Excitons in extremely shallow quantum wells

J. Kossut
Institute of Physics, Polish Academy of Sciences, Aleja Lotnikow 32/46, 02-668 Warszawa, Poland

J. K. Furdyna and M. Dobrowolska
Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556
(Received 21 October 1996)

Excitons in extremely shallow semiconductor quantum wells are considered in the limit when both the conduction band and the valence band confining potentials are small compared to the binding energy of a three-dimensional (3D) exciton. Under these circumstances it is found that the quantization of the center-of-mass motion can make a sizable contribution to energies of excitonic optical transitions. A simple effective Hamiltonian is derived for describing this situation, with a potential that confines the motion of the exciton center of mass. The shape of the potential is approximated either by a parabolic profile (when quantum wells are narrow compared with the 3D exciton Bohr radius), or by a rectangular potential (for wide quantum wells), and the resultant eigenvalue problem is solved accordingly. The results are compared to experimental data obtained in magnetooptical studies of $ZnSe/Zn_{1-x}Mn_xSe$ spin superlattices, giving excellent quantitative agreement. [S0163-1829(97)03536-4]

I. INTRODUCTION

Most of the usual variational approaches to the problem of exciton energy in quasi-two-dimensional semiconductor quantum structures assume that the ground state wave function of the exciton can be approximated by a product of $\chi_1(z_e)\chi_1(z_h)$ and an appropriate ''excitonic'' envelope, e.g., $e^{-r/\lambda}$, where $\chi_n(z_e)$ and $\chi_m(z_h)$ are the wave functions of the confined electron and hole, respectively, both localized in the well region, and, r is their relative motion variable while λ represents an effective Bohr radius of the exciton (usually found in a variational procedure).[1] This approximation is suitable for relatively deep quantum wells, when the Coulomb potential of the electron-hole interaction does not lead to significant admixtures of excited states of the electron and/or the hole. Such assumption can be expected to work provided that the characteristic energy of the Coulomb interaction [$\varepsilon_{3D}=(\mu e^4/2\kappa^2\hbar^2)$, where κ denotes the dielectric constant of the material and μ the reduced mass] is small compared to interlevel distances of the electron or the hole confined in the quantum well.[2] The interlevel distance decreases, of course, with decreasing depth of the quantum well, as well as with increasing quantum well width. A situation can be achieved when the above form of the exciton trial wave function is no longer justified.

Recently, there has been considerable interest specifically in quantum wells with small confinement, as illustrated by a number of papers published (see, e.g., Refs. 1–8) where subtleties of the transition from three-dimensional (3D) to two-dimensional behavior were studied as the quantum wells becomes progressively deeper. These works are of obvious importance in view of the role played by excitons with confinement-enhanced binding energies in optical phenomena of semiconducting heterostructures (and, thus, in optoelectronic devices). In particular, Ref. 4 notes that even extremely shallow quantum wells in the $GaAs/Ga_{1-x}Al_xAs$ system ($x=0.01$, width $w=200$ Å) do exhibit experimentally measurable deviations of the exciton energy from its value characteristic for three dimensions. It is, therefore, important to develop a reliable theory of the exciton in such weakly confined systems. It is obvious that one needs to go beyond the simple trial wave functions given above in order to treat this small well depth limit. II-VI spin superlattices[9–11] represent a system with small (vanishing in the absence of an external magnetic field) offsets in both the conduction and the valence bands. It is the study of this system that gave initial motivation for the present work.

Various improvements of the theory of excitons in configurations involving weak confining potentials have been suggested to amend the consistency of the approach[12–22] In the majority of quantum well systems, the holes are the first to become delocalized (since the valence band offset is usually smaller than that of the conduction band). Therefore, it is often assumed that the electrons remain strongly localized by the quantum well potential [and thus describable in terms of $\chi_1(x_e)$], and then an effective Schrödinger equation is derived for an exciton whose potential experienced by the holes contains a term proportional to Refs. 13–18,

$$\frac{\int|\chi_1(z_e)|^2dz_e}{\kappa r}, \tag{1}$$

where r is the length of the relative variable of motion given by

$$r=\sqrt{(x_h-x_e)^2+(y_h-y_e)^2+(z_h-z_e)^2}. \tag{2}$$

A more general procedure was constructed in Ref. 19, which allows for both types of particles to be only very weakly localized in the quantum well region. Unfortunately, the latter approach relies on a lengthy variational self-consistent calculation that is not at all transparent.

