Exciton binding energies in a dielectric quantum well in a magnetic field

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We study the effect of a magnetic field applied along the growth axis on exciton binding energies in dielectric quantum-well structures, in which the dielectric constant of the confining barriers is significantly smaller than that of the well material. The anisotropic electron-hole Coulomb interaction potential is obtained analytically by solving the Poisson equation in the layered geometry of quantum wells. Confinement is provided by the image charge distribution arising from the mismatch of dielectric constants at the interfaces, in addition to that of the quantum-well potential and the applied magnetic field. Exciton binding energies are calculated using the Gaussian-type orbital expansion method. Significantly enhanced binding energies are obtained for the excitons in various dielectric quantum-well structures and their behavior in a magnetic field is discussed.

I. INTRODUCTION

The enhancement of the Coulomb interaction in a thin semiconductor layer sandwiched by insulators was first pointed out by Keldysh in 1979.[1,2] A quantum well can be called "dielectric" when the dielectric constant of the barrier material is significantly smaller than that of the well material, as in the case of a GaAs-ZnSe quantum well (QW) and others constructed according to the same principle. Image charges arise due to the mismatch of dielectric constants at the interfaces. Dielectric quantum wells have recently received increasing attention because of their potential to sustain electro-optic operations with greater range of applicable electric fields.[3–8] Recent progress in the fabrication of such structures has prompted further interest in studying properties of excitons and their dependence on various material parameters and applied fields.[9–14] Binding energies of excitons can be significantly enhanced because of the additional confinement effect produced by the image charge distribution.

Calculations of the binding energies and their variations with the applied fields are needed to obtain accurate values of the optical transition energies of excitons in such quantum wells. Dielectric quantum wells differ from the nondielectric quantum wells in one essential aspect, i.e., in addition to the usual quantum confinement provided by the band offsets at the interfaces and possibly also by external fields, confinement effect due to the image charge distributions is also significant. The Coulomb interaction between an electron and a hole is no longer isotropic; it not only depends on $z_e - z_h$ (where z is the direction normal to the interfaces), but also involves $z_e + z_h$. A comprehensive theoretical treatment of excitons in dielectric quantum-well structures was given by Kumagai and Takagahara,[4] in the absence of external fields. They used an image charge method to obtain the Coulomb attraction between an electron and a hole in the dielectric quantum wells. The image charge method, although very simple and intuitive when there is only one interface involved, becomes increasingly cumbersome to use in more complex geometries of quantum-well structures. For example, it would be practically impossible to use the image charge method in the coupled double quantum wells and superlattices.

We have developed a formalism for the calculation of binding energies of excitons in the "dielectric quantum wells," in the presence of a magnetic field applied along the growth axis. In this paper, we obtain the electron-hole Coulomb potential analytically by solving the first-principle Poisson equation in the layered geometry of quantum wells, which, in principle, can be readily used in the more complex dielectric quantum-well structures. In the next section, we consider excitons in a dielectric quantum well depicted in Fig. 1, and describe the variational formalism in which binding energies are calculated with the Gaussian-type orbital expansion method.[15–20] Several semiconductor quantum-well structures with significant dielectric confinement are considered. In Sec.

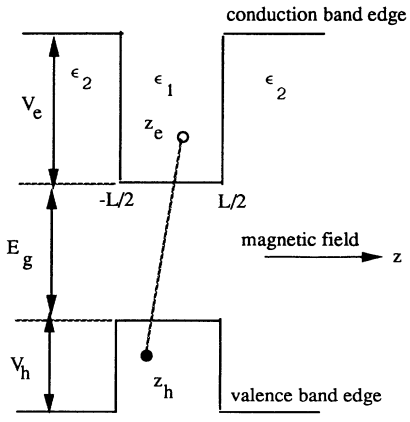

FIG. 1. Schematic band diagram for a dielectric quantum-well structure. The dielectric constant of the well material is ε_1, that of the barrier material is ε_2 ($\varepsilon_2 < \varepsilon_1$). The magnetic field **B** is applied parallel to the growth direction of the structure.

III, we give the results of the exciton binding energies in some representative dielectric quantum-well structures and discuss their variations as functions of the strength of the magnetic field and the size of the quantum well. A summary is provided in Sec. IV.

II. FORMALISM

We consider a dielectric quantum well of width L depicted in Fig. 1, with the magnetic field **B** applied along the growth direction (chosen as the z axis). The origin is chosen at the center of the well. The dielectric constant in the well is ε_1, that in the barrier is ε_2 ($\varepsilon_2<\varepsilon_1$).

