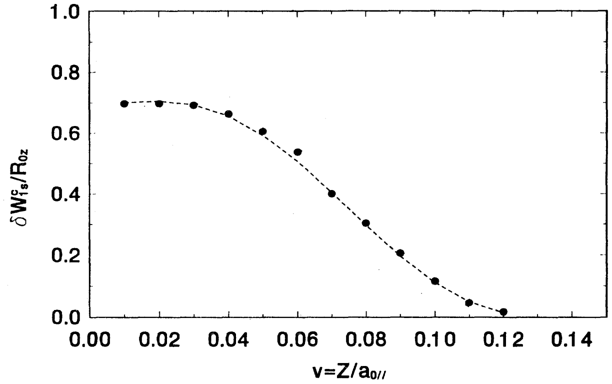

FIG. 2. $\delta W^c_{n=1}$ [defined in Eq. (4)] function versus Z. The energies are expressed in Rydberg unit: $R_{0z}=\mu_z e^4/[2(4\pi\varepsilon\varepsilon_0)^2\hbar^2]$. The lengths are expressed in Bohr radius unit: $a_{0\|}$ ($v=Z/a_{0\|}$). The calculated values of $\delta W^c_{n=1}(v)$ are represented by the circles. For $v>0.12$, $\delta W^c_{n=1}(v)\approx 0$. $\delta W^c_{n=1}(v)$ can be fitted by the polynomial expression, given in Table I, in the interval $0<v<0.12$ (dashed line).

We must not forget that the masses of the particles along the growth axis are finite, therefore, the relative motion of the electron-hole pair along this axis provides a kinetic energy, which could contribute to some extent to the exciton binding energy. This kinetic-energy function is noted as $W_n^c(Z)$, and is such that

$$W_n^c(Z)=\frac{\hbar^2}{2\mu_Z}\int_0^{+\infty}2\pi\rho d\rho\left|\frac{\partial g_n(\rho;Z)}{\partial Z}\right|^2, \qquad (4)$$

which is also analog with the Born Oppenheimer's theory.

The binding energy is defined as the energy difference between the bottom of the electron-hole pair continuum and the lowest excitonic bound state. In term of quantities defined above, we obtain the binding energy:

$$\begin{aligned}E_n^B(Z)={}&[E_n^{2D}(Z)+W_n^c(Z)]\\&-\lim_{m\to+\infty}[E_m^{2D}(Z)+W_m^c(Z)]\ . \qquad (5)\end{aligned}$$

Equation (5) may be simplified as follows. Note first that $\lim_{m\to+\infty}E_m^{2D}(Z)=0$ for all Z [continuum solution of Eq. (1b) first appears at zero energy]. Although the functions $W_n^c(Z)$ are comparable to the two-dimensional binding energies $E_n^{2D}(Z)$, a numerical evaluation has shown that the difference $\delta W_n^c(Z)=W_n^c(Z)-W^c_{m\to+\infty}(Z)$ contributes to at most 10% of the total exciton binding energy. Therefore, except for $n=1$, we can neglect the δW_n^c contribution. In addition, $\delta W^c_{n=1}(Z)$ is significantly different from zero only for arguments whose magnitudes are smaller than 0.12 times the exciton Bohr radius, as shown on the Fig. 2.

The expression (3) of Leavitt and Little does not take into account the kinetic-energy function $\delta W^c_{n=1}(Z)$. Since we do not neglect this term (for $n=1$), we substitute [Eq. (3)] by the following expression:

$$E_n^B=\int_{-\infty}^{+\infty}dz_e\int_{-\infty}^{+\infty}dz_h\Phi(z_e,z_h)|E_n^B(Z)|\ , \qquad (6)$$

where $E_n^B(Z)=E_n^{2D}(Z)+\delta W_n^c(Z)$ if $n=1$, and $E_n^B(Z)=E_n^{2D}(Z)$ if $n>1$.

In Table I, we propose a set of analytical functions, which fit E_n^{2D} and $\delta W^c_{n=1}$ (expressed in a Rydberg unit) versus Z (expressed in a Bohr radius unit). These functions are useful when computing the exciton binding energy [using Eq. (3) or Eq. (6)], whatever the values of the parameters of the material composing the quantum structure.

