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Hydrogenic impurities in parabolic quantum-well wires in a magnetic field

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The properties of a hydrogenic impurity in a parabolic GaAs quantum-well wire in the presence of the magnetic field are investigated using the finite-difference method within the quasi-one-dimensional effective potential model. The magnetic effects on the energies and binding energies of the ground and lowest excited states of a hydrogenic impurity in a parabolic GaAs quantum-well wire are studied for various parabolic potentials. The calculated results indicate that the interplay of the spatial confinement and the magnetic confinement of electrons in the quantum-well wires leads to complicated binding energies of the hydrogenic impurity, and high magnetic fields significantly increase the binding energies of the hydrogenic impurity in the case of weak spatial confinement. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2206415]

I. INTRODUCTION

Recent advances in semiconductor technology have made possible the fabrication of low-dimensional semiconductor heterostructures such as two-dimensional semiconductor quantum wells (QWs), one-dimensional semiconductor quantum-well wires (QWWs), and zero-dimensional semiconductor quantum dots (QDs). The investigation of these structures has attracted much attention because of their potential applications in high performance devices since they are predicted to offer superior optical and electrical characteristics.[1,2]

During the past few decades, the properties of low-dimensional systems composed of semiconductor materials have been extensively investigated.[3–19] Among the various systems currently under investigation, quasi-one-dimensional (1D) QWWs have received considerable attention. The theoretical and experimental studies of the electronic properties of shallow donor impurities in 1D QWWs are essential for understanding the behavior of these systems. A number of studies concerning hydrogenic impurities in cylindrical and rectangular QWWs in the absence of a magnetic field have been carried out.[3–5] The large binding energies of a hydrogenic impurity result from enhanced Coulomb coupling between electrons and donors due to the localization of electrons in the nanostructures. The achievement of large binding energies of hydrogenic impurities is considered as an important goal in the field of semiconductor nanostructures. As in all other nanostructures, the spatial confinement of the wave function, which depends on both the shape of the potential and the position of the impurity in the structure, plays an important role in these QWWs. An applied uniform magnetic field is one of the main probes used for studying the physical properties of nanostructures. The application of a magnetic field modifies the symmetry of the electron motion and the nature of the electron wave function. The quantizations caused by the magnetic field and the spatial confinement of electrons overlap in low-dimensional semiconductor heterostructures. These effects lead to more complicated energy levels and binding energies of the hydrogenic impurity and produce several interesting physical phenomena.[6–8] The problems of a hydrogenic impurity or an exciton in QWWs with various potential barriers in the presence of a magnetic field have been treated by many authors.[9–13] Zounoubi *et al.* has estimated the binding energy and the polarizability of a shallow donor confined to a GaAs QWW with a rectangular cross section in the presence of an axial magnetic field.[9] Kyrychenko and Kossut have studied the dependence of exciton binding energy on a magnetic field in T-shaped QWW structures.[10] Branis *et al.* performed a calculation of the ground-state binding energy of a hydrogenic impurity in a cylindrical QWW with infinite or finite confining potentials in a magnetic field parallel to the wire.[11] Aktas and coworkers investigated the effects of both electric and magnetic fields on the binding energy of a shallow donor impurity in a coaxial GaAs–(Ga, Al)As QWW. They calculated the binding energy as a function of impurity position and barrier thickness for various values of the applied magnetic and electric fields.[12,13] Recently, Bednarek *et al.* have proposed an analytical 1D formula for the effective interaction potential between confined charge carriers. They applied both the 1D model with an effective potential and the full three-dimensional (3D) approach to an exciton confined in a QWW and discussed the applicability of the effective 1D interaction potential to real 3D nanostructures by comparing the results of the 1D and 3D approaches.[14] There are relatively few quantitative studies on parabolic QWWs in a magnetic field.

In this paper, we report the calculation of the energies and binding energies of the ground and lowest excited states of a hydrogenic impurity in parabolic GaAs QWWs in a magnetic field parallel to the wire. We also calculate the distance between the electron and the donor. These calculations are done using the finite-difference method within the 1D effective potential model.[14] The calculated results indicate that the interplay of the spatial confinement and the magnetic confinement of the electron in the QWW leads to complicated binding energies of the hydrogenic impurity,

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and high magnetic fields significantly enhance the binding energies of the hydrogenic impurity in the case of weak spatial confinement. The paper is organized as follows: In Sec. II we present our theoretical model, our numerical results and discussion are presented in Sec. III, and finally in Sec. IV the conclusions obtained are summarized briefly.

