# Effect of a magnetic field on the energy levels of donor impurities in the ZnO parabolic quantum well*

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**Abstract:** Energy levels of a donor impurity in the ZnO parabolic quantum well under the magnetic field are investigated using the variational method. The binding energy of the ground state, the energies of 2p± state and $1s \rightarrow 2p_{\pm}$ transition energies of a hydrogenic donor in the ZnO parabolic quantum well are numerically calculated as a function of the strength of magnetic field for different parabolic potential fields. The results show that the external magnetic field has an obvious influence on the binding energies and the $1s \rightarrow 2p_{\pm}$ transition energies of a hydrogenic donor. The 1s to $2p_{\pm}$ transition energy increases linearly with the strength of magnetic field, but the 1s to $2p_{-}$ transition energy decreases when the strength of magnetic field increases for the small field strength. Compared to the GaAs parabolic well, the donors are more tightly bound to the ZnO parabolic well and the influence of external magnetic field on the binding energy of a donor is much stronger in the ZnO parabolic well.

**Key words:** parabolic quantum well; donor; magnetic field; $1s \rightarrow 2p_{\pm}$ transition energy

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## 1. Introduction

ZnO is an important II–VI semiconductor material with a wide direct band gap, which has a large exciton binding energy at room temperature, even larger than the ionization energy at the same temperature. Nowadays ZnO is widely used for production of blue-ultraviolet light-emitting devices and detectors[1, 2]. In Refs. [3, 4], ZnO quantum well structures have been fabricated to realize high efficiency luminescence in light-emitting devices. Compared to square quantum wells, the optical transition between the size-quantized electron subbands are easier to implement and the optical nonlinearities are stronger in the parabolic quantum wells (PQWs). Therefore the parabolic quantum wells have attracted substantial interest in the research community[5–7].

Leavitt[8] has calculated the binding energy of a hydrogenic impurity in GaAs/$Al_xGa_{1-x}$As PQWs using variational methods. Niculescu[9] has calculated the energies of ground and first excited states of a donor in a finite-PQW without a magnetic field. The results show that the effect of the finite well is to lower the binding energies and the infinite-PQW approximation is valid for the excited states. The effect of a magnetic field on the donor states in a PQW has been examined by Zhang and Rustigi[10], and this is the first calculation on the hydrogenic impurity in a parabolic well with a magnetic field. However, they only calculate the energy levels of a hygrogenic impurity in a PQW. Blinowski and Szwacka[11] have studied $D^0$ and $D^-$ centers in bulk crystals and in parabolic quantum wells with magnetic fields; Li[12] has investigated the effect of a spatially dependent effective mass (SDEM) on the binding energies of 1s- and 2p-like state for the hydrogenic impurity in a finite PQW with a magnetic field. They have obtained the binding energy as a function of the well width and a magnetic field. Their results indicated that the binding energy is greater than that without the effect of a SDEM. Sa and Guan[13] investigated the energy levels of a hydrogenic impurity in the GaN/$Al_xGa_{1-x}$N PQW with the magnetic field, but they only calculate the energy and binding energy of the ground state. So far little research has been conducted to investigate the 1s to $2p_{+}$ transition energies for the donor impurity in the PQW with a magnetic field.

The purpose of this paper is to apply the variational method to investigate the energy levels and optical transition of the donor impurity in a ZnO PQW with a magnetic field. The binding energy of the ground state, $2p_{\pm}$ state energy and the $1s \rightarrow 2p_{\pm}$ transition energy of a donor as a function of the magnetic field have been obtained by numeric calculation. The results show that an external magnetic field has a great effect on the binding energies and $1s \rightarrow 2p_{\pm}$ transition energies of a hydrogenic donor.

## 2. Theory and calculation

We consider a parabolic quantum well with a hydrogenic impurity located at the bottom of it. A uniform magnetic field $B$ is considered perpendicular to the quantum well layer. In the effective mass approximation, the Hamiltonian of this system can be written as

$$H = \frac{1}{2m^*}\left[-i\hbar\nabla - \frac{e\boldsymbol{A}}{c}\right]^2 - \frac{e^2}{\varepsilon_0 r} + \frac{1}{2}m\omega^2 z^2, \quad (1)$$

where $\varepsilon_0$ is the static dielectric constant to the medium, $m^*$ is the effective mass of the electron, $\omega$ is the harmonic oscillator