We assume that each exciton can be associated with a pair (i,j) of electron and hole subbands, where $(i,j)=1,2,3\dots$ are the states in order of increasing energies. Therefore, we can write $\phi_{ij}(z_e,z_h)=f_i^{(e)}(z_e)f_j^{(h)}(z_h)$. The states are described by single-band envelope functions $f_i^{(e)}$ and $f_j^{(h)}$, satisfying

$$\left[-\frac{\hbar}{2}\frac{\partial}{\partial z_\alpha}\frac{1}{m_\alpha}\frac{\partial}{\partial z_\alpha}+V_\alpha(z_\alpha)-E_i^{(\alpha)}\right]f_i^{(\alpha)}(z_\alpha)=0$$
$$\text{where } \alpha=e \text{ or } h \qquad (7)$$

On the figures 3(a) and 3(b), the 1*s*- and 2*s*-e_1h_1 associated exciton binding energies are calculated for a GaAs/$\text{Ga}_{0.7}\text{Al}_{0.3}$As single quantum well. Our results are compared to Leavitt and Little calculations (for E^B_{1s}) on the one hand, and with Greene, Bajaj, and Phelps[15] calculation (for E^B_{1s} and E^B_{2s}) on the other hand. Here, we have used the diagonal approximation. The agreement with the multiparameter variational method of Greene and Bajaj is excellent. In Fig. 3(a), the comparison between our results and Leavitt and Little's ones show that the $\delta W_1^c(Z)$ term is not negligible in the case of small quantum well width. Henceforth we are able to calculate the binding energy, whatever the heterostructure

TABLE I. This table summarizes the parameters of the polynomial expressions, which fit the $E_n^{2D}(v)$ and $\delta W_{n=1}^c(v)$ functions plotted on Figs. 1 and 2.

$$E_n^{2D}(v)/R_{\parallel 0} = m_1/(1+v) + m_2/(1+v)^2 + m_3/(1+v)^3 + m_4 v$$

n	m_1	m_2	m_3	m_4
1	2.816 024	−5.497 548	6.680 902	−0.019 755
2	0.778 004	−0.866 559	0.533 742	0.003 448
3	0.378 807	−0.416 971	0.198 414	0.003 618
4	0.167 364	−0.106 859	0.021 518	0.002 672

$$\delta W_{n=1}^c(v)/R_{z0} = p_0 + p_1 v + p_2 v^2 + p_3 v^3 + p_4 v^4 + p_5 v^5$$

p_0	p_1	p_2	p_3	p_4	p_5
0.7	−0.8982	154.973	−5841.52	51894.8	−139716

confinement potential and whatever the state of the exciton. A microcomputer takes between ten and twenty seconds to obtain each eigenvalue. The other big advantage of this method is its ability to be extended to the case of an exciton under an arbitrary magnetic field applied parallel to the heterostructure growth axis.

II. EXCITON IN A HETEROSTRUCTURE SUBMITTED TO MAGNETIC FIELD ALONG THE GROWTH AXIS

In this section we develop a method, which is an extension of the one accounted in the first section for arbitrary intensity of the magnetic field applied perpendicular to the layers. The main difficulty resides in the simultaneous presence of the Coulomb interaction and of the harmonic potential created by the field **B**. When one of these two effects dominate, the other can be treated as a perturbation. It is very convenient to introduce the parameter $\gamma = \hbar\omega_c/2R_0$, where $\hbar\omega_c$ is the cyclotron energy and R_0^* the effective Rydberg of the exciton. For example, if the cyclotron energy is small in comparison with the exciton Rydberg, diamagnetic effects proportional to the square of B are expected. On the contrary, for strong-field values, a Landau quantization of the states induces a linear variation of the exciton transition associated lines versus the magnetic field. But, it is often a difficult problem to connect the different energy levels and states at intermediate field. Note that, in this section we only consider the effect of the field on the orbital part of the wave functions (i.e., the Zeeman spin splitting is not treated here).

The field in the Faraday geometry only affects the in-plane radial motion, therefore, the previous 2D-