II. THEORY AND CALCULATION

For simplicity, we assume that the hydrogenic impurity is located at the center of the wire along the z direction. In this problem the electron is free to move in the longitudinal direction (which is the direction of the z axis) and is confined by parabolic lateral confinement along the x and y axes. Within the effective-mass approximation, the system is described by the Hamiltonian

$$H=\frac{1}{2m_e^*}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right)^2+\frac{1}{2}m_e^*\omega^2\rho^2-\frac{e^2}{\varepsilon r}, \qquad (1)$$

where e and m_e^* are, respectively, the electronic charge and the effective mass, $\mathbf{p}$ is the momentum, ε is the dielectric constant of the material of the parabolic GaAs QWW, ω is the harmonic oscillator frequency, ρ is the distance from the axis of the wire, and $r=\sqrt{\rho^2+z^2}$ gives the distance of the electron from the donor. $\mathbf{A}$ is the potential vector of the magnetic field, which is written as $\mathbf{A}=\frac{1}{2}\mathbf{B}\times\mathbf{r}$, with $\mathbf{B}=B\hat{z}$. We have used the effective electron Bohr radius in GaAs, $a^*=\hbar^2\varepsilon/m_e^*e^2$, as the unit of length and the effective electron Rydberg $\mathrm{Ry}=e^2/2\varepsilon a^*$ as the unit of energy. In these units, the Hamiltonian (1) can be rewritten as

$$H=-\nabla^2+\gamma L_z+(\tfrac{1}{4}\gamma^2+\gamma_p^2)\rho^2-\frac{2}{r}. \qquad (2)$$

Here, L_z is the z component of the angular momentum operator of an electron (in unit of $\hbar$). The γ and γ_p are dimensionless measures of the magnetic field and the parabolic potential, respectively, which are defined as $\gamma=e\hbar B/2m_e^*c\mathrm{Ry}$ and $\gamma_p=\hbar\omega/2\mathrm{Ry}$.

A. The ground state

We assume that the electron is in the ground state of transverse motion. The electron wave function for this potential can be separated in cylindrical coordinates as[14]

$$\psi(r)=\psi_\perp(\rho,\varphi)\psi_\parallel(z), \qquad (3)$$

where

$$\psi_\perp(\rho,\varphi)=\frac{(\frac{1}{4}\gamma^2+\gamma_p^2)^{1/4}}{\sqrt{\pi}}\exp\left[-\tfrac{1}{2}\sqrt{\tfrac{1}{4}\gamma^2+\gamma_p^2}\rho^2\right], \qquad (4)$$

and $\psi_\parallel(z)$ is the electron's longitudinal wave function. We can obtain the effective interaction potential energy

$$V_{\mathrm{eff}}(z)=2\sqrt{\pi}(\tfrac{1}{4}\gamma^2+\gamma_p^2)^{1/4}\,\mathrm{erfc}\,x[(\tfrac{1}{4}\gamma^2+\gamma_p^2)^{1/4}|z|]. \qquad (5)$$

Here, $\mathrm{erfc}\,x(t)=\exp(t^2)\mathrm{erfc}(t)$ is the exponentially scaled complementary error function, which can be calculated using standard numerical procedures, and $\mathrm{erfc}(t)$ is the complementary error function. We define the operator $H_\parallel$ as the Hamiltonian for the longitudinal motion which satisfies the equation

$$H_\parallel\psi_\parallel(z)=\int\rho d\rho d\varphi\psi_\perp^*(\rho,\varphi)H\psi_\perp(\rho,\varphi)\psi_\parallel(z). \qquad (6)$$

Equation (6) yields

$$H_\parallel=2\sqrt{\tfrac{1}{4}\gamma^2+\gamma_p^2}-\frac{\partial^2}{\partial z^2}-V_{\mathrm{eff}}(z). \qquad (7)$$

The eigenvalue problem for Hamiltonian (7) depends on only one coordinate. Therefore, it can be treated with the finite-difference method on a one-dimensional mesh.

The ground-state binding energy E_b of the impurity is defined as the ground-state energy of the system without the impurity minus the ground-state energy with the impurity ($E_{\min}$):

$$E_b=E_0-E_{\min}. \qquad (8)$$

Here, E_0 is the ground-state energy of the system without the impurity, which can be shown to be

$$E_0=\sqrt{\gamma^2+4\gamma_p^2}. \qquad (9)$$

The ground-state energy $E_{\min}$ of the system described by Hamiltonian (7) can be evaluated using the finite-difference method with a one-dimensional mesh.

