# Binding energy of shallow donors in a quantum well in the presence of a tilted magnetic field

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We present the results of variational calculations of the binding energy of a neutral donor in a quantum well (QW) in the presence of a magnetic field tilted relative to the QW plane. Assuming that the donor is located in the center of the QW, we perform calculations for parameters of a rectangular CdTe quantum well with CdMgTe barriers. We present the dependence of the binding energy of a neutral donor on the tilt angle and on the magnitude of the applied magnetic field. As a key result, we show that measurement of the binding energy of a donor at two angles of the magnetic field with respect to the quantum well plane can be used to unambiguously determine the conduction band offset of the materials building up heterostructure.

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Much work has already been done on calculating the energies and wave functions of electronic states in semiconductor quantum wells (QW's) in the presence of an applied magnetic field. Most of these theoretical studies have focused on the binding energy of the neutral donor[1–4] ($D^0$), charged donor,[1,5,6] neutral exciton,[7–10] and charged exciton[9–12] (trion) states as a function of magnetic field. The vast majority of these calculations treat the most straightforward case, where the magnetic field is applied parallel to the direction of growth of the QW. Experimental and theoretical results show that in this geometry the binding energy of the above complexes increases with increasing magnetic field.[9,12] In spite of considerable progress in this area, little attention has been paid to the dependence of the binding energy on the tilt angle of the field relative to the QW plane.[13–15]

The objective of the present work is to determine the dependence of the binding energy of a neutral donor on the tilt angle $\theta$ between two limiting geometries, the first geometry (denoted below as case I) corresponding to the magnetic field $\vec{B}$ aligned along the growth axis of the QW (designated as the $z$ direction); and the second limit (denoted as case II) corresponding to external magnetic field applied in the plane of the QW. In our notation described below, in case I we define the tilt angle as $\theta=0°$ and in case II as $\theta=90°$ (see Fig. 1 for details).

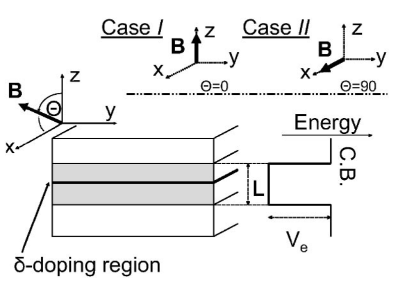


FIG. 1. Proposed experimental geometry. CdTe QW is grown in the $z$ direction: $L$ is the QW width and $V_e$ is the QW height. The donors are incorporated into the system by the $\delta$-doping technique only in the center of the well. The edge of the conduction band is sketched on the right-hand side. The magnetic field $\vec{B}$ lies in the $XZ$ plane. Case I corresponds to $\vec{B}=B\vec{e}_z$ and case II corresponds to $\vec{B}=B\vec{e}_x$.

It is well established that the binding energy of different electronic complexes stemming from the Coulomb interaction increases as the dimensionality of the quantum structure decreases—i.e., as we progress from quasi-two- to quasi-one- and eventually to quasi-zero-dimensional quantum structures.[16] An external magnetic field localizes the charged particles in the plane perpendicular to $\vec{B}$ in the form of its cyclotron motion, while the particle can move freely in the direction of the applied field, constituting in effect one-dimensional localization.[17] One should note that in this case the density of states also has the character of a one-dimensional system, manifesting itself as peaks at the Landau level positions. For an electron subjected simultaneously to the potential of the QW and of an external magnetic field, "total" localization of a particle is different in the two limiting cases defined above. In case I, the combined action of QW confinement and magnetic localization have different directions, which then manifests itself as quasi-zero-dimensional localization. In case II, the QW and the magnetic confinements have the same direction, so that the electron retains its quasi-one-dimensional character associated with the magnetic confinement. This implies that the binding energy of a donor should be larger in case I than in case II. When the tilt angle $\theta$ increases, we can then say that the dimensionality of an electron is between quasi-zero and quasi-one, and we expect the binding energy of $D^0$ to be a *monotonic* function of the tilt angle $\theta$.