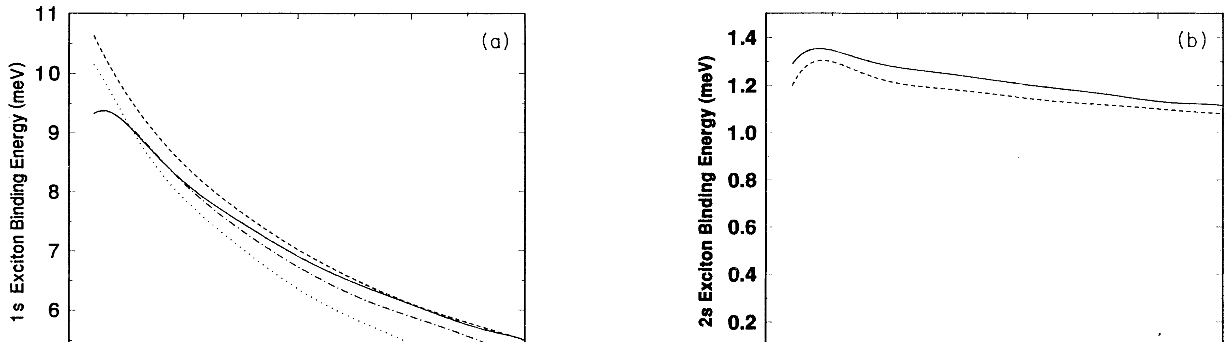

FIG. 3. (a) 1s heavy-hole exciton binding energy E_1H_1 for a GaAs/Ga$_{0.7}$Al$_{0.3}$As single quantum well calculated by several authors. The parameters used are $m_e = 0.067$, $\gamma_1(\mathrm{GaAs}) = 7.36$, $\gamma_2(\mathrm{GaAs}) = 2.57$, $\varepsilon = 12.5$; the conduction- and valence-band offsets are, respectively, CBO = 322.8 meV and VBO = 57 meV. These parameters are those used in the following references. Dotted line: Priester, Allan, and Lannoo (Ref. 14); dashed line: Leavitt and Little (Ref. 3); dot-dashed line: Greene, Bajaj, and Phelps (Ref. 15); solid line: our numerical calculation. (b) 2s heavy-hole exciton binding energy E_1H_1 for the same GaAs/Ga$_{0.7}$Al$_{0.3}$As single quantum well. The parameters used are the same as those of (a). The dashed and the solid curve represent the Greene, Bajaj, and Phelps (Ref. 15) results and our calculation, respectively. The difference between the two methods is smaller than 0.2 meV, which is below the experimental accuracy. The origin of this small difference comes from the fact that we neglect the $\delta W_{n=2}^c$ term in this case.

Hamiltonian H^{2D} is the only operator that is affected by the field:

$$H^{2D}=-\frac{\hbar^2\nabla_{\parallel}^2}{2\mu_{\parallel}}-\frac{e^2}{4\pi\varepsilon\sqrt{\rho^2+Z^2}}+\frac{e^2B^2}{8\mu_{\parallel}}\rho^2 , \tag{8a}$$

$$[H^{2D}-E_n^{2D}(Z;B)]g_n(Z;B)=0 . \tag{8b}$$

Equation (8a) is written in the Lorentz gauge, which preserves the cylindrical symmetry of the problem. We only consider the exciton s states, (i.e., without any orbital moment). The total potential is the sum of Coulomb potential and of harmonic potential, due to the field **B**. It is shown on the Fig. 4.

The exciton wave function is now

$$\Psi_{ijn}(\mathbf{r}_e,\mathbf{r}_h;B)=f_i^{(e)}(z_e)f_j^{(h)}(z_h)g_n(\rho;Z;B) . \tag{9}$$

The functions E_n^{2D} and g_n are now dependent on two parameters: Z and B. The field, because of its geometry, does not affect the Z motion and we can consider these two parameters as independent. Thus, $\delta W_{n=1}^c(Z)$, which represents the kinetic energy of the exciton along the growth axis, should not be strongly affected by the field. $\delta W_{n=1}^c(Z)$ is independent of the sign of the field, this property implies that this function does not have a first-order field dependence. Therefore it is not surprising, as we will see later on, that the reliability of our results is not affected by taking the same function $\delta W_{n=1}^c(Z)$, whatever the intensity of the magnetic field. We also assume that the envelope functions $f_i^{(e)}(z_e)$ and $f_j^{(h)}(z_h)$ are not affected by the field.