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Table 1. Ground state energy in an effective Rydberg constant of hydrogenic impurity in the GaAs/$Al_xGa_{1-x}$As PQW with a magnetic field. The values without parentheses are the results of the present work and the values in parentheses represent the results of Zhang and Rustgi[10]. $\alpha$ is the parabolic parameter.

| $\alpha$ | 0.2 | 0.2 | 0.2 | 1 | 1 | 1 | 2 | 2 | 2 |
|---|---|---|---|---|---|---|---|---|---|
| $\gamma$ | 0 | 1 | 10 | 0 | 1 | 10 | 0 | 1 | 10 |
| $1s_0$ | (−0.8759) | (−0.5614) | (6.5521) | (0.3058) | (0.5565) | (7.3286) | (2.0763) | (2.2955) | (8.7963) |
| $1s_0$ | −0.8781 | −0.5614 | 6.5867 | 0.3094 | 0.5588 | 7.3414 | 2.0797 | 2.2977 | 8.8116 |

frequency, $c$ is velocity of light, and $r = \sqrt{\rho^2 + z^2}$ gives the distance of the electron from the donor. $\boldsymbol{A}$ is the potential vector of the magnetic field, which can be written as $\boldsymbol{A} = \frac{1}{2}\boldsymbol{B} \times \boldsymbol{r}$.

If the effective Rydberg constant $R_y = m^* e^4 / 2\varepsilon_0^2 \hbar^2$ is the energy unit and the effective Bohr radius $a_B = \varepsilon_0 \hbar^2 / m^* e^2$ is the length unit, the Hamiltonian can be expressed as

$$H^* = -\nabla^2 - \frac{2}{r} + \gamma L_z + \frac{\gamma^2}{4}\rho^2 + 4\alpha^2 z^2, \tag{2}$$

where $L_z$ is the $z$ component of the angular momentum operator of an electron (in unit of $\hbar$). The $\gamma$ and $\alpha$ are dimensionless measures of the magnetic field and the parabolic potential, which are defined as $\gamma = \frac{\hbar}{2R_y}\frac{eB}{m^* c}$ and $\alpha = \frac{\hbar\omega}{4R_y}$.

We apply the variational approach to solve the nonlinear Schrödinger equation (2). The trial wavefunction for the ground state is given by

$$\psi = \exp\left(-\xi\sqrt{\rho^2 + z^2} - \eta\rho^2 - \zeta z^2\right), \tag{3}$$

and the trial wavefunction for the first excited state is given by

$$\psi = \rho \exp(im\phi) \exp(-\xi\sqrt{\rho^2 + z^2} - \eta\rho^2 - \zeta z^2), \tag{4}$$

where $\xi$, $\eta$ and $\zeta$ are the variational parameters and $m$ is magnetic quantum number.

The energies of the ground state and the first excited state are determined by minimizing the expectation value of the Hamiltonian:

$$E = \frac{\langle\psi|\, H^* \,|\psi\rangle}{\langle\psi \mid \psi\rangle}. \tag{5}$$

The binding energy of the ground state is defined as

$$E_b = E_0 + \gamma - E_1, \tag{6}$$

where $E_0$ is the energy of a free electron in a PQW without a magnetic field and $\gamma$ is the energy of the first Landau level. Greene and Bajaj[14] have used this method to calculate the ground state binding energy of a donor in a square quantum well. The ground state energy $E_1$ can be expressed as

$$E_1 = I / I_0, \tag{7}$$

where

$$I_0 = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\infty} \rho \mathrm{d}\rho \times \int_{-\infty}^{\infty} \mathrm{d}z \exp\left(-2\xi\sqrt{\rho^2 + z^2} - 2\eta\rho^2 - 2\zeta z^2\right), \tag{8}$$

and

$$I = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\infty} \rho \mathrm{d}\rho \times \int_{-\infty}^{\infty} \mathrm{d}z\, F_1 \exp\left(-2\xi\sqrt{\rho^2 + z^2} - 2\eta\rho^2 - 2\zeta z^2\right), \tag{9}$$

with

$$F_1 = \frac{2\xi - 2}{\sqrt{\rho^2 + z^2}} - \xi^2 + \left(0.25\gamma^2 - 4\eta^2\right)\rho^2 + 4\eta + (4\alpha^2 - 4\xi^2)z^2 + 2\zeta - \frac{4\xi\eta\rho^2}{\sqrt{\rho^2 + z^2}} - \frac{4\xi\zeta z^2}{\sqrt{\rho^2 + z^2}}. \tag{10}$$

The transition energy from the 1s state to $2p_\pm$ state is defined as

$$\Delta E = E_2 - E_1, \tag{11}$$

where $E_2$ is the first excited energy.