The Hamiltonian of a shallow donor embedded in a symmetric square quantum well is modeled by the Hamiltonian

$$H=\frac{[\vec{p}-e\vec{A}(\vec{r})]^2}{2m_e^*}+V^{QW}(z)-\frac{e^2}{4\pi\epsilon\epsilon_0}\frac{1}{|\vec{r}-\vec{R}_0|}-\mu_B g_e^*\vec{B}\vec{s}. \quad (1)$$

The first part of the Hamiltonian is the kinetic energy of a delocalized conduction electron (where $e$ is the electron charge and $m_e^*$ is its effective mass) in the presence of a tilted magnetic field $\vec{B}=B(\sin(\theta),0,\cos(\theta))$ lying in the $XZ$ plane (see Fig. 1). We have chosen an asymmetric gauge for vector potential $\vec{A}(\vec{r})=B(0,x\cos(\theta)-z\sin(\theta),0)$. For $\theta=0°$ (case I), the magnetic field $\vec{B}$ is parallel to the $OZ$ axis, and for $\theta = 90°$ (case II) it lies in the $XY$ plane (i.e., in the plane of the QW) (see Fig. 1). The profile of the potential energy of the QW is described by the second term in Eq. (1): $V^{QW}(z)=0$ if $|z|>L/2$ and $V^{QW}(z)=-V_e$ if $|z|<L/2$, where $L$ is the width of the QW and $V_e$ is the height of its barrier. The energy scale is chosen by defining the conduction band edge of the barriers as zero. The third term in Eq. (1) is the Coulomb energy of a shallow donor located at point $\vec{R}_0$. We assumed that the donor center is located at the center of the QW, so we can set $\vec{R}_0=\vec{0}$ without losing physical generality. The last expression in Eq. (1) is the Zeeman Hamiltonian, in which $g_e^*$ is the effective $g$ factor of conduction electrons.

So far the problem of the Hamiltonian of a donor in a QW has not been solved analytically (even the case of a free electron in a QW in a tilted magnetic field remains analytically unsolved[18–20]), so that in our work we have used a variational approach. We propose the following form of the trial wave function of a two-component spinor,

$$\Psi_\pm = f_\pm(\vec{r}) \cdot \chi_\pm = \sum_{i=0}^{N_1}\sum_{j=0}^{N_2}\sum_{k=0}^{N_3} C_{ijk}^{\pm}\phi_i(\alpha x)\phi_j(\alpha y)\phi_k(\alpha z)\cdot\chi_\pm, \tag{2}$$

where $\phi_i$ are one-dimensional harmonic oscillator functions (Gaussian functions) and $\chi_\pm$ are spin states. Note that Gaussian trial wave functions have been successfully used in Refs. 1 and 10 for calculating donor and trion states, respectively. The nonlinear variational parameter $\alpha$ (the scaling parameter) and the linear variational parameters $C_{ijk}^{\pm}$ were determined using the Ritz variational method. In Eq. (2) the number of the basis functions has to be finite, and in this connection we have checked that $N_1=N_2=N_3=10$ are sufficient to ensure that the results do not depend on the cutoff of the number of basis functions.

The orbital part of the total wave function of a donor $\Psi_\pm$, Eq. (2), is denoted by $f_\pm(\vec{r})$, $\chi_\pm$ being the spin part. It is easy to show by direct substitution that the two spinors $\chi^\dagger = (\cos(\theta/2), \sin(\theta/2))$ and $\chi^\dagger = (-\sin(\theta/2), \cos(\theta/2))$ solve the Schrödinger equation that contains the Hamiltonian given by Eq. (1). Then the orbital part $f_\pm(\vec{r})$ of the spinor function $\Psi_\pm$ satisfies the following eigenequation:

$$\left\{\frac{[\vec{p}-e\vec{A}(\vec{r})]^2}{2m_e^*} + V^{QW}(z) - \frac{e^2}{4\pi\epsilon\epsilon_0}\frac{1}{|\vec{r}|} \mp \frac{1}{2}\mu_B g_e^* B\right\} f_\pm(\vec{r}) = E_\pm f_\pm(\vec{r}). \tag{3}$$

Additionally, as seen from the above equation, $f_\pm(\vec{r})$ has the same functional form for both spin configurations $\chi_\pm$.