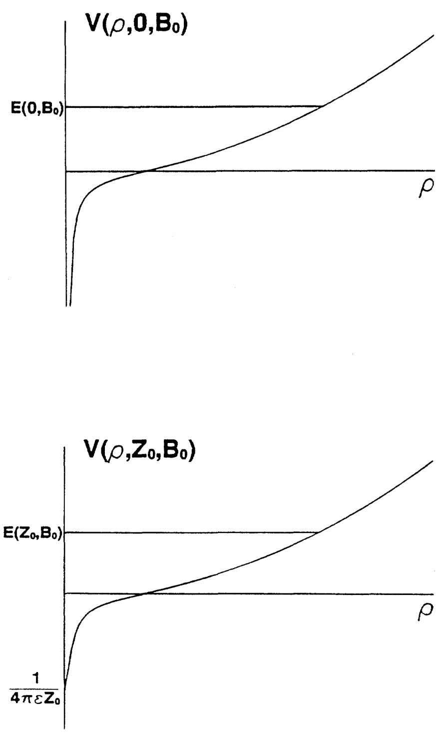

FIG. 4. $V(\rho;Z;B)$ is the sum of the Coulomb interaction (with a $\mathbf{r}=0$ singularity) and of the harmonic potential, due to the magnetic field. $E_n^{2D}(Z_0;B_0)$ is the corresponding eigenenergy.

While a variational resolution of Eq. (8b) is difficult to achieve, the numerical resolution of this one-dimensional equation is easy. Once again, in this case, the magnetoexciton binding energy is

$$E_{ijn}^B(B)=\int_{-\infty}^{+\infty}dz_e\int_{-\infty}^{+\infty}dz_h|f_i^{(e)}(z_e)|^2 \times|f_j^{(h)}(z_h)|^2|E_n^{2D}(Z;B)| , \tag{10}$$

with $E_n^B(Z,B)=E_n^{2D}(Z,B)+\delta W_n^c(Z)$ for $n=1$ and $E_n^B(Z,B)=E_n^{2D}(Z,B)$ for $n>1$.

In Fig. 5, we compare our results with the ones of Greene and Bajaj[19] for a 1s exciton in a GaAs/$Ga_xAl_{1-x}As$ quantum well submitted to a magnetic field parallel to the growth axis. The agreement between the two methods is excellent and proves the reliability of our calculations. Whereas Greene and Bajaj use a great set of basis states of functions, we only use the function written in Eq. (9). This allows us to follow the evolution of a ns exciton state from the weak- to the strong-field values, by simply counting the number of zeros in the $g_n(\rho;Z;B)$ function along the ρ direction. Let us call $\mathscr{n}$ this number: $\mathscr{n}=0$ represents the fundamental state of the potential, $\mathscr{n}=1$ is the first excited state, etc. At low field $\mathscr{n}=n-1$. (n is the quantum number for the exciton states.) At high field $\mathscr{n}=N$ (N is the quantum number for the Landau states). At intermediate field the harmonic and Coulomb parts of the potential are of the same order of magnitude. Strictly speaking, we do not have a pure exciton or a pure Landau level, the description of the magnetoexciton state is very convenient when using the number of zeros $\mathscr{n}$ as the invariant of the problem.

Figure 6 presents a fit of the experimental results obtained for a $CdTe/Cd_{0.78}Zn_{0.22}Te$ quantum well grown on a $Cd_{0.78}Zn_{0.22}Te$ substrate. In the II-VI heterostructures, we often have to deal with the case $\gamma\approx1$, because of the comparatively high value of the effective Rydberg $\mathscr{R}$ in compounds such as CdTe. The agreement with our cal-

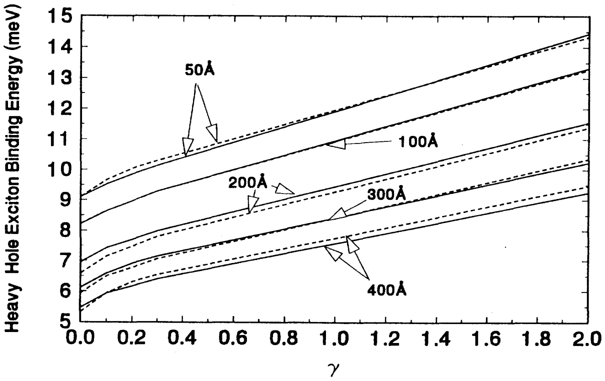

FIG. 5. e_1h_1 exciton binding energy for a few single $Ga_{0.7}Al_{0.3}As$ quantum wells of various thicknesses, with a magnetic field applied parallel to their growth axis. We compare our results (solid curves) to the Greene and Bajaj (Ref. 19) results (dashed curves). Once again, we can see that the difference between the two methods is experimentally unobservable.