## 3. Numerical results and discussion

We first calculated the ground state energy of a hydrogenic impurity in the GaAs/$Al_xGa_{1-x}$As PQW with a magnetic field using our method and compare our results to those from Ref. [10]. The results are shown in Table 1. The comparison shows that our results are consistent with those in Ref. [10] and the present calculation is quite accurate.

Then we have calculated the binding energies of the ground state, the first excited state energies and the $1s \rightarrow 2p_\pm$ transition energies of a hydrogenic impurity in the ZnO PQW with a magnetic field and the results have been shown in Figs. 1–3. The effective mass of 0.24 and the dielectric constant of 8.656 have been used for the ZnO PQW in our calculations and we assume they are the same throughout the whole quantum well. For the parameter of ZnO PQW, the length and energy units become $a_B = 19.08$ Å and $R_y = 43.7$ meV.

In Fig. 1 we have showed the ground-state binding energies of the hydrogenic impurity in the ZnO PQW as a function of magnetic field for different $\alpha$. For a given parabolic potential $\alpha$, the binding energies are found to increase with an increase of magnetic field $\gamma$. This result indicates that the magnetic field applied along the growth axis of the quantum well structure leads to the additional quantum confinement and effectively increases the donor binding energies. For given values of $B$, the binding energy for $\alpha = 2$ is larger than those for $\alpha = 1$. This is due to the fact that the increase in the value of $\alpha$ results in the reduction in the size of quantum well, which causes wave

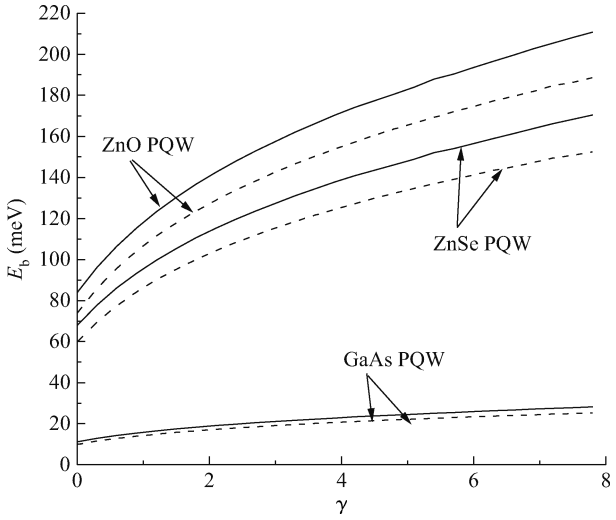


Fig. 1. Binding energy of the ground state of the hydrogenic impurity in the PQW as a function of $\gamma$. The solid curves correspond to $\alpha = 2$, and the dashed curves correspond to $\alpha = 1$.

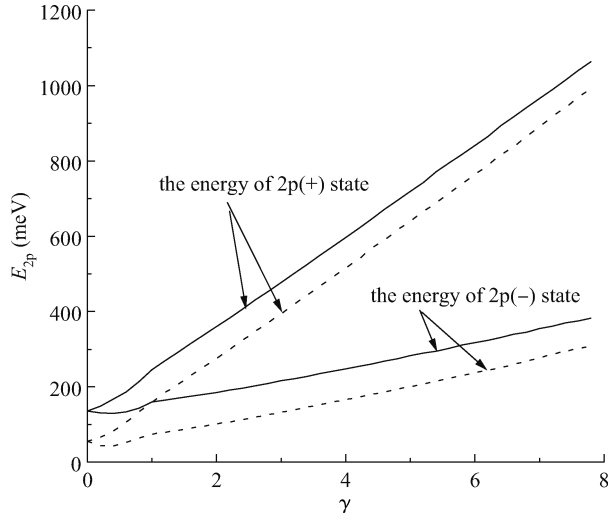


Fig. 2. The $2p_{\pm}$ state energy of a hydrogenic impurity in the ZnO PQW as a function of $\gamma$. The dashed curves: $\alpha = 1$, and the solid curves: $\alpha = 2$.

functions to become more compressed and leads to more binding. We also plotted the binding energy of the hydrogenic impurity in the ZnSe PQW and the GaAs PQW in Fig. 1. ZnSe is another II–VI semiconductor material with a wide direct band gap[15, 16], but the binding energy of a donor in the ZnSe PQW is lower than that in the ZnO PQW, which indicates that the hydrogenic impurities are more tightly bound to the ZnO PQW compared with the ZnSe PQW. From Fig. 1, it can be seen that the binding energies of the hydrogenic impurity in the GaAs PQW are totally insensitive to the magnetic field comparison with the ZnO PQW and ZnSe PQW. The binding energy of hydrogenic impurity in GaAs PQW is far less than those in the ZnO PQW and ZnSe PQW, due to the small effective mass and the large static dielectric constant of GaAs.