Because of the difference in the dielectric constants, the electron not only sees the hole, but also its image charge distribution, and vice versa for the hole. In what follows, we solve the first-principle Poisson equation in the layered quantum-well geometry to obtain the expression of the potential between the electron and the hole, with the effect of image charge distributions properly accounted for.

The electrostatic potential $\Phi(\mathbf{r})$ produced by a unit charge at $(\rho=0, z=z_0)$ satisfies

$$\varepsilon\nabla^2\Phi(\mathbf{r})=-4\pi\delta(z-z_0)\ , \tag{1}$$

the solution of which in the cylindrical coordinates is independent of the azimuthal angle φ. We therefore can write $\Phi(\mathbf{r})$ in the general form,[21]

$$\Phi(\mathbf{r})=\int_0^\infty d\kappa\, f(z,z_0;\kappa)J_0(\kappa\rho)\ , \tag{2}$$

where $J_0(\kappa\rho)$ is the Bessel function of the zeroth order, $f(z,z_0;\kappa)$ is a function to be determined from boundary conditions on $\Phi(\mathbf{r})$, i.e., $\Phi(\mathbf{r})$ and $\varepsilon_i\partial\Phi_i(\mathbf{r})/\partial z$ be continuous across the interfaces at $z=\pm L/2$. Since $\Phi(\mathbf{r})$ is uniquely determined by the function $f(z,z_0;\kappa)$, we need only to obtain its expression for possible combinations of z and z_0. For that purpose, we divide the quantum-well structure into three regions for z and for z_0, depending on whether $z(z_0)$ is in the quantum well or in the barrier. A schematic diagram is provided in Fig. 2. For z_0 locations inside and outside the quantum well, we obtain expression of $f(z,z_0;\kappa)$ as a function of z,[22] and similar expressions of $f(z,z_0;\kappa)$ as function of z_0 if z locations are specified instead.

The derivation of the expressions for ($|z_0|<L/2$) is provided as an example; other expressions for z_0 outside the quantum well can be obtained similarly. $f(z,z_0;\kappa)$ in the quantum well and the barrier regions can be written as

$$f_{12}(z,z_0;\kappa)=De^{\kappa z}\quad (z<-L/2,\ |z_0|<L/2)\ , \tag{3.1}$$

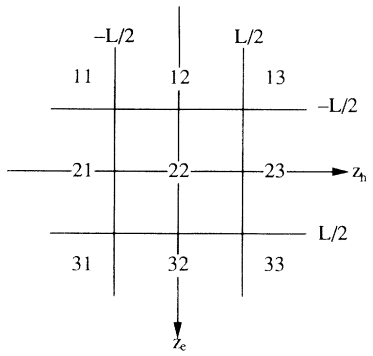

FIG. 2. Schematic diagram for regions in a dielectric quantum structure. z_e is the z coordinate of the electron, z_h the z coordinate of the hole. The first index denotes the region for the electron, the second index that of the hole.

$$f_{22}(z,z_0;\kappa)=e^{-\kappa|z-z_0|}+Ae^{-\kappa z}+Be^{\kappa z}\quad (|z|<L/2,\ |z_0|<L/2)\ , \tag{3.2}$$

$$f_{32}(z,z_0;\kappa)=Ce^{-\kappa z}\quad (z>L/2,\ |z_0|<L/2)\ , \tag{3.3}$$

where the term $e^{-\kappa|z-z_0|}$ would be the expression for the isotropic Coulomb interaction; the first index in f_{ij} indicates the region for z, the second index the region for z_0; A, B, C, D are constants to be determined. At $z=-L/2<z_0$,

$$f_{21}=f_{22},\quad \varepsilon_2\frac{\partial f_{12}}{\partial z}=\varepsilon_1\frac{\partial f_{22}}{\partial z}\ , \tag{4.1}$$

and at $z=L/2>z_0$,

$$f_{32}=f_{22},\quad \varepsilon_2\frac{\partial f_{32}}{\partial z}=\varepsilon_1\frac{\partial f_{22}}{\partial z}\ , \tag{4.2}$$