A systematic theoretical study of the problem of excitons in a shallow quantum well has been very recently published in Ref. 22. In this variational approach the authors made use of a class of trial wave functions that are suitable for both shallow and deep quantum wells. The primary aim of the study in Ref. 22 was to analyze the transition from a three-dimensional exciton behavior to the 2D regime driven by an application an in-plane magnetic field. For reasons stated below, the results obtained in Ref. 22 are of special interest to that aspect of our study which concentrates on diluted magnetic semiconductor quantum structures. The authors of Ref. 22 noticed that in the case of shallow quantum wells (when the well depth does not exceed the three-dimensional exciton binding energy ε_{3D}), the wave function of the exciton can be well approximated by a product of a function depending only on the relative motion variable of the electron and the hole comprising the exciton by a wave function depending only on the center-of-mass variable. (The decomposition of the two-particle problem into independent relative motion and center-of-mass motions is not, strictly speaking, possible in the presence of the quantum well potential which breaks the translational invariance of the system.) This particular case is referred to in Ref. 22 as 3D-like regime (as opposed to a 2D-like regime, where the coupling of the center-of-mass and relative motions of the electron and the hole becomes important). In other words, the problem becomes that of a nearly 3D relative variable eigenproblem, with the center-of-mass motion subject to quantization by a potential arising from the confining potential due to the presence of the quantum well. In this paper we shall use the same assumption concerning the form of the exciton wave function. We shall show further that this is an approximately justified approach in the particular case of $Zn_{0.96}Mn_{0.04}Se/ZnSe$ spin superlattices of interest to us. In these systems it is only in the presence of an external magnetic field that the confining potentials in certain layers of the structure become appreciable. In contrast to Refs. 6,22, however, in these structures involving diluted magnetic semiconductors (DMS's)[26] we can neglect the direct influence of the magnetic field via the $\vec{A}\cdot\vec{p}$ term in the Hamiltonian on the motion of the particles. The magnetic field will enter the problem only through modifications of the depth of the quantum wells related to the spin splitting of the conduction and the valence band edges. This approximation is very well justified in view of the smallness of cyclotron energies for the holes and electrons compared to their giant spin splitting characteristic for DMS's arising from the very strong coupling of electron and hole spins to localized magnetic moments of Mn ions.

In the present paper we attempt to find a formulation that would be essentially analytical, and would make the physics underlying the problem as explicit as possible. We find, as mentioned, that the correction to the energy of the nearly three-dimensional exciton occurring in small-offset structures can be expressed in terms of a quantized energy of its center-of-mass motion (in the z direction), which is neglected in most earlier analyses (Refs. 6,22,23 being exceptions). In this respect, the present paper emphasizes the importance of an aspect of excitonic energetics that was completely ignored in the majority of the papers so far. In the next section we formulate the model, and we solve it for various exciton energies. We illustrate the ranges of parameters in which the model is applicable by using various semiconductor systems as examples. Then, in Sec. III, we use the equations which have been derived to specifically calculate the optical transition energies in $ZnSe/Zn_{1-x}Mn_xSe$ spin superlattices, and we find that the model yields corrections that are quantitatively consistent with recent experimental observations of Dai *et al.*[10]

II. FORMULATION OF THE MODEL

We shall assume that both the conduction and the valence band are nondegenerate (apart from spin degeneracy), and that they have simple isotropic and parabolic dispersions characterized by the masses m_e and m_h (the heavy hole mass), respectively. These simplifications are justified by the relatively large splitting between the heavy and the light hole subbands usually present in strained heterostructures. The Hamiltonian of an exciton in such a system is

$$H_{\rm ex}=\frac{p_e^2}{2m_e}+\frac{p_h^2}{2m_h}+V_e(z_e)+V_h(z_h)-\frac{e^2}{\kappa|\vec{r}_e-\vec{r}_h|}, \quad (3)$$

where E_g is the band gap of the ''barrier'' material, while the potentials due to the band edge discontinuities are

$$V_e(z_e)=\begin{cases} E_g-V_e^0 & \text{for } -\dfrac{w}{2}\leqslant z_e\leqslant\dfrac{w}{2}, \\ E_g & \text{otherwise,}\end{cases} \quad (4)$$

$$V_h(z_h)=\begin{cases} V_h^0 & \text{if } -\dfrac{w}{2}\leqslant z_h\leqslant\dfrac{w}{2}, \\ 0 & \text{otherwise,}\end{cases} \quad (5)$$

w being the width of the quantum well. With the present approach it is, in principle, possible to consider the case where the quantum wells for the electrons and for the holes occur in spatially different regions of the structure (as in the case of type-II structures). However, here we shall limit ourselves to the simplest type-I situation, with both the holes and the electrons experiencing the well potential for $|z_i|\leqslant(w/2)$ $(i=e,h)$. We are thus assuming that V_e^0 and V_h^0 are positive quantities in Eqs. (4)–(5). (In the above expressions the zero of the energy scale was taken at the valence band edge of the ''barrier'' material, and the origin of z is taken at the center of the well.)