In order to demonstrate the tilt angle dependence of the binding energy of $D^0$, we performed calculations for two barrier heights, $V_e=200$ meV and 20 meV. These two choices of barrier heights correspond to a 19% and 2% content of manganese in the barriers, respectively. Additionally, for each $V_e$ we chose $L=100$ and 300 Å and $B=0$, 1, 4, 9, and 16 T, corresponding to magnetic lengths $\lambda_c=\infty$, 256, 130, 85, and 65 Å. Finally, results for $L=50$ Å QW and different barrier heights are presented. In calculations we used: $m_e^*=0.1$ of free electron mass for both the QW and the barrier, and dielectric constant $\epsilon=10.4$, which give the characteristic Coulomb scales: $\text{Ry}^*=12.6$ meV and $a_B^*=55$ Å.

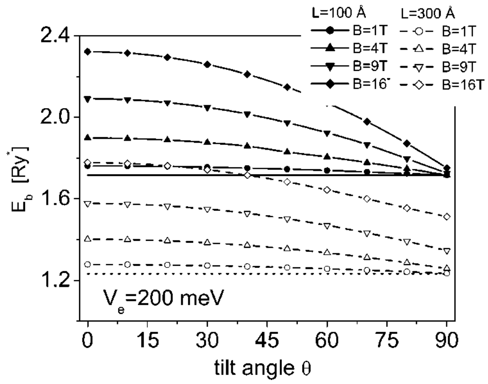


FIG. 2. Donor binding energy $E_b$ in a rectangular $CdTe/Cd_{0.81}Mg_{0.19}Te$ QW as a function of tilt angle $\theta$ of external magnetic field $B$ for different magnetic field values (different symbols), calculated for two QW widths $L$. Solid lines correspond to $L=100$ Å and dashed lines to $L=300$ Å. Lines without symbols correspond to $B=0$ T.

The donor binding energy $E_b$ is obtained as a difference between the ground-state energies of the free electron and of the donor ($E_\pm$) with the same electron spin configuration.[17] This definition implies that the Zeeman Hamiltonian does not contribute to the binding energy of $D^0$.

We will be interested mainly in the variation of $E_b$ with the inclination $\theta$ and the magnitude of the magnetic field, $E_b=E_b(\theta,B)$. It must be noted that $E_b$ also depends on other parameters—e.g., the barrier height—but these are kept constant in each variational process.

In Fig. 2 we present the binding energy of the donor ground state as a function of tilt angle $\theta$ for $V_e=200$ meV at different magnetic fields, as well as for two different QW widths $L=100$ and 300 Å. First we discuss the $L=100$ Å case, represented by solid lines in Fig. 2. At $B=0$ T, the binding energy of the neutral donor is about $1.7\ \text{Ry}^* = 21.4$ meV and is increased by 70% compared to the binding energy of a donor in three dimensions (in this case $L \sim 2a_B$). Next, for $B\neq 0$ T, the binding energy is a *monotonically* decreasing function of the tilt angle: at a given magnetic field $B=\text{const}$, the binding energy is highest for $\theta=0°$ and decreases for $\theta>0°$. Inspection of Fig. 2 shows that for $\theta=0°$ the difference $E_b(B=16T)-E_b(B=0T)$ is $0.6\ \text{Ry}^* = 8$ meV, while for $\theta=90°$ it is only $0.05\ \text{Ry}^*=0.6$ meV (see also Fig. 3). These totaly different values in the two limiting field orientations (cases I and II) are related to the fact that the QW width is smaller than (or comparable to) the characteristic magnetic length $\lambda_c$ at fields up to 16 T. If the magnetic field is applied along the $z$ direction ($\theta=0°$), the electron is localized in $x$ and $y$ directions by the external magnetic field, as discussed at the outset (the bigger the field, the larger the magnetic localization). When this effect is combined with QW confinement, the electron becomes localized in all three directions. As the magnetic field is changing from 0 T to 16 T, the initially quasi-two-dimensional electron is becoming increasingly quasi-zero-dimensional. We thus