The average distance between the ground-state electron and the donor along the quantum wire can be obtained by

$$\langle|z|\rangle=\frac{\int\psi_\parallel^*(z)|z|\psi_\parallel(z)dz}{\int|\psi_\parallel(z)|^2dz}. \qquad (10)$$

B. The lowest excited state

If the electron is in the lowest excited state of transverse motion, the electron wave function of the lowest excited state can be approximated in cylindrical coordinates by the product

$$\psi^{sp}(r)=\psi_\perp^{sp}(\rho,\varphi)\psi_\parallel^{sp}(z), \qquad (11)$$

where

$$\psi_\perp^{sp}(\rho,\varphi)=\sqrt{\frac{\frac{1}{4}\gamma^2+\gamma_p^2}{\pi}}\rho\exp(-\tfrac{1}{2}\sqrt{\tfrac{1}{4}\gamma^2+\gamma_p^2}\rho^2)e^{i\varphi} \qquad (12)$$

and $\psi_\parallel^{sp}(z)$ is the electron's longitudinal wave function. We can obtain the effective interaction potential energy of the lowest excited state as

$$V_{\mathrm{eff}}^{sp}(z)=[\sqrt{\pi}(\tfrac{1}{4}\gamma^2+\gamma_p^2)^{1/4}-2\sqrt{\pi}(\tfrac{1}{4}\gamma^2+\gamma_p^2)^{3/4}]\times\mathrm{erfc}[(\tfrac{1}{4}\gamma^2+\gamma_p^2)^{1/4}|z|]+2\sqrt{\tfrac{1}{4}\gamma^2+\gamma_p^2}|z|. \qquad (13)$$

Similarly as in Sec. II A, the Hamiltonian for the longitudinal motion is

$$H_\parallel^{sp}=4\sqrt{\tfrac{1}{4}\gamma^2+\gamma_p^2}+\gamma-\frac{\partial^2}{\partial z^2}-V_{\mathrm{eff}}^{sp}(z). \qquad (14)$$

The binding energy E_b^{sp} of the lowest excited state of the impurity is defined as the energy of the lowest excited state

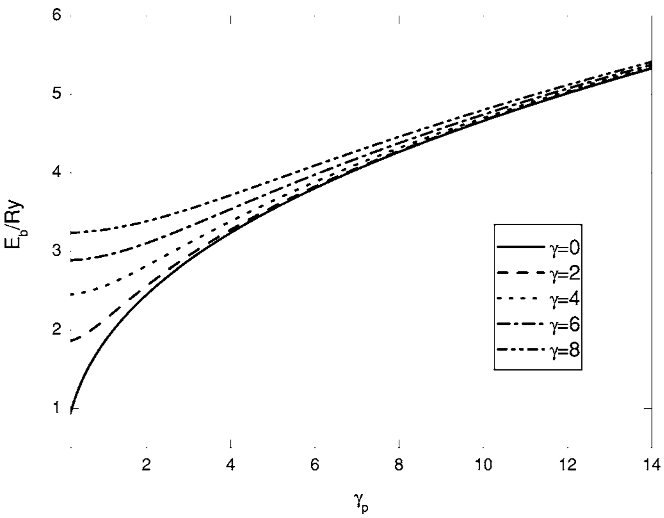

FIG. 1. Ground-state binding energy of a hydrogenic impurity in a parabolic GaAs QWW as a function of the parabolic potential γ_p for various values of the magnetic field.

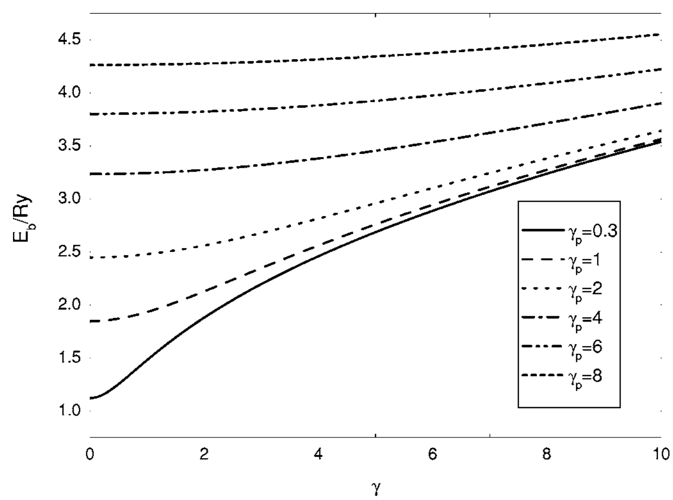

FIG. 2. Ground-state binding energy of a hydrogenic impurity in a parabolic GaAs QWW as a function of the magnetic field for various values of the parabolic potential.