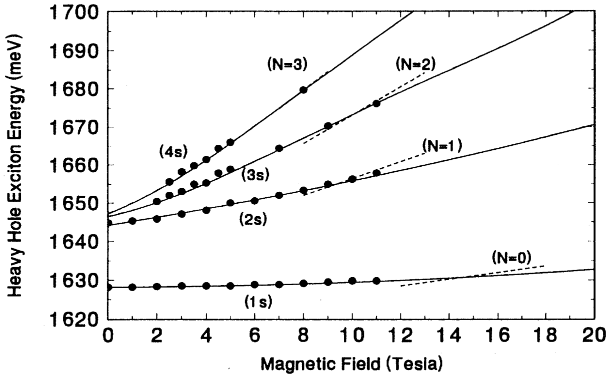

FIG. 6. Exciton energy variation of the heavy-hole e_1h_1 exciton in a 57 Å CdTe/$Cd_{0.78}Zn_{0.22}Te$ single quantum well grown on a $Cd_{0.78}Zn_{0.22}Te$ substrate (strained structure). Circles are the experimental points obtained at the temperature $T=2$ K. We have chosen $m_{h\parallel}=0.5m_0$. We have taken a dielectric constant $\varepsilon=10$; The conduction- and valence-band offset are, respectively, CBO = 1.01 meV and VBO = 35 meV. The CdTe gap is 1606 meV (Ref. 22), at $T=2$ K. The agreement between the experimental and theoretical results allows us to identify, without any ambiguity, the 1*s*, 2*s*, 3*s*, and 4*s* exciton states. The dashed lines represent the slopes of the Landau levels $N=0$, 1, 2, 3.

culations is excellent, and allows us to clearly identify the 1*s*, 2*s*, 3*s*, and 4*s* heavy exciton states. We would like to emphasize that in order to fit all of the sample data, we have used a single parameter: $m_{h\parallel}=0.5m_0$.

The methods that already exist in the literature are variational and, in this case, less flexible. The method introduced here has the overwhelming advantage of being fast and accurate, in addition to keeping the flexibility of the Leavitt and Little calculations, i.e., it is still applicable to a great variety of heterostructures.

III. SMALL VALENCE-BAND DISCONTINUITIES

In this section, we are going to extend the previous method to the case of small (even zero) valence-band offsets. The case of a small (even zero) conduction-band offset is strictly equivalent. When the valence-band potential is small enough compared to the Coulomb attraction between the electron and the hole, the quantum potential is not strong enough to confine the hole that is attracted in the neighborhood of the electron. In that case, the single hole subband envelope function $f_j^{(h)}(z_h)$ [defined in Eq. (7)] is not sufficient to correctly describe the hole confinement along the growth axis. However, we assume that the electron is sufficiently well confined to consider that its wave function $f_i^{(e)}(z_e)$ is not alterated by the electron-hole Coulomb attraction (i.e., the electron confinement is large compared to the electrostatic interaction). One possibility would be to achieve a calculation, which takes into account the admixing of the different hole subbands by the electrostatic potential.[20] Another solution would be to calculate the exact envelope function of the hole in an effective potential $V^{\rm eff}(z_h)$, which is the sum of the heterostructure potential and of the Coulomb interaction with the electron. $V^{\rm eff}(z_h)$ is averaged over the electron motion (z_e) and over the in-plane (ρ) relative motion. This method has been proposed by Peter *et al.*,[21] but they achieved a variational resolution as well. Applying this method to the calculation developed in Sec. I, and integrating the Schrödinger equation over z_e and ρ, we obtain

$$V_{i,n}^{\rm eff}(z_h;B)=E_{\rm gap}+E_i^{(e)}+V_h(z_h)+\int_{-\infty}^{+\infty}dz_e|f_i^{(e)}(z_e)|^2[E_n^{\rm 2D}(Z,B)+W_n^c(Z,B)]\ . \qquad (11)$$

The associated energy is E_{ijn}. The approximation we make here is to substitute $W_n^c(Z)$ by $\delta W_n^c(Z)=W_n^c(Z)-W_\infty^c(Z)$, to take into account the Coulomb potential continuum effect. A rigorous treatment should consist in recalculating the energy associated with the effective potential $V^{\rm eff}$, with the term $W_\infty^c(Z)$ instead of $W_n^c(Z)$ and in subtracting from this energy, the value E_{ijn} in order to obtain E_{ijn}^B. We have not done it here, because in the case of small valence-band confinement, the contribution of the correction due to the kinetic terms W^c is at most 0.5 meV, which is far from being important comparatively to the total exciton binding energy. Thus, the effective Schrödinger equation describing the exciton is

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z_h}\frac{1}{m_{hz}}\frac{\partial}{\partial z_h}+V_{i,n}^{\rm eff}(z_h)-E_{ijn}(B)\right]F_j^{(h)}(z_h;B)=0\ . \qquad (12)$$

$F_j^{(h)}(z_h;B)$ is the eigenfunction of the hole confined to the effective potential $V^{\rm eff}(z_h;B)$.