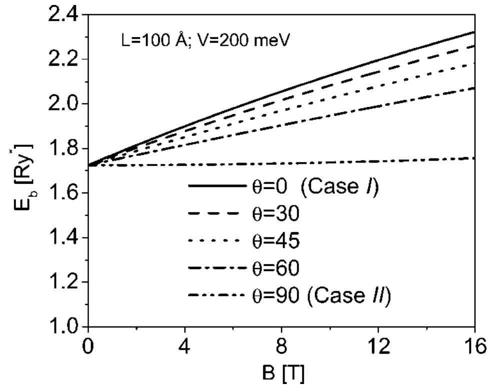


FIG. 3. Donor binding energy $E_b$ in a $CdTe/Cd_{0.81}Mg_{0.19}Te$ QW ($L=100$ Å) as a function of a magnetic field $B$ for $\theta=0°$ (case I) and 30°, 45°, 60°, and 90° (case II). In case II, the binding energy is practically independent of the magnetic field $B$ ($B<16$ T).

expect that the binding energy will increase substantially in this situation. On the other hand, if the magnetic field is aligned in the $x$ direction, magnetic localization involves the $y$ and $z$ directions with characteristic lengths $\lambda_c$. Since the QW also confines the electron motion in the $z$ direction and does not restrict its motion along $x$, the combined effects of magnetic and of QW localization now result in a one-dimensional motion. As seen in Fig. 2, even up to $B=16$ T the magnetic localization now has practically no effect, and binding energy practically does not depend on $B$.

In contrast with $L=100$ Å, for a wider QW ($L=300$ Å) the changes in binding energy produced by the magnetic field are quite visible at $\theta=90°$, as seen in Fig. 2. For such a wide QW, the change of $E_b$ as $B$ increases from 0 to 16 T is 0.3 Ry* =4 meV. Now $L=300$ Å and the binding energy is only 1.2 Ry* (without a magnetic field) so that the system is nearly three dimensional ($a_B \ll L$), in contrast to the two-dimensional character obtained for $L=100$ Å. Thus for all values of $\theta$ the magnetic field effectively localizes the particle in both dimensions perpendicular to the direction of the applied field. This explains why the curves for $E_b$ are much more flat for $L=300$ Å than for $L=100$ Å, particularly at higher values of $B$. We expect that, when we increase the QW width even more, $E_b$ should become even more flat, eventually approaching the three-dimensional limit, where it ceases to depend on the tilt angle even for large $B$. Our calculations clearly confirm this trend.

In Fig. 3 we show the dependence of the donor binding energy $E_b$ for a $CdTe/Cd_{0.81}Mg_{0.19}Te$ quantum well as a function of the magnetic field $B$, for five different values of the tilt angle $\theta$. As before we have chosen the magnetic field range to be $0 \leq B \leq 16$ T, which is the most widely accessible field range in photoluminescence (PL) spectroscopy. For case I, the increase in magnetic field has a clearly visible impact on $E_b(B)$. In contrast, $E_b$ is practically constant for case II. While the series of curves presented in Fig. 3 seems to be linear, our results for the binding energy have, in fact, a square-root dependence on the external magnetic field. Such a dependence is in accordance with the results obtained in Ref. 1. The apparent linearity of the curves is due to the fact that at the highest field we consider ($B=16$ T) the ratio

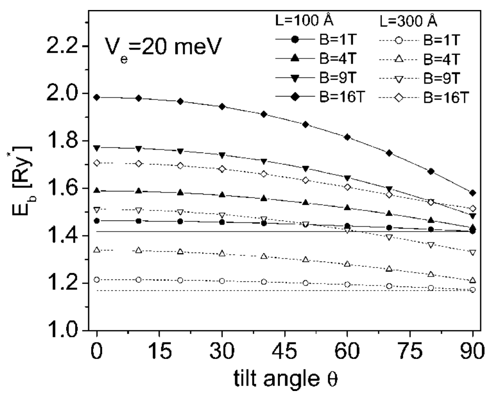


FIG. 4. Donor binding energy $E_b$ in a rectangular $CdTe/Cd_{0.98}Mg_{0.02}Te$ QW as a function of tilt angle $\theta$ of external magnetic field $B$ for different magnetic field values (different symbols), calculated for two QW widths $L$. Solid lines correspond to $L=100$ Å and dashed lines to $L=300$ Å. Lines without symbols correspond to $B=0$ T.