Introducing, as usual, the center of mass and the relative motion variables defined by

$$(m_e+m_h)\vec{R}=m_e\vec{r}_e+m_h\vec{r}_h, \quad (6)$$

$$\vec{r}=\vec{r}_e-\vec{r}_h, \quad (7)$$

and substituting them into Eq. (3), we obtain

$$H_{\rm ex}=E_g+\frac{P_\perp^2}{2M}+\frac{P_Z^2}{2M}+\left(\frac{\vec{\pi}^2}{2\mu}-\frac{e^2}{\kappa r}\right)+V_e\left(Z+\frac{m_h}{M}z\right)+V_h\left(Z-\frac{m_e}{M}z\right), \quad (8)$$

where the reduced mass μ and that of the center-of-mass M are given by

$$\mu^{-1}=m_e^{-1}+m_h^{-1}, \tag{9}$$

$$M=m_e+m_h. \tag{10}$$

In the above expression, $\vec{\pi}$ denotes the momentum operator related to the relative variable $\vec{r}$, while $\vec{P}_\perp$ and $\vec{P}_Z$ are the components (two-dimensional and one-dimensional, respectively) of the momentum relative to the center-of-mass variable $\vec{R}$. The second and the third terms in Eq. (8) represent the kinetic energy of the center-of-mass motion. The fourth and fifth terms in the parentheses in Eq. (8) correspond to the three-dimensional relative motion of the exciton. The remaining two terms mix the two types of variables. If these two terms are weak, then one can solve the equation approximately, using the solution for the ground state of the exciton in the form

$$\psi_{\rm ex}(\vec{r},\vec{R})=\frac{1}{\sqrt{S}}e^{i\vec{K}_\perp\cdot\vec{R}_\perp}\frac{1}{\sqrt{\pi a_B^3}}e^{-r/a_B}F(Z), \tag{11}$$

where $a_B=\hbar^2\kappa/\mu e^2$ is the three-dimensional exciton Bohr radius, S is the area of the sample, $\vec{R}_\perp$ is the (two-dimensional) in-plane vector related to the quasifree center-of-mass motion, and $\vec{K}_\perp$ is the corresponding momentum. The function $F(Z)$ (normalized to unity) is yet to be determined.

The energy of the exciton described by the wave function, Eq. (11) can now be calculated:

$$\begin{aligned}\langle\psi_{\rm ex}|H_{\rm ex}|\psi_{\rm ex}\rangle=E_g-\varepsilon_{\rm 3D}+\frac{\hbar^2K_\perp^2}{2M}+\left\langle F(Z)\right|\frac{P_Z^2}{2M}\\ +\frac{1}{\pi a_B^3}\int e^{-2(r/a_B)}\left[V_e\left(Z+\frac{m_h}{M}z\right)\right.\\ \left.+V_h\left(Z-\frac{m_e}{M}z\right)\right]d^3r\left|F(Z)\right\rangle.\end{aligned} \tag{12}$$

The last term in the above expression can be treated (after carrying out the integration over the three-dimensional relative variable) as a matrix element of an effective Hamiltonian which describes the motion of the excitonic center of mass in the Z direction. The corresponding eigenvalue problem then becomes

$$H^{\rm eff}F(Z)=\left[\frac{P_Z^2}{2M}+V^{\rm eff}(Z)\right]F(Z)=\varepsilon F(Z), \tag{13}$$

where ε gives the correction to the energy of the three-dimensional exciton due to its center-of-mass motion in the z direction that is weakly perturbed by the rectangular well potential. Here

$$V^{\rm eff}=V_e^{\rm eff}(Z)+V_h^{\rm eff}(Z), \tag{14}$$

with

$$V_e^{\rm eff}(Z)=\begin{cases}-\frac{1}{2}V_e^0\left\{\left[-1-\left(\frac{w}{2}-Z\right)\frac{1}{a_B}\frac{M}{m_h}\right]e^{-(2/a_B)[(w/2)-Z](M/m_h)}+\left[1-\left(\frac{w}{2}+Z\right)\frac{1}{a_B}\frac{M}{m_h}\right]e^{(2/a_B)[(w/2)+Z](M/m_h)}\right\} & \text{for } Z<-\frac{w}{2}\\ -\frac{1}{2}V_e^0\left\{\left[-1-\left(\frac{w}{2}+Z\right)\frac{1}{a_B}\frac{M}{m_h}\right]e^{-(2/a_B)[(w/2)+Z](M/m_h)}+\left[-1-\left(\frac{w}{2}-Z\right)\frac{1}{a_B}\frac{M}{m_h}\right]e^{-(2/a_B)[(w/2)-Z](M/m_h)}+2\right\} & \text{for } -\frac{w}{2}<Z<\frac{w}{2}\\ -\frac{1}{2}V_e^0\left\{\left[-1-\left(\frac{w}{2}+Z\right)\frac{1}{a_B}\frac{M}{m_h}\right]e^{-(2/a_B)[(w/2)+Z](M/m_h)}+\left[1-\left(\frac{w}{2}-Z\right)\frac{1}{a_B}\frac{M}{m_h}\right]e^{(2/a_B)[(w/2)-Z](M/m_h)}\right\} & \text{for } Z>\frac{w}{2}\end{cases} \tag{15}$$

