

Donor-bound electrons in quantum rings under magnetic fields

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We theoretically study donor-bound electron states in two-dimensional quantum rings of finite width. A strong magnetic field is applied perpendicular to the plane of the quantum ring. The resulting electronic states are obtained within the effective-mass approximation. For on-center donors, the radial Hamiltonian for the envelope function is exactly diagonalized, and the corresponding energy levels for different angular momenta are studied as a function of the applied magnetic field. Confinement properties change rapidly with the external magnetic field. An abrupt change of the localization properties appears at a critical magnetic field, since the electron is mainly localized around the impurity. This transition gives rise to well-defined anticrossing of levels as a function of the magnetic field. Intraband transitions are found to carry relevant information of these confining properties of the rings.

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I. INTRODUCTION

Recent advances in nanofabrication of quantum devices enable the study of the electronic properties of quantum rings (QRs) in a very controllable way.¹⁻³ QRs are small semiconductor ring-shape structures in which electrons are confined in all spatial dimensions. As a consequence, discreteness of energy and charge arises, such as in atomic systems. In contrast to real atoms, different regimes can be studied by continuously changing the applied external potential, which can compete with the quantum confinement. As a consequence, QRs are very promising systems due to their physical properties as well as their potential application in electronic devices. Currently, researchers are investigating a variety of magnetic QRs, with or without impurities, due to their potential uses in high-density memory devices and spintronics (see Ref. 4 and references therein). In magnetic QRs, electronic quantum confinement is achieved solely by inhomogeneous magnetic fields, giving rise to a parabolic potential across the width of the ring. Parabolic confining potentials are amenable of analytical calculations since the center-of-mass motion of excitons can be separated from the relative electron-hole motion.^{5,6} In contrast, band-edge offsets give rise to the confining potential in QRs based on semiconductor heterostructures.⁷ In this case, calculation of the effects of the Coulomb interaction is more complex.

In this work, we consider on-center donors in a two-dimensional (2D) QR made of two different III-V semiconductors. The conduction-band-edge offset at the heterojunctions confines the electrons and gives rise to finite-size effects since the QR is assumed to be of finite width. Donor binding energies are also modified due to the presence of a QR as compared to bulk semiconductors. Therefore, binding energy carries information about the confinement properties of electrons in QRs. In addition, a strong magnetic field is applied perpendicular to the plane of the QR. The binding energy of a single electron bound to an on-center donor is obtained by exact diagonalization of the radial Hamiltonian. As a major result, we find a strong dependence of the confining properties of the QR on the magnetic field. In particular, an abrupt transition of the localization properties of the

electronic envelope function is observed at a critical magnetic field. Consequently, spectroscopy studies of donor-bound electrons provide a unique tool to characterize the confining properties of QRs.

II. THEORETICAL MODEL

We will focus on electron states close to the bottom of the conduction band and neglect nonparabolicity effects hereafter. Then, a one-band effective mass Hamiltonian suffices to obtain accurate results. For simplicity, we assume the same effective mass m^* at the Γ valley in both semiconductors, namely, inside and outside the QR.

For the moment, we will neglect the Coulomb potential due to the presence of an ionized donor. As mentioned above, a magnetic field of magnitude B is applied normally to the plane of the QR. Within these assumptions, and due to the axial symmetry of the system, the envelope function is factorized as⁷

$$\chi(\rho, \phi) = \frac{e^{i\ell\phi}}{\sqrt{2\pi}} R(\rho), \quad (1)$$

where ρ is the in-plane radial coordinate, ϕ is the polar angle, and $\ell=0, \pm 1, \pm 2, \dots$ is the quantum number determining the angular momentum $\ell\hbar$.

The radial function $R(\rho)$ in Eq. (1) satisfies the following effective-mass equation:

$$\left[-\frac{\hbar^2}{2m^*} \frac{1}{\rho} \frac{d}{d\rho} \left(\rho \frac{d}{d\rho} \right) + \frac{\hbar^2}{2m^*} \frac{\ell^2}{\rho^2} + \frac{m^*}{8} \omega_c^2 \rho^2 + V(\rho) \right] R(\rho) = \left(E - \frac{\ell}{2} \hbar \omega_c \right) R(\rho), \quad (2)$$

where the cyclotron frequency is $\omega_c = eB/m^*c$ and $V(\rho)$ has two contributions, $V(\rho) = V_R(\rho) + V_C(\rho)$. The conduction-band-edge profile contribution along the radial direction of the QR is given by

$$V_R(\rho) = \begin{cases} 0, & \rho_1 < \rho < \rho_2 \\ V_0, & \text{otherwise,} \end{cases} \quad (3)$$

with $V_0 > 0$. Here, ρ_1 and ρ_2 are the inner and outer radii of the QR, respectively. The contribution of a single ionized donor at the center of the QR (which does not break the axial symmetry) could be described in terms of a Coulomb term of the form

$$V_C(\rho) = -\frac{e^2}{\epsilon_r \rho}, \quad (4)$$

ϵ_r being the relative dielectric constant of the semiconductors. Solution of Eq. (2) without impurity ($V_C=0$) is given in Ref. 7 and, for brevity, is not quoted here.