which lead to a set of linear equations

$$A+Be^{\kappa L}-C=-e^{\kappa z_0}\ , \tag{5.1}$$

$$A-Be^{\kappa L}-C\tilde{\varepsilon}=-e^{\kappa z_0}\ , \tag{5.2}$$

$$Ae^{\kappa L}+B-D=-e^{-\kappa z_0}\ , \tag{5.3}$$

$$Ae^{\kappa L}-B+D\tilde{\varepsilon}=e^{-\kappa z_0}\ , \tag{5.4}$$

where $\tilde{\varepsilon}=\varepsilon_2/\varepsilon_1<1$. We obtain the following expression of the electron-hole Coulomb interaction after substituting the solution of the above equation into Eqs. (3) and (2) (in units of the effective Rydberg),

$$H_C=-2\int_0^\infty d\kappa\, v_{jl}(z_e,z_h;\kappa)J_0(\kappa\rho)\ , \tag{6}$$

where

$$v_{11}(\kappa)=\frac{1}{\tilde{\varepsilon}}\left[e^{-\kappa|z_e-z_h|}-\frac{e^{\kappa(L+z_e+z_h)}\sinh\kappa L}{\sinh(\kappa L+\eta)}\right]\quad (z_e<-L/2,\ z_h<-L/2)\ , \tag{7.1}$$

$$\nu_{12}(\kappa)=\frac{2}{(1+\bar{\varepsilon})}\frac{e^{\kappa z_e+(\kappa L+\eta)/2}\cosh[\kappa z_h-(\kappa L+\eta)/2]}{\sinh(\kappa L+\eta)} \quad (z_e<-L/2,\ |z_h|\le L/2)\ , \tag{7.2}$$

$$\nu_{13}(\kappa)=\frac{2}{(1+\bar{\varepsilon})^2}\frac{e^{\kappa(L+z_e-z_h)+\eta}}{\sinh(\kappa L+\eta)} \quad (z_e<-L/2,\ z_h>L/2); \tag{7.3}$$

$$\nu_{21}(\kappa)=\frac{2}{(1+\bar{\varepsilon})}\frac{e^{\kappa z_h+(\kappa L+\eta)/2}\cosh[\kappa z_e-(\kappa L+\eta)/2]}{\sinh(\kappa L+\eta)} \quad (|z_e|\le L/2,\ z_h<-L/2)\ , \tag{7.4}$$

$$\nu_{22}(\kappa)=\frac{2\cosh[\kappa z_>-(\kappa L+\eta)/2]\cosh[\kappa z_<+(\kappa L+\eta)/2]}{\sinh(\kappa L+\eta)} \quad (|z_e|\le L/2,\ |z_h|\le L/2)\ , \tag{7.5}$$

$$\nu_{23}(\kappa)=\frac{2}{(1+\bar{\varepsilon})}\frac{e^{-\kappa z_h+(\kappa L+\eta)/2}\cosh[\kappa z_e+(\kappa L+\eta)/2]}{\sinh(\kappa L+\eta)} \quad (|z_e\le L/2,\ z_h>L/2)\ ; \tag{7.6}$$

$$\nu_{31}(\kappa)=\frac{2}{(1+\bar{\varepsilon})^2}\frac{e^{\kappa(L-z_e+z_h)+\eta}}{\sinh(\kappa L+\eta)} \quad (z_e>L/2,\ z_h<-L/2)\ , \tag{7.7}$$

$$\nu_{32}(\kappa)=\frac{2}{(1+\bar{\varepsilon})}\frac{e^{-\kappa z_e+(\kappa L+\eta)/2}\cosh[\kappa z_h+(\kappa L+\eta)/2]}{\sinh(\kappa L+\eta)} \quad (z_e>L/2,\ |z_h|\le L/2)\ , \tag{7.8}$$

$$\nu_{33}(\kappa)=\frac{1}{\bar{\varepsilon}}\left[e^{-\kappa|z_e-z_h|}-\frac{e^{\kappa(L-z_e-z_h)}\sinh\kappa L}{\sinh(\kappa L+\eta)}\right] \quad (z_e>L/2,\ z_h>L/2)\ ; \tag{7.9}$$

where $\eta=\ln[(1+\bar{\varepsilon})/(1-\bar{\varepsilon})]$, $z_>=\max(z_e,z_h)$, and $z_<=\min(m_e,z_h)$. It is easy to see that if the dielectric constants were the same across the interfaces (normal quantum-well case), then $\eta\to\infty$ and $\nu(z_e,z_h;\kappa)\to e^{-\kappa|z_e-z_h|}$, one recovers the usual expression for the Coulomb interaction $H_C=-2/r$. It is also easy to verify that a power-series expansion of the function $1/\sinh(\kappa L+\eta)$ in terms of $e^{-n\kappa L}$ $(n=1,\ldots,\infty)$ leads to the image change summations of the various terms in H_C. At this point we would also like to compare our expression for $\nu(z_e,z_h;\kappa)$ with that derived by Jain and Allen[23] for a structure consisting of a film containing a finite number of equally spaced layers of two-dimensional gas. Even though the structure we consider is different from that studied by Jain and Allen, our expression for $\nu(z_e,z_h;\kappa)$ goes over to their expression in the limit $L\to\infty$ in our case and d (spacing between two adjacent layers) goes to infinity in their case.