and

$$V_h^{\rm eff}(Z)=\begin{cases}-\frac{1}{2}V_h^0\left\{\left[1+\left(\frac{w}{2}-Z\right)\frac{1}{a_B}\frac{M}{m_e}\right]e^{-(2/a_B)[(w/2)-Z](M/m_e)}+\left[-1+\left(\frac{w}{2}+Z\right)\frac{1}{a_B}\frac{M}{m_e}\right]e^{(2/a_B)[(w/2)+Z](M/m_e)}\right\} & \text{for } Z<-\frac{w}{2}\\ -\frac{1}{2}V_h^0\left\{\left[1+\left(\frac{w}{2}-Z\right)\frac{1}{a_B}\frac{M}{m_e}\right]e^{-(2/a_B)[(w/2)-Z](M/m_e)}+\left[1+\left(\frac{w}{2}+Z\right)\frac{1}{a_B}\frac{M}{m_e}\right]e^{-(2/a_B)[(w/2)+Z](M/m_e)}-2\right\} & \text{for } -\frac{w}{2}<Z<\frac{w}{2}\\ -\frac{1}{2}V_h^0\left\{\left[-1+\left(\frac{w}{2}-Z\right)\frac{1}{a_B}\frac{M}{m_e}\right]e^{(2/a_B)[(w/2)-Z](M/m_e)}+\left[1+\left(\frac{w}{2}+Z\right)\frac{1}{a_B}\frac{M}{m_e}\right]e^{-(2/a_B)[(w/2)+Z](M/_e)}\right\} & \text{for } Z>\frac{w}{2}.\end{cases} \tag{16}$$

Figure 1 shows a sketch of the effective potential $V^{\rm eff}(Z)$ for $Ga_xAl_{1-x}As/GaAs$ quantum wells, for width w smaller than, equal to, and greater than a_B, respectively. The overall shape of the effective potential gradually changes from rectangularlike to paraboliclike, as we reduce the quantum well width. This suggests that, when $a_B/w<1$, we can approximate the eigenvalues of Eq. (13) by solutions of the Schrödinger equation for a particle of mass M in a rectangular well with width w, and with depth ε_0 given by

$$\begin{aligned}\varepsilon_0=-(|V_e^0|+|V_h^0|)+|V_e^0|\left(1+\frac{1}{2}\frac{w}{a_B}\frac{M}{m_h}\right)e^{-(w/a_B)(M/m_h)}\\ +|V_h^0|\left(1+\frac{1}{2}\frac{w}{a_B}\frac{M}{m_e}\right)e^{-(w/a_B)(M/m_e)}.\end{aligned} \tag{17}$$

These eigenvalues can be easily found numerically in a standard way.[1] In the opposite limit, when $a_B/w>1$, the eigenvalues of Eq. (13) can be approximated by solutions of the

Schrödinger equation for a particle with mass M moving in a parabolic potential,

$$V_{\text{parab}}^{\text{eff}}(Z)=\varepsilon_0+\frac{w}{a_B^3}M^3\left[V_e^0 e^{-(w/a_B)(M/m_h)}\frac{1}{m_h^3}+V_h^0 e^{-(w/a_B)(M/m_e)}\frac{1}{m_e^3}\right]Z^2. \tag{18}$$

In general, solutions for a parabolic quantum well of a finite depth are obtained numerically.[24] However, when the well is sufficiently deep (i.e., when $|\varepsilon_0|>\frac{1}{2}\hbar\omega$, see below), we can approximate the eigenvalues by

$$\varepsilon=\varepsilon_0+\frac{1}{2}\hbar\omega, \tag{19}$$

where

$$\omega=\sqrt{2\left(|V_e^0|e^{-(w/a_B)(M/m_h)}\frac{1}{m_h^3}+|V_h^0|e^{-(w/a_B)(M/m_e)}\frac{1}{m_h^3}\right)\frac{wM^2}{a_B^3}}. \tag{20}$$

We see immediately from Eqs. (17) and (20) that, for $(w/a_B)\to\infty$, we have $\varepsilon_0\to-(|V_e^0|+|V_h^0|)$. For $(w/a_B)\to 0$, on the other hand, we have

$$\varepsilon_0=\frac{1}{2}\frac{w}{a_B}M\left(|V_e^0|\frac{1}{m_h}+|V_h^0|\frac{1}{m_e}\right) \tag{21}$$

and

$$\omega=\frac{M}{a_B}\sqrt{|V_e^0|\frac{1}{m_h^3}+|V_h^0|\frac{1}{m_e^3}}. \tag{22}$$

In the intermediate case of $a_B\approx w$, we can numerically integrate Eq. (13) using one of the appropriate routines for finding solutions of differential equations. As shown in Ref. 25, the Schrödinger equation is very efficiently solved by the so called shooting method. We have used it in our approach to Eq. (13).

The sum of $E_g+\varepsilon-\varepsilon_{3D}$ represents now the total energy of the exciton in the ground state. Thus, $|\varepsilon-\varepsilon_{3D}|$ can be interpreted as the binding energy of a nearly three-dimensional exciton, weakly perturbed by the presence of a shallow quantum well. Since ε is a negative quantity, we obtain an enhancement of the binding energy due to the presence of the well potential. The ''weakness'' of the perturbation required at the outset of our calculation—and justifying our entire approach—can now be put on a more quantitative grounds by demanding that $|\varepsilon|<|\varepsilon_{3D}|$.