Once again we deal with a one-dimensional differential

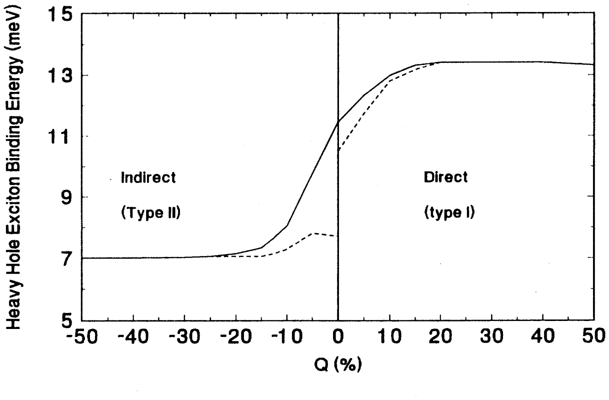

FIG. 7. 1*s* heavy-hole exciton binding energy in a multiple quantum well versus the relative valence-band offset $Q=\mathrm{VBO}/\Delta E_g$, $\Delta E_g=80$ meV, the thickness of wells and barriers is 100 Å. Calculations are carried out in the diagonal approximation and are represented by the solid curve. The dashed curves represent the calculations achieved with simply a square quantum well hole envelope function (i.e., $f_j^{(h)}(z_h)$, with our notation [see Eq. (7)]).

equation that we solve numerically. Without any Coulomb interaction, the energy of the free-electron-hole pair is $E_{fp}(B)=E_i^{(e)}+E_j^{(h)}+E_{\text{gap}}+(N+\frac{1}{2})\hbar\omega_c$, where $N=n-1$. The exciton binding energy is then obtained by subtracting the exciton energy E_{ijn} to the free-electron-hole pair energy:

$$E_{ijn}^{B}(B)=E_{fp}(B)-E_{ijn}(B) \quad (E_{ijn}^{B}>0) \ . \tag{13}$$

Figure 7 shows the binding energy of an e_1h_1 exciton confined to a multiple quantum well versus the relative valence-band offset $Q=\text{VBO}/\Delta E_g$. VBO is the valence band offset defined as the difference between the edge of the valence bands in the barriers and in the well. ΔE_g is the band-gap difference between barriers and well. For $Q>0$, both the electron and the hole are confined to the same layer (type-I confinement), thus they create a direct exciton (in the real space). When $Q<0$, the electron and the hole are situated in separate layers (type-II confinement), and give rise to an indirect exciton. We can see that for the small values of Q ($|Q|<10\%$, the hole confinement, due to the quantum well potential, begins to disappear and the calculation developed in the first section is not valid yet. Outside this interval (i.e., $|Q|>10\%$), the 1*s* heavy hole exciton binding energy (E_{hh}^{B}) is almost quite constant. For $Q>10\%$, the electron-hole proximity increases the binding energy and $E_{\text{hh}}^{B}\approx 13.5$ meV (type I) and for $Q<-10\%$, the separation of the two particles by the quantum potential decreases the binding energy and $E_{\text{hh}}^{B}\approx 7$ meV (type II). The value of the exciton binding energy drops very rapidly from type-I to type-II confinement in the interval $|Q|<10\%$. For $Q=0$, we cross the bulk exciton binding energy $E_{\text{hh}}^{B}\approx 10$ meV.[22] This calculation is very useful, especially in the case of the semimagnetic heterostructures, such as CdTe/Cd$_x$Mn$_{1-x}$Te,[1,11] where the type-I–type-II transition can be tuned by a magnetic field.

CONCLUSION

The exciton binding-energy calculations developed here are reliable, whatever the profile of the heterostructure potential along the growth axis—even in the case of a flat valence-band profile—whatever the value of a magnetic field applied perpendicular to the layers, and whatever the *s* state of the exciton. The last, but not least, advantage of such a calculation is that it is fast to compute. To our knowledge, it is the first time that a reliable exciton binding-energy calculation provides such flexibility. It can be applicable to the very large field of various already existing or future heterostructures. Thus, it is an efficient tool for anyone who wishes to quantitatively interpret experimental results.

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