of the system without the impurity minus the energy of the lowest excited state with the impurity ($E_{\min}^{sp}$):

$$E_b^{sp} = E_0^{sp} - E_{\min}^{sp}. \quad (15)$$

Here, E_0^{sp} is the energy of the lowest excited state of the system without the impurity, which can be shown to be

$$E_0^{sp} = \sqrt{\gamma^2 + 4\gamma_p^2} + \gamma. \quad (16)$$

The energy $E_{\min}^{sp}$ of the lowest excited state of the system described by Hamiltonian (14) can be evaluated using the finite-difference method with a one-dimensional mesh.

III. RESULTS AND DISCUSSION

We have calculated the energies and binding energies of the ground and lowest excited states of a hydrogenic impurity located at the center of a parabolic GaAs QWW in a magnetic field parallel to the wire. We also calculated the distance between the electron and the donor. The values of the parameters for GaAs QWWs used in our calculations are $\varepsilon=12.5$ and $m_e^*=0.067m_0$,[15] where m_0 is the free-electron mass. For these parameter values, $a^*=98.7$ Å and Ry $=5.83$ meV.

Figure 1 shows the ground-state binding energy of a hydrogenic impurity in a parabolic GaAs QWW as a function of the parabolic potential γ_p for various values of the magnetic field. The binding energy of the hydrogenic impurity increases with increasing the parabolic potential which confines the electron close to the donor. In the strong spatial confinement range ($\gamma_p>6$), the binding energy of the hydrogenic impurity is insensitive to magnetic fields and diverges as the parabolic potential approaches infinity, indicating that the main contribution to the binding energies of the hydrogenic impurity comes from the spatial confinement of electrons, which prevails over the magnetic confinement of electrons. In the intermediate range of the spatial confinement ($2<\gamma_p<6$), the effect of the magnetic confinement of electrons combines with the effect of the spatial confinement of electrons, and the effect of the magnetic confinement on the binding energy of the hydrogenic impurity becomes more apparent with the decrease of the parabolic potentials. In the weak spatial confinement range ($\gamma_p<2$), the binding energy of the hydrogenic impurity increases with the increasing magnetic field and converges asymptotically to the corresponding bulk value as the parabolic potential is further decreased. In the limit of weak confinement, the binding energy of the ground state for $\gamma=0$ approaches the bulk case result: the Rydberg constant Ry.

In Fig. 2, the ground-state binding energy of a hydrogenic impurity in a parabolic GaAs QWW is plotted as a function of the magnetic field for various parabolic potentials γ_p. Since the electron is strongly confined in a small volume by the strong parabolic potential, in the case of strong spatial confinement ($\gamma_p>6$), the binding energy of the hydrogenic impurity is totally insensitive to the magnetic field. As the spatial confinement decreases, the binding energy of the hydrogenic impurity increases slowly firstly and then increases linearly with the increasing magnetic field. This phenomenon stems from the complicated interplay of the magnetic confinement and the spatial confinement of electrons. The spatial confinement plays a more important role than the magnetic confinement for diluted magnetic fields, which leads to the complicated binding energies of the hydrogenic impurity. For weak spatial confinement, it is clear that high magnetic fields increase the binding energies of the hydrogenic impurity. Increasing magnetic field decreases the cyclotron radius of the electron and increases the binding energy.

In Figs. 3 and 4 the energies and binding energies of the ground state (solid curve) and the lowest excited state (dashed curve) of a hydrogenic impurity in a parabolic GaAs QWW are plotted as functions of the magnetic field for the parabolic potentials of $\gamma_p=0.3$, 1, 2, and 3, respectively. The energies of the ground state are lower than those of the lowest excited state for certain parabolic potentials, while the binding energies of the ground state are higher than those of the lowest excited state for certain parabolic potentials. The reason is that the average distance between the electron and the donor in the lowest excited state is greater than that in the