Figure 2 shows $|\varepsilon-\varepsilon_{3D}|$ calculated for GaAs quantum wells surrounded by $Ga_{0.99}Al_{0.01}As$ barriers. The curves for the parabolic approximation and the rectangular approximation are drawn only in the regions where Eq. (19) and Eq. (17) are, respectively, applicable. An experimental point from Ref. 4 for $w=200$ Å is also shown.

III. APPLICATION TO $ZnSe/Zn_xMn_{1-x}Se$ SPIN SUPERLATTICES

We apply the above formulation specifically to spin superlattices involving ZnSe and DMS's $Zn_{0.96}Mn_{0.04}Se$ layers.[26] DMS's are characterized by a strong spin splitting of the conduction band edge and, particularly, the valence band edge. The origin of the splitting lies in the strong sp-d coupling of the spins of band carriers and those localized on Mn ions. The splitting is proportional to the magnetization of the DMS material. The idea of a spin superlattice[9] involves alternating layers of nonmagnetic and DMS materials, where the materials are chosen in such a way that, in the absence of an external magnetic field, both constituents have the same value of the energy gap, and their conduction and valence band edges are aligned. After application of a magnetic field, however, the band edges in both types of layers begin to shift with respect to one another, because the spin splitting in the nonmagnetic component is negligible compared to that in the DMS layer. Depending on the spin of the particle (up or down) a well may be created in this way for, say, the spin-up electrons in the DMS layers, while the spin-down electrons experience a quantum well in the nonmagnetic layers of the heterostructure. The amount of Mn in the DMS layers in $ZnSe/Zn_{0.96}Mn_{0.04}Se$ superlattice was chosen to make the energy gaps of the two constutuents equal making use of a small bowing of the ΔE_g vs x relationship. Similar spatial separation of the spin species occurs in the valence band.[10] The idea of a spin superlattice has been realized in practice in $ZnSe/Zn_xMn_{1-x}Se$ (Ref. 10) and in $ZnSe/Zn_xFe_{1-x}Se$ (Ref. 11) DMS systems.

As a result, when studying spin superlattices, one deals with systems of quantum wells whose barrier heights depend on the magnetic field, growing from zero to a maximum value determined by the saturation magnetization. In the particular case of a $ZnSe/Zn_{0.96}Mn_{0.04}Se$ spin superlattice, the maximum band discontinuity in the heavy hole band is of the order of 30 meV at liquid helium temperatures. For the conduction band, the maximum band discontinuity is even smaller, due to a smaller exchange coupling constant for the s-like electrons.[26,27] Thus, the depth of the quantum wells that form in these spin superlattices is (in magnetic fields smaller than those corresponding to saturation of the magnetization) comparable or smaller than the exciton binding energy in the bulk material, which is ~ 22.1 meV. In this situation the usual approaches to the exciton problem appears to be inappropriate.

The authors of Ref. 10 used the value of the three-dimensional exciton binding energy for calculating the transition energies to be compared with those observed in their magnetoabsorption experiments. They noted a conspicuous deviation of the calculated transition energies, which consistently overestimated the observed values. The deviations also showed a clear trend of increasing with the field. Already in