Since no analytical solution of the resulting equation is found, we solved it numerically. To this end, we introduce a dimensionless coordinate $z = \rho/a^*$, where $a^* = \epsilon_r \hbar^2 / e^2 m^*$ is the effective Bohr radius. We set an integration interval $0 < z < z_A$ with the condition $z_A \gg \rho_2/a^*$. Then, we take an integration step $s = z_A/N$, where N is a positive integer, and define the grid points $z_k = sk$ with $k=0, \dots, N$. Using a standard finite-difference approach, the resulting discrete equation is found to be

$$-\left(1 + \frac{1}{2k}\right)R_{k+1} - \left(1 - \frac{1}{2k}\right)R_{k-1} + \left[\frac{\ell^2}{k^2} + \left(\frac{a^*}{l_m}\right)^4 s^4 k^2 - 2\frac{s}{k} + s^2 \frac{V_k}{R_y^*}\right]R_k = \left[s^2 \frac{E}{R_y^*} - 2 - s^2 \ell \left(\frac{a^*}{l_m}\right)^2\right]R_k, \quad (5)$$

where $k=1, \dots, N-1$. Here, $l_m = \sqrt{\hbar/m^* \omega_c}$ is the magnetic length, $R_y^* = \hbar^2/2m^* a^{*2}$ is the effective Rydberg, $R_n = R(z_n a^*)$, and $V_k = V(z_k a^*)$. Boundary conditions read $R(\rho) \sim \rho^\ell$ for $\rho \rightarrow 0$ and $R(\rho) = 0$ for $\rho \rightarrow \infty$. Notice that the resulting matrix is tridiagonal but nonsymmetric, although their eigenvalues are real.

In our next step, we calculate the optical absorption spectrum of the QR in the midinfrared due to bound-to-bound intraband transitions. Hereafter, we neglect bound-to-continuum absorption since it is usually 3 orders of magnitude smaller in zero-dimensional structures.⁸ We focus on transitions from the ground state of the QR, $|1,0\rangle$, to higher bound states, $|n,\ell\rangle$. Therefore, the absorption coefficient is calculated as

$$\alpha(\omega) \sim \sum_{n\ell} |\langle 1,0 | \mathbf{e} \cdot \boldsymbol{\rho} | n,\ell \rangle|^2 \delta(E_{n\ell} - E_{10} - \hbar\omega), \quad (6a)$$

where the unit vector \mathbf{e} indicates the direction of polarization of light. For in-plane polarization, the so-called normal incidence, the transition matrix element is

$$\langle 1,0 | \mathbf{e} \cdot \boldsymbol{\rho} | n,\ell \rangle = \frac{1}{2\pi} (e_x + i e_y) \delta_{|\ell|,1} \int_0^\infty d\rho \rho^2 R_{10}(\rho) R_{n\ell}(\rho), \quad (6b)$$

which yields the selection rule $\ell = \pm 1$.

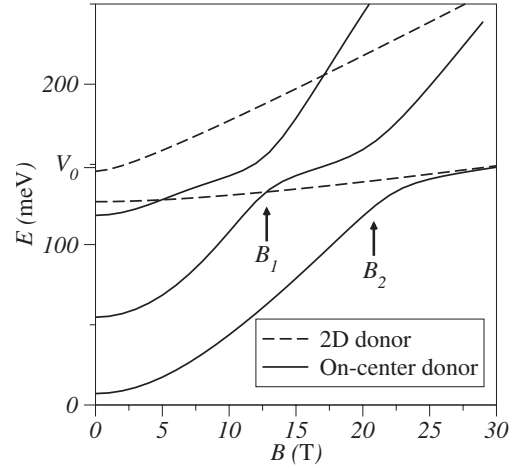


FIG. 1. Lowest energy levels with $\ell=0$ as a function of the applied magnetic field. Solid lines correspond to an on-center donor in a QR. Dashed lines correspond to an isolated 2D donor.

III. NUMERICAL RESULTS

We have performed numerical calculations in order to study the effect of the ionized donor on the electronic levels of the QR. Hereafter, we will focus on GaAs-In_{0.2}Ga_{0.8}As QRs and assume a constant effective mass $m^* = 0.0576$ in units of the free-electron mass. The inner and outer radii are set $\rho_1 = 10$ nm and $\rho_2 = 26$ nm, respectively.³ The effective Bohr radius is found to be $a^* = 10$ nm, and the magnetic length is given by $l_m = (26/\sqrt{B})$ nm, where B is expressed in tesla. The effective Rydberg is $R_y^* = 5.4$ meV in this material system. The conduction-band offset is $V_0 = 148$ meV. As we are interested in bound electrons, the value z_A was set in such a way that $|R(z_A a^*)| < 10^{-10} \text{ nm}^{-1}$. We have diagonalized the matrix Hamiltonian arising in Eq. (5) with $s=0.01$ and $N=1000$, corresponding to electronic states of on-center donor-bound electrons. This value of the grid size is enough to get accurate results.

Figure 1 shows the lowest energy levels with $\ell=0$ as a function of the applied magnetic field. Energy is measured from the bottom of the potential well. Results are compared to the energy levels of an isolated 2D donor. The obtained binding energy of the ground state in the latter case is $4R_y^* = 21.6$ meV for $B=0$, within the numerical uncertainty (recall that the potential energy at large distances is nonvanishing, $V_0 = 148$ meV; see the tick mark on the vertical axis in Fig. 1). This value is in perfect agreement with the analytic solution of the 2D Coulomb problem.⁹ Increasing the magnetic field yields an increase of the energy, as expected (see dashed lines in Fig. 1).

When the donor is placed at the center of the QR, the confining properties of the ground state at low fields are mainly determined by the conduction-band-edge offset, while the effects of the Coulomb interaction are negligible. The explanation lies in the fact that the potential well due to the QR is rather wide ($\rho_2 - \rho_1 = 16$ nm) and deep ($V_0 = 148$ meV). Therefore, the electron localizes at the well of the QR, with an energy much lower than that of the isolated 2D donor (see Fig. 1).