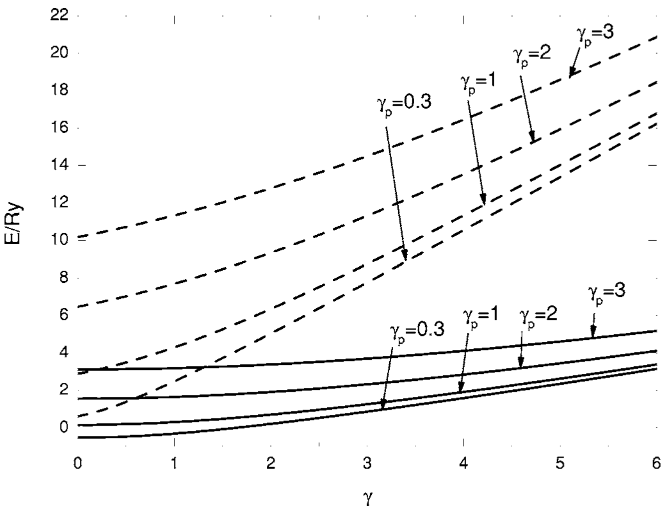

FIG. 3. The energies of the ground state (solid curve) and the lowest excited state (dashed curve) of a hydrogenic impurity in a parabolic GaAs QWW as functions of the magnetic field for parabolic potentials of γ_p=0.3, 1, 2, and 3.

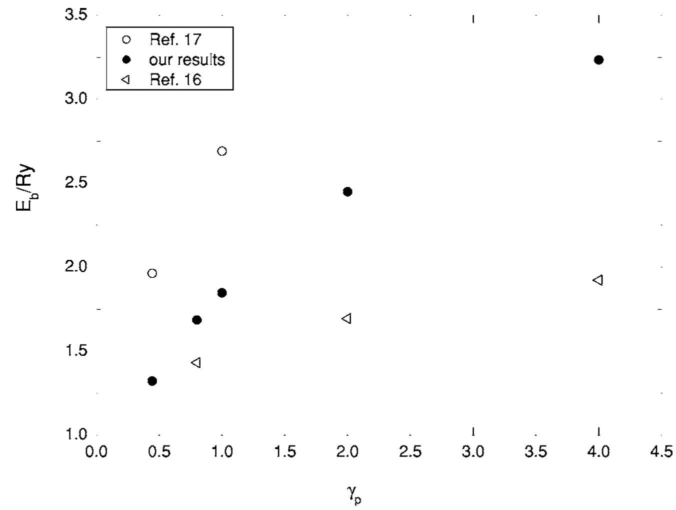

FIG. 5. Ground-state binding energy of a hydrogenic impurity in a parabolic GaAs QWW (●, our results), parabolic GaAs QW (◁, Ref. 16), and parabolic GaAs QD (○, Ref. 17) with various values of parabolic potential in a magnetic field of γ=0.

ground state. From Fig. 3, we can see that the energy of the hydrogenic impurity increases with the increasing magnetic field and the energy levels of the hydrogenic impurity in two states in different parabolic QWWs cross. The complex interplay of the magnetic confinement and the spatial confinement of electrons in QWWs leads to a rich structure of the hydrogenic impurity energy spectrum. The effect of the magnetic field on the binding energy of the lowest excited state is similar to that of the ground state.

In Fig. 5, we plot the ground-state binding energy of a hydrogenic impurity in parabolic GaAs QWWs, parabolic GaAs QWs,[16] and parabolic GaAs QDs (Ref. 17) for various parabolic potentials with γ=0. We can determine the applicability of 1D effective interaction potential. The ground-state binding energies in our results are larger than those in parabolic GaAs QWs and smaller than those in parabolic GaAs QDs. It is well known that the reduction of dimensionality increases the effective strength of the Coulomb interaction. The binding energy of a hydrogenic impurity is increased by the reduction of dimensionality.

Figure 6 shows the average distance between the ground-state electron and the donor along the quantum wire axis as a function of the parabolic potential γ_p for various values of the magnetic field. The electron becomes more localized with the increase of the parabolic potential. Figure 7 shows the distance as a function of the magnetic field for various values of the parabolic potential γ_p. The magnetic field shrinks the distance between the electron and the donor in parabolic GaAs QWWs, and the distance becomes more sensitive to the magnetic field with the decrease of the parabolic potential.