Within the framework of an effective-mass approximation, the Hamiltonian of an exciton in the quantum-well structure is written as

$$H=H_e+H_h+H_{\rm ex}^B\ , \tag{8}$$

where

$$H_e=-\frac{\partial}{\partial z_e}\frac{\mu_0}{m_e}\frac{\partial}{\partial z_e}+V_{\rm QW}^e(z_e)+V_{\rm SE}^e(z_e)\ , \tag{9.1}$$

$$H_h=-\frac{\partial}{\partial z_h}\frac{\mu_0}{m_h}\frac{\partial}{\partial z_h}+V_{\rm QW}^h(z_h)+V_{\rm SE}^h(z_h)\ , \tag{9.2}$$

$$H_{\rm ex}^B=\frac{\mu_0}{\mu(z_e,z_h)}\left[-\left[\frac{\partial}{\rho\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{\partial^2}{\rho^2\partial\varphi^2}\right]+\gamma L_z+\frac{\gamma^2\rho^2}{4}\right]+H_C(z_e,z_h;\rho)\ ; \tag{9.3}$$

$\rho=\sqrt{(x_e-x_h)^2+(y_e-y_h)^2}$, m_e is the effective mass of the electron, $\mu(z_e,z_h)$ is the reduced mass of the exciton defined by

$$\mu^{-1}=m_e^{-1}+\tfrac{1}{4}[(2\mp1)m_{\rm hh}^{-1}+(2\pm1)m_{\rm lh}^{-1}]\ , \tag{10}$$

where the upper sign denotes the heavy-hole exciton, the lower sign the light-hole exciton; $m_{\rm hh}$ ($m_{\rm lh}$) is the effective mass of the heavy (light) hole in the growth direction; μ_0 is the reduced exciton mass inside the quantum well. In Eqs. (9), all the lengths have been scaled in terms of the effective Bohr radius $a_B=\varepsilon_1\hbar^2/\mu_0e^2$ and all energies in the effective Rydberg $R=e^2/2\varepsilon_1a_B$; $\gamma=\hbar eB/2\mu_0cR$ is energy of the first Landau level, L_z is the z component of the angular momentum (in units of $\hbar$); and H_C is the term describing the anisotropic Coulomb attraction between the electron and the hole in a dielectric quantum-well structure. $V_{\rm QW}^c(z_c)$ $(c=e,h)$ is the confining potential profile for the electron (hole), and

$$V_{\rm SE}^c(z)=\int_0^\infty\frac{d\kappa}{\sinh(\kappa L+\eta)}\begin{cases}-\dfrac{\sinh\kappa L}{\bar{\varepsilon}}e^{-2\kappa(|z_c|-L/2)}, & |z_c|>\dfrac{L}{2}\quad(c=e,h),\\ \cosh2\kappa z_c+e^{-\kappa L-\eta}, & |z_c|\le\dfrac{L}{2}\quad(c=e,h),\end{cases} \tag{11}$$

is the self-polarization energy from the interaction between the electron (hole) and its image charge distribution.

Next we write the wave function $\Psi(z_e,z_h;\rho,\varphi)$ in the following form[24]:

$$\Psi(z_e,z_h;\rho,\varphi)=F_e(z_e)F_h(z_h)\phi(\rho,\varphi;z_e-z_h)\ . \tag{12}$$

$F_e(z_e)$ and $F_h(z_h)$ are subband wave functions for the electron and the hole, respectively, that satisfy the following two equations:

$$H_eF_e(z_e)=E_eF_e(z_e)\ , \tag{13.1}$$

$$H_hF_h(z_h)=E_hF_h(z_h)\ , \tag{13.2}$$

where E_e and E_h are the subband energies of the electron and the hole, respectively. It has been shown[22] that the effect of the self-polarization energy can be satisfactorily accounted for by a shift in the subband energy, without significant modification of the subband wave functions. Since such shifts are canceled out in the results for the exciton binding energies, $V_{SE}(z)$ will be replaced by the calculated shifts in the subband energies in the Hamiltonian in the rest of this paper. $\phi(\rho,\varphi;z)$, as a function describing the binding between the electron and the hole, is expressed as an expansion in Gaussian-type orbitals,[25,26]

$$\phi(\rho,\varphi;z)=\frac{1}{\sqrt{2\pi}}e^{-\beta\rho^2}\sum_{i=1}c_ie^{-\alpha_i(\rho^2+z^2)}\ , \tag{14}$$

where β is a variational parameter and α_i are the Gaussian-type orbital expansion coefficients adopted from the variational results of Huzinaga.[27] The total energy E for the exciton is obtained from the Schrödinger equation $H\Psi=E\Psi$ and is subsequently minimized with respect to the variational parameter β. The remaining expansion coefficients c_i are also determined from the minimization of the total energy. The binding energy of a exciton state is defined as

$$E_B=E_e+E_h+\gamma-E\ . \tag{15}$$

III. RESULTS AND DISCUSSION

We have calculated the binding energies of the heavy-hole and light-hole excitons in the GaAs-AlAs and GaAs-ZnSe dielectric quantum wells, in the presence of an applied magnetic field. The electron and hole masses and other parameters used in our calculations are listed in Table I. For the HH exciton, $\mu_0=0.04m_0$, $a_B=167$ Å, and $R=3.4$ meV. For the lh exciton, $\mu_0=0.05m_0$, $a_B=135$ Å, and $R=4.2$ meV.

TABLE I. Material parameters used in the calculation.

	GaAs[a]	AlAs	ZnSe[b]
$m_e(m_0)$	0.067	0.15[a]	0.17
$m_{hh}(m_0)$	0.35	0.40[a]	0.76
$m_{lh}(m_0)$	0.08	0.18[a]	0.16
V_e (meV)		1060[b]	340
V_h (meV)		550[b]	960
dielectric constant ε	12.5	10.1[b]	7.6

[a]Reference 20.
[b]Reference 4.

Before proceeding further, we would like to comment on the origin of the discrepancy between the results for exciton binding energy obtained for a GaAs-$Al_{0.3}Ga_{0.7}As$ dielectric QW in Ref. 4 Kumagai and Takagahara (KT) and Ref. 6 Tran Thoai, Zimmermann, Grundmann, and Bimberg (TZGB). The result given by KT does not exhibit a maximum in the binding energy at small QW sizes, which contradicts an earlier theoretical prediction by Greene, Bajaj, and Phelps.[24] On the other hand, the exciton binding energy calculated by TZGB has the predicted behavior as QW size gets smaller; these authors tentatively attribute the difference to the inclusion of *convergent* self-polarization energy terms in their calculation. However, a careful comparison of the Coulomb potential terms given by KT with our analytical expressions in Eqs. (7) reveals two sign errors in their Eqs. (C20) and (C21). The exciton binding energy has the correct behavior when these errors are corrected, irrespective of the contribution from the self-polarization energy terms. We have therefore convincingly shown not only the merits of the first-principle analytical approach to obtain the expression for the Coulomb interaction, but also the insignificance of the contribution from the self-polarization energy to the exciton binding energy.

In order to see how the image charge contribution would enhance the exciton binding energies, we consider a GaAs-AlAs quantum well, where the dielectric constants of the well and the barriers are not very different. Calculations are first performed with an isotropic Coulomb attraction by using the dielectric constant of

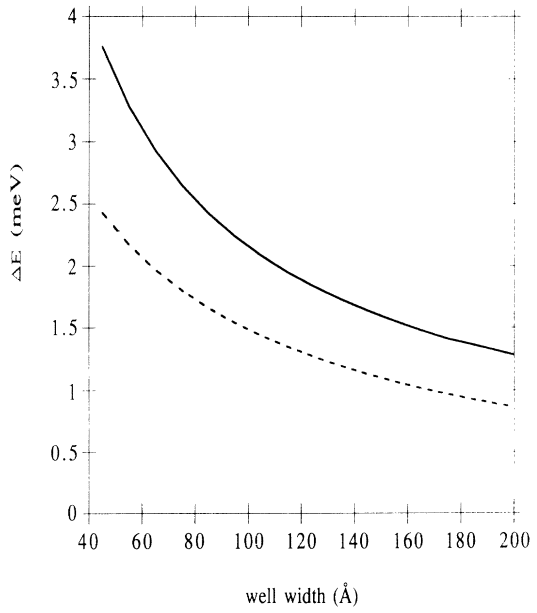

FIG. 3. Variation of the enhancement of the binding energy of a heavy-hole exciton (ΔE) due to image charge contribution as a function of well width in GaAs-AlAs (dashed line: — — —) and GaAs-ZnSe (solid line: ——) quantum wells for the magnetic field $\mathbf{B}=0$.

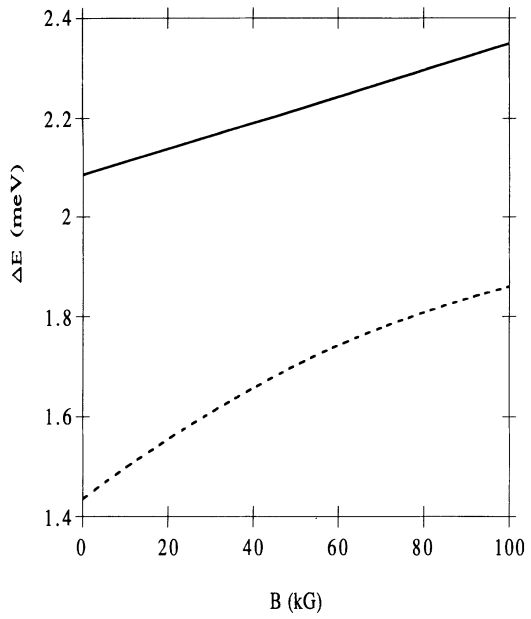

FIG. 4. Variation of the enhancement of the binding energy of a heavy-hole exciton (ΔE) due to image charge contribution as a function of magnetic field B in GaAs-AlAs (dashed line: — — —) and GaAs-ZnSe (solid line: ——) quantum-well structures. The width of the quantum well is chosen to be 100 Å.

GaAs for both the well and the barriers (the normal quantum-well case). Then the calculations are repeated with the actual anisotropic Coulomb attraction by using the different dielectric constants for the well and the barriers. In Fig. 3 we display the variation in the enhancement of the binding energy of a heavy-hole exciton (ΔE) due to image charge contribution in a GaAs-AlAs quantum well (dotted line) as a function of well width for $B=0$. The value of ΔE varies from about 1 meV for wide wells to about 2.5 meV for narrow wells. We see that contribution of the image charge distribution is significant even in a quantum-well structure where the dielectric constants of the well and barrier materials are not too different. Physically, the electron and the hole are compelled to the center of the quantum well by their image charges, so the average electron-hole distance is smaller in a quantum well when the dielectric constant of the barrier material is smaller than that of the well material. We also display the variation in ΔE as a function of well width in a GaAs-ZnSe quantum well for $B=0$. We find that in this structure the variation of ΔE is somewhat larger due to the larger difference in the values of the dielectric constants of the well and barrier materials.

Aside from the expected increase in binding energies due to smaller average electron-hole distance when the quantum-well size gets smaller, we find that at zero-field the exciton binding energies in such structures can exceed the conventional two-dimensional limit, i.e., four times the relative Rydberg. This unique property is attributed to the dielectric confinement effect in such structures. In Fig. 4 we show the variation of ΔE as a function of the applied magnetic field in a GaAs-AlAs quantum well (dotted line) and in a GaAs-ZnSe quantum well (solid line) for a well width of 100 Å. We find that the magnitude of the variation in ΔE is larger in a GaAs-AlAs quantum-well structure due to the smaller value of the exciton binding energy and hence the weaker Coulomb interaction between the electron and the hole. We have also calculated the variation of ΔE for the light-hole excitons as functions of well width and magnetic field in GaAs-AlAs and GaAs-ZnSe quantum-well structures and find a similar behavior.

IV. SUMMARY

In conclusion, we have developed a formalism for studying the exciton states in a dielectric quantum-well structure in the presence of a magnetic field applied along the growth direction, and have obtained expressions of the anisotropic electron-hole Coulomb interaction in the dielectric quantum-well structures, by solving the Poisson equation in the layered quantum-well geometries. We have shown the merit of the first-principle analytical approach to obtain the expression of the Coulomb interaction in a dielectric quantum-well structure, and discussed the relevance of the self-polarization energy in the calculation of exciton binding energies. We have calculated the binding energies of excitons in several dielectric quantum-well structures and have discussed their behavior as a function of well width and applied magnetic field.

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