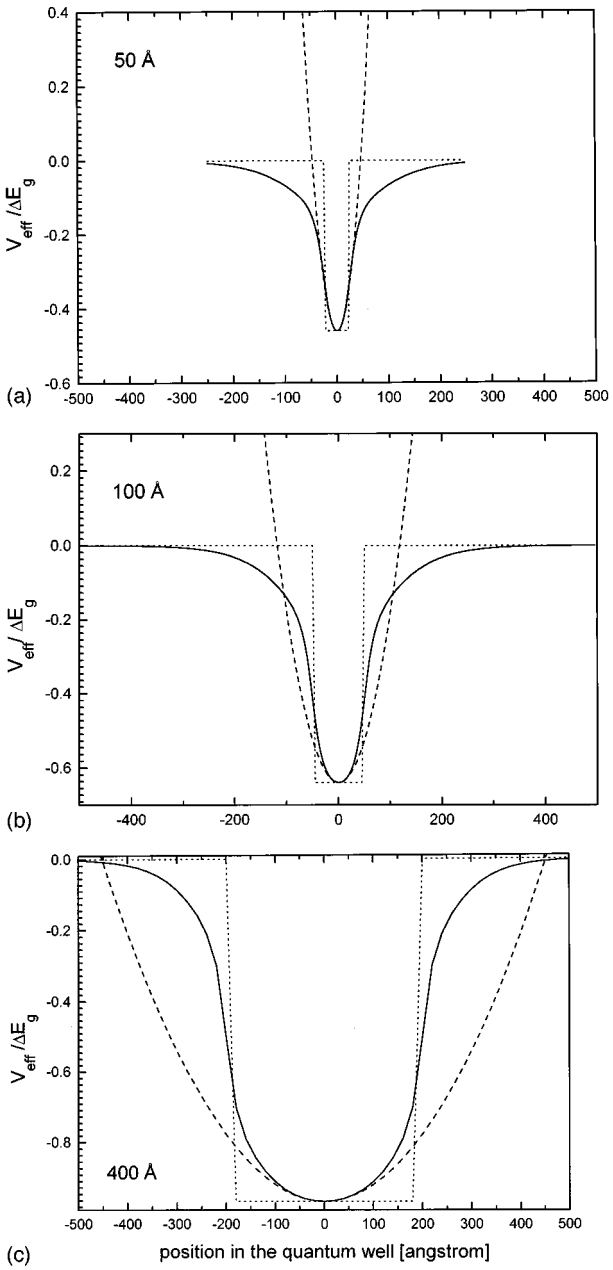

FIG. 1. Calculated shapes of the effective potential given by Eq. (14) for three values of the quantum well width: (a) $w=50$ Å, (b) $w=100$ Å, and (c) $w=400$ Å. Material parameters were taken as for GaAs/$Ga_{1-x}Al_x$As quantum wells ($m_e=0.067$, $m_h=0.38$, $\kappa=12.56$), which lead to $a_B=116$ Å. The potential is in units of the energy gap discontinuity ΔE_g (which depends on x), with the valence band offset constituting 35% of this value and the conduction band offset being equal to 65% of ΔE_g. The dotted and dashed lines show the approximate rectangular and parabolic potentials, respectively.

Ref. 10 a hypothesis was put forward that the aforementioned discrepancies between calculations and experimental data could be related to modifications of the exciton binding energy due to the presence of a shallow potential of the (field-induced) quantum well.

To check this hypothesis, we calculated the energy of the exciton *via* the procedure developed in the previous section, with V_e^0 and V_h^0 calculated using the standard expressions for

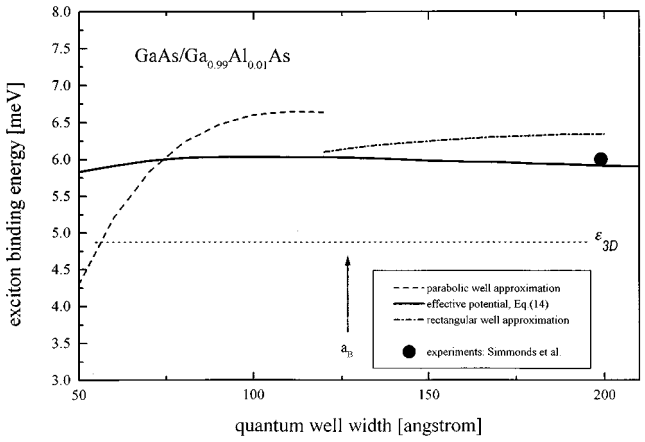

FIG. 2. The energy of the exciton in a shallow GaAs/$Ga_{0.99}Al_{0.01}$As quantum well as a function of the well width. Dash-dotted line corresponds to the solution of the rectangular well eigenproblem, Eq. (17), dashed line shows the solutions of the eigenproblem with an (infinite) parabolic potential with parameters given by Eq. (18); and the solid line shows the solution with the general form of the potential, Eq. (14) obtained by the shooting method. The dashed and dash-dotted lines are plotted only in the regions of applicability of the respective approximations. An experimental point from Ref. 4 is also shown. The thin dotted line indicates the binding energy of a 3D exciton.

the band-edge variation of a DMS material in a magnetic field B:

$$V_e^0=\left|\tfrac{1}{2}\alpha x N_0\langle S_z\rangle\right| \tag{23}$$

and

$$V_h^0=\left|\tfrac{1}{2}\beta x N_0\langle S_z\rangle\right|, \tag{24}$$

where $|\alpha|N_0=0.27$ eV, $|\beta|N_0=0.9$ eV,[26,27] and $\langle S_z\rangle$ is the average component of the Mn-spin along the field direction is given by

$$\langle S_z\rangle=3\coth\left[\frac{3g_{\mathrm{Mn}}\mu_B B}{k_B(T+T_0)}\right]-\frac{1}{2}\coth\left[\frac{g_{\mathrm{Mn}}\mu_B B}{2k_B(T+T_0)}\right]. \tag{25}$$

Here $g_{\mathrm{Mn}}=2$, μ_B is the Bohr magneton, k_B—the Boltzmann constant, T—the temperature, and $T_0=1.4$ K. This expression proved very accurate in describing the spin splitting in the bulk $Zn_{0.96}Mn_{0.04}Se$ (c.f. Ref. 10). Using the effective mass values for the electrons and the heavy holes in ZnSe ($m_e=0.133$ and $m_h=0.775$) and the dielectric constant in this material ($\kappa=8.8$), we can calculate the relevant quantities, and convince ourselves that for the well widths in the samples studied in Ref. 10 (73 Å and 105 Å) we can accurately approximate the potential $V^{\mathrm{eff}}(Z)$, Eq. (14), by a rectangular potential with a depth given by Eq. (17) in the entire range of the fields studied (up to 5 T). Solving for the eigenvalues, we obtain the exciton energy $|\varepsilon-\varepsilon_{3D}|$ as a function of the magnetic field B. The results are shown in Fig. 3, together with the three-dimensional exciton binding energy.