Figure 2 shows the energy levels of the first excited state of a hydrogenic impurity in the ZnO PQW as functions of the magnetic field strength $\gamma$ for different $\alpha$. It can be seen that the

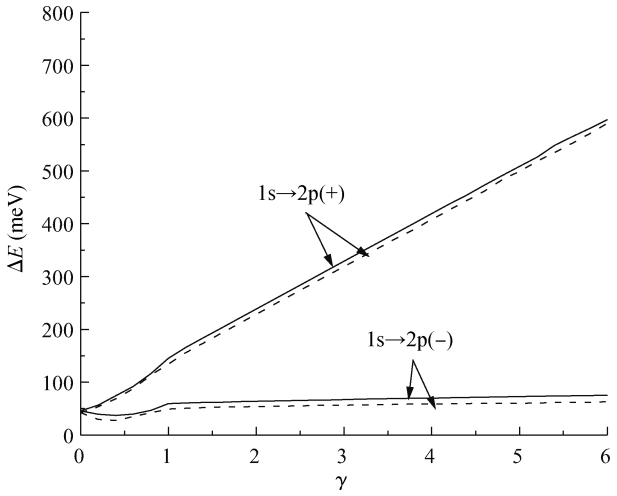


Fig. 3. The $1s \rightarrow 2p_{\pm}$ transition energies of a hydrogenic impurity in the ZnO PQW as a function of $\gamma$ . The dashed curves: $\alpha = 1$, and the solid curves: $\alpha = 2$.

energies of the $2p_+$ state increase nearly linearly with increasing $\gamma$. However, the energies of the $2p_-$ state first decrease and achieve their minima around $\gamma = 0.5$, then increase linearly with increasing $\gamma$. The result is consistent with those obtained by Zhang[10] and indicates that the $2p_-$ state is an unbound state when $\gamma < 0.5$. The complex interaction of the magnetic confinement and the spatial confinement of electrons in ZnO PQWs leads to a rich structure in energy spectrum of the hydrogenic impurity and make the behavior of the $2p_-$ state at small $\gamma$ values quite complicated.

In Fig. 3 we show the influence of the magnetic field on the $1s \rightarrow 2p_{\pm}$ transition energies of the hydrogenic impurity in the ZnO PQW for different parabolic parameters $\alpha$. The $1s \rightarrow 2p_-$ transition energies have their minima around $\gamma = 0.5$, which are consistent with the previous work obtained by qualitative analysis[11]. We also found that $1s \rightarrow 2p_-$ transition energies are insensitive to the magnetic field when the $\gamma > 0.5$ but the $1s \rightarrow 2p_+$ transition energies are very sensitive to the magnetic field. What is more interesting is that the $2p_+$ state energy level can be obtained from the $2p_-$ state energy level by adding $2\gamma$ for a given value of $\alpha$ and $\gamma$. The obvious influence of the parabolic parameter $\alpha$ on the transition energy cannot be found in Fig. 3 because the main contribution to the transition energies of the hydrogenic impurity comes from the magnetic confinement of electrons.

## 4. Conclusions

In the presence of the magnetic field, the binding energies of the ground state and $1s \rightarrow 2p_{\pm}$ transition energies of a hydrogenic impurity in the ZnO PQW have been calculated using the variational approach. We have investigated the spatial confinement, the magnetic confinement of the electron and the coulomb interaction between electron and donor. The magnetic field applied along the growth axis of the quantum well structure leads to additional quantum confinement, which increases both the donor binding energy and the transition energy between the 1s and $2p_+$ donor states. The $1s \rightarrow 2p_-$ transition energies show extraordinary behavior at small $\gamma$ values, which

decreases with increasing $\gamma$ when $\gamma < 0.5$. We also found that the binding energy of the hydrogenic impurity in the ZnO PQW is larger than those in the ZnSe and the GaAs PQW. The calculation method of this work provides a numerical solution for the ZnO parabolic quantum well system in the presence of a magnetic field.

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