IV. CONCLUSIONS

In the presence of the magnetic field, the energies and binding energies of the ground and lowest excited states of a

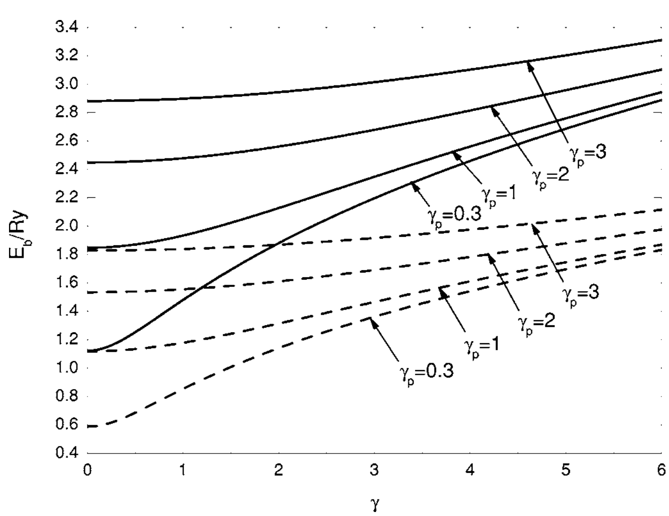

FIG. 4. The binding energies of the ground state (solid curve) and the lowest excited state (dashed curve) of a hydrogenic impurity in a parabolic GaAs QWW as a function of the magnetic field for parabolic potentials of γ_p =0.3, 1, 2, and 3.

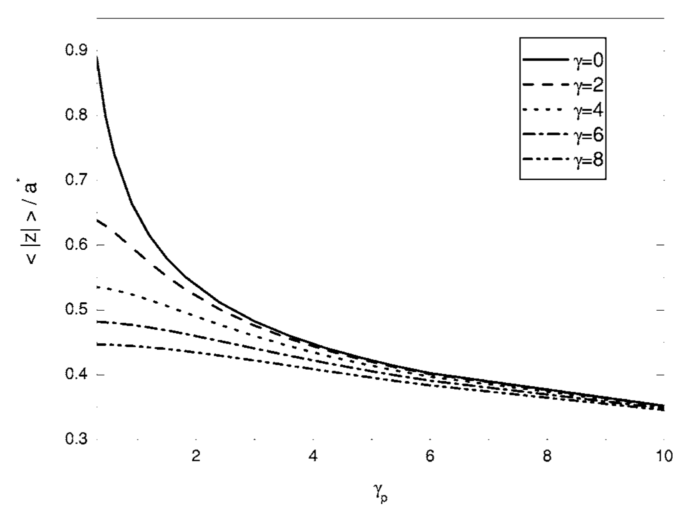

FIG. 6. The average distance between the ground-state electron and the donor along the quantum wire as a function of the parabolic potential γ_p for various values of the magnetic field.

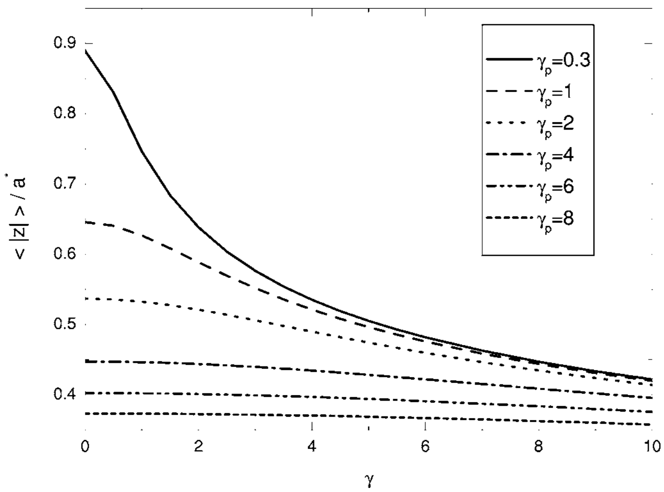

FIG. 7. The average distance between the ground-state electron and the donor along the quantum wire as a function of the magnetic field for various values of the parabolic potential γ_p.

hydrogenic impurity in a parabolic GaAs QWW have been calculated using the finite-difference method within the 1D effective potential model. We have considered the spatial confinement and the magnetic confinement of electrons and the Coulomb interaction between electrons and donors. The complex interplay of the spatial confinement and the magnetic confinement of electrons leads to the complicated magnetic field dependence of the binding energy of the hydrogenic impurity in parabolic GaAs QWWs. The calculated distance between the electron and the donor provides a clear picture of the behavior of a hydrogenic impurity in a parabolic potential QWW. The calculation method provides a numerical solution for the parabolic QWW system in the presence of a magnetic field. The theoretical model of the parabolic potential QWW and the calculation method can be extended to other low-dimensional quantum systems in the presence of a magnetic field.

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