In Fig. 4 we compare the optical transition energies calculated using both the three-dimensional exciton binding energy and the exciton energies obtained in the present approach with those observed experimentally.[10] The calculated

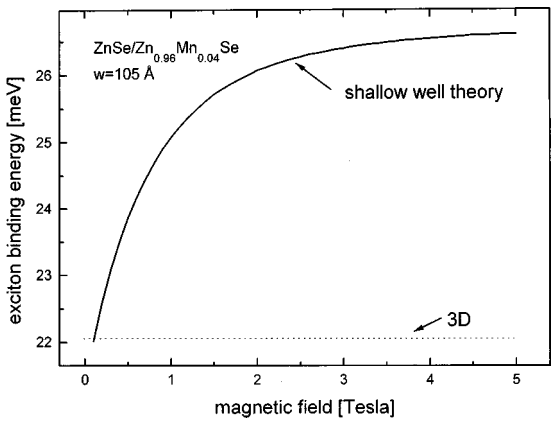

FIG. 3. Exciton binding energies in $ZnSe/Zn_{0.96}Mn_{0.04}Se$ spin superlattices with layer thicknesses of 105 Å for both materials as a function of magnetic field at $T=1.5$ K. For comparison, the value of the three-dimensional exciton binding energy is also shown by the dashed line.

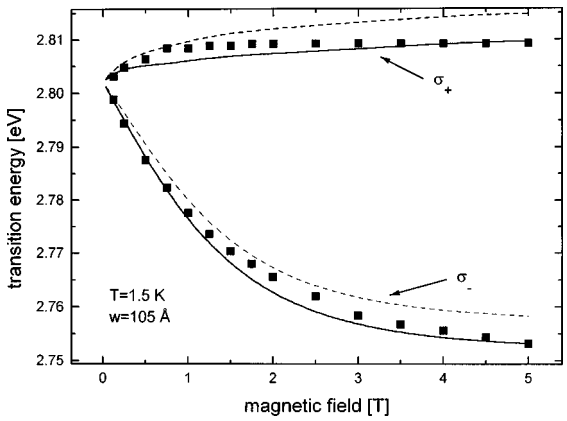

FIG. 4. Comparison of the measured energies at $T=1.5$ K of optical transitions in $ZnSe/Zn_{0.96}Mn_{0.04}Se$ spin superlattice (Ref. 10) (symbols) with calculations assuming either uncorrected, three-dimensional exciton energies [broken lines (Ref. 10)] or those calculated using the present approach (solid lines) within the rectangular well approximation.

values based on the quantization of the exciton center-of-mass motion in the z direction are in good agreement with the observations, giving a marked improvement over those using the 3D approach, and confirming the original conjecture concerning the source of the deviations noted in Ref. 10.

Let us check the validity of the assumptions used in the derivation of the above results. First, notice that dropping the terms in the Hamiltonian of the electron and the hole that are due to the direct influence of a magnetic field through $\vec{A}\cdot\vec{p}$ terms (see, Ref. 22) is perfectly justified. This is because $\hbar\Omega_c$ (where $\Omega_c=eB/c\mu$) is much smaller (maximum 2%) in the entire range of the magnetic field considered in Ref. 10 than the total spin splitting of the valence and conduction band edges, which determines the depth of the quantum well. In fact $\hbar\Omega_c$ becomes equal to the total depth of the quantum well only in fields as large as 500 T (the quantum well varies only slightly with B in the high magnetic field region due to saturation of the magnetization).

Second, the relatively large value of the 3D exciton binding energy ε_{3D} in II-VI compounds justifies the use of wave functions in the form of the product of functions depending separately on r and $(\vec{R}_\perp, Z)$. In fact, in our case we have $\varepsilon_{3D}=22.1$ meV, and the depth of the quantum well in the conduction band at $B=5$ T (i.e., at the maximum field considered here) is $V_e^0\approx 11$ meV, while that in the valence band is $V_h^0\approx 43$ meV. While, strictly speaking, the depth of the quantum well at the highest magnetic field considered in Ref. 10 does exceed ε_{3D}, an inspection of Figs. 1 and 2 in Ref. 22 convince us that even for quantum wells as deep as $\sim 2\varepsilon_{3D}$ the crossover from the 3D-like regime to the 2D-like regime is rather slow. This gives some confidence in the separable wave function used by us. Nevertheless, it is possible that the deviations between our calculations and the experimental data in Fig. 4 are related to the onset of the 3D→2D crossover, and constitutes a limitation of the present method.

IV. CONCLUSIONS

We have developed a simple theory of excitons in very shallow quantum wells, which includes the energy corrections due to size quantization of the center-of-mass motion. We were able to solve the problem analytically assuming realistic parameters for the quantum wells. In particular, the energy corrections derived by us satisfactorily explain deviations between calculated and observed values of magneto-optical transition energies in DMS spin superlattices, where an external magnetic field creates shallow but well-defined quantum wells.

Similar conclusion concerning the importance of the exciton center-of-mass quantization in shallow quantum wells were arrived at in recent theoretical calculations[22] (see, also, Ref. 6). Let us note, however, that although the application of the magnetic field drives the transition from a 3D-like to a 2D-like exciton regime, as concluded in Ref. 22, in our case this occurs also in the configuration with B pointing along the growth axis of the structure (z direction). This is in contrast to the case considered in Ref. 22, where only the in-plane component of the field induces the transition.