$\gamma \equiv \hbar\omega_c/2\text{Ry}^*$ is only 0.74. The $E_b(B) \propto \sqrt{B}$ scaling behavior becomes apparent for a much wider range of magnetic fields: $0 \leq \gamma \leq 5$, and note that $\gamma=5$ corresponds to $B=108$ T.

In Fig. 4 we present results for $V_e=20$ meV. Comparing Figs. 2 and 4, we see that the binding energy of the donor is larger for $V_e=200$ meV than for $V_e=20$ meV. This well-known fact originates from the larger quantum confinement of the deeper QW. The characteristics of the results in Fig. 4 are similar to those in Fig. 2, including the *monotonic* behavior of $E_b$. Comparing the curves in Fig. 2 with corresponding curves in Fig. 4, we see that the latter clearly are more flat. This again confirms that in the three-dimensional case; i.e., as $V_e \to 0$, we should have no $\theta$ dependence (straight horizontal lines).

In Fig. 5 we show the difference $E_{diff}$ between the binding energy of a donor at $\theta=0°$ and its binding energy at $\theta=90°$ as a function of the height of the barrier $V_e$—i.e., $E_{diff} = E(\theta=0°) - E(\theta=90°)$. At $B=7$ T and $V_e>50$ meV, the difference $E_{diff}$ is practically constant and relatively small (only 3.7 meV), but at $B=16$ T it does not saturate until $V_e \approx 75$ meV and its value is twice as high—i.e., 7.5 meV. This

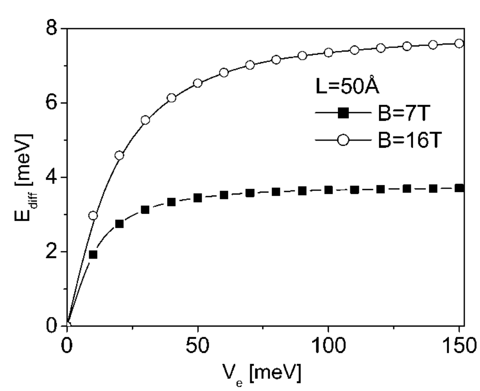


FIG. 5. Difference $E_{diff}$ of the binding energy of a donor for $\theta=0$ and $\theta=90°$ in a QW with $L=50$ Å as a function of barrier height $V_e$. Solid symbols correspond to $B=7$ T and open symbols to $B=16$ T.

feature can be utilized as a tool for determining the conduction band offset, at least in QW's with moderate barrier heights.[21] Note that the bigger the magnetic field, the larger the offset which can be measured using this method.

In Ref. 15, Fig. 6, the binding energy of the donor as a function of tilt angle is a nonmonotonic function showing a maximum at $\theta=45°$, in contrast to the monotonic behavior reported here. In our opinion this is related to the approach employed by the authors of Ref. 15, in which a real QW is transformed into two QW's oriented at right angles to one another. In Ref. 13 the same group, using the same approximation, calculated the exciton binding energy as a function of tilt angle (see Fig. 7 in Ref. 13). Unfortunately, the approach used in the latter reference does not provide the results for the range of $\theta$ between 0° and 15° and between 75° and 90°, which appears to be an artifact of the technique used in Refs. 13 and 15.

We have shown the results of variational calculations of the binding energy of a neutral donor in a rectangular QW as a function of the angle of an external magnetic field tilted with respect to the growth direction of the QW. For a given magnetic field, the largest binding energy is found to correspond to the case when the magnetic field is perpendicular to the plane of the QW. We find that the binding energy of $D^0$ is a *monotonic* function of the tilt angle $\theta$, decreasing with increasing tilt angle, in contrast with earlier calculations reported in Refs. 13 and 15. Our results reduce to the three-dimensional limit when either the QW width increases or the barrier height decreases, providing a "reality check" of the method used. We have shown that for the $CdTe/Cd_{1-x}Mg_xTe$ quantum well $(x<0.1)$, the conduction band offset can be determined by measuring the binding energy of the neutral donor at two perpendicular directions of the applied magnetic field, $\theta=0$ and 90°. To our knowledge this technique of determining conduction band offsets has not been previously recognized.

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