ACKNOWLEDGMENT

This work was supported by the NSF Grant No. DMR 92-08400.

[1] G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures* (Halstead Press, New York, 1988).

[2] L. C. Andreani and A. Pasquarello, Phys. Rev. B **42**, 8928 (1990).

[3] Q. X. Zhao, P. O. Holtz, C. I. Harris, B. Monemar, and E. Veje, Phys. Rev. B **50**, 2023 (1994).

[4] P. E. Simmonds, M. J. Birkett, M. S. Skolnick, W. I. E. Tagg, P. Sobkowicz, G. W. Smith, and D. M. Whittaker, Phys. Rev. B **50**, 11 251 (1994).

[5] I. Brener, W. H. Knox, K. W. Goosen, and J. E. Cunningham, Phys. Rev. Lett. **70**, 319 (1993).

[6] M. Fritze, I. E. Perakis, A. Getter, W. Knox, K. W. Goosen, J. E. Cunnigham, and S. A. Jackson, Phys. Rev. Lett. **76**, 106 (1996).
[7] A. Alexandrou, M. K. Jackson, D. Hulin, N. Magnea, H. Mariette, and Y. Merle d'Aubigneé, Phys. Rev. B **50**, 2727 (1994).
[8] V. Voliotis, R. Grousson, P. Lavallard, and R. Planel, Phys. Rev. B **52**, 10 725 (1995).
[9] M. von Ortenberg, Phys. Rev. Lett. **49**, 1041 (1982).
[10] N. Dai, L. R. Ram-Mohan, H. Luo, G. Yang, F. C. Zhang, M. Dobrowolska, and J. K. Furdyna, Phys. Rev. B **50**, 18 153 (1994).
[11] X. C. Liu, W. C. Chou, A. Petrou, J. Warnock, B. T. Jonker, G. A. Prinz, and J. J. Krebs, in *Proceedings of the 20th International Conference on the Physics of Semiconductors, Thessaloniki*, edited by E. M. Anastassakis and J. D. Joannopoulos (World Scientific, Singapore, 1990), p. 621.
[12] W. J. Walecki, A. V. Nurmikko, N. Samarth, H. Luo, J. K. Furdyna, and N. Otsuka, Appl. Phys. Lett. **57**, 466 (1990).
[13] C. Delalande, Superlattices Microstruct. **12**, 387 (1992).
[14] E. I. Ivchenko, A. V. Kavokin, V. P. Kochereshko, G. R. Posina, I. N. Uraltsev, D. R. Yakovlev, R. N. Bicknell-Tassius, A. Waag, and G. Landwehr, Phys. Rev. B **46**, 7713 (1990).
[15] E. Deleporte, J. M. Berroir, G. Bastard, C. Delalande, J. M. Hong, and L. L. Chang, Phys. Rev. B **42**, 5891 (1990).
[16] Ji-Wei and A. V. Nurmikko, Phys. Rev. B **38**, 1504 (1988).
[17] S. K. Chang, A. V. Nurmikko, J. W. Liu, L. A. Kolodziejski, and R. L. Gunshor, Phys. Rev. B **37**, 1191 (1988).
[18] G. Peter, E. Deleporte, G. Bastard, J. M. Berroir, C. Delalande, D. Gil, J. M. Hong, and L. L. Chang, J. Lumin. **52**, 147 (1992).
[19] J. Warnock, B. T. Jonker, A. Petrou, W. C. Chou, and X. Liu, Phys. Rev. B **48**, 17 321 (1993).
[20] P. Peyla, R. Romestain, Y. Merle d'Aubigné, G. Fishman, A. Wasiela, and H. Mariette, Phys. Rev. B **52**, 12 026 (1995).
[21] R. P. Leavit and J. W. Little, Phys. Rev. B **42**, 11 774 (1990).
[22] A. Getter, I. E. Perakis, and S. A. Jackson, Solid State Commun. **98**, 379 (1996).
[23] J. Kossut and J. K. Furdyna, Acta Phys. Pol. A **86**, 528 (1995).
[24] W.-P. Yuen, Phys. Rev. B **48**, 17 316 (1993).
[25] S. E. Koonin and D. C. Meredith, *Computational Physics* (Addison-Wesley, New York, 1989).
[26] For a review of diluted magnetic semiconductors see, *Diluted Magnetic Semiconductors*, edited by J. K. Furdyna and J. Kossut, Semiconductors and Semimetals, Vol. 25 (Academic, Boston 1988).
[27] J. Kossut and W. Dobrowolski, in *Handbook of Magnetic Materials*, edited by K. H. J. Buschow (Elsevier, Amsterdam, 1993), Vol. 7, Chap. 4, pp. 231–305; *Semiconductors. Physics of II-VI and I-V Compounds, Semimagnetic Semiconductors*, edited by G. Madelung, Landolt Bornstein, New Series, Group III, Vol. 17, Pt. b (Springer, Berlin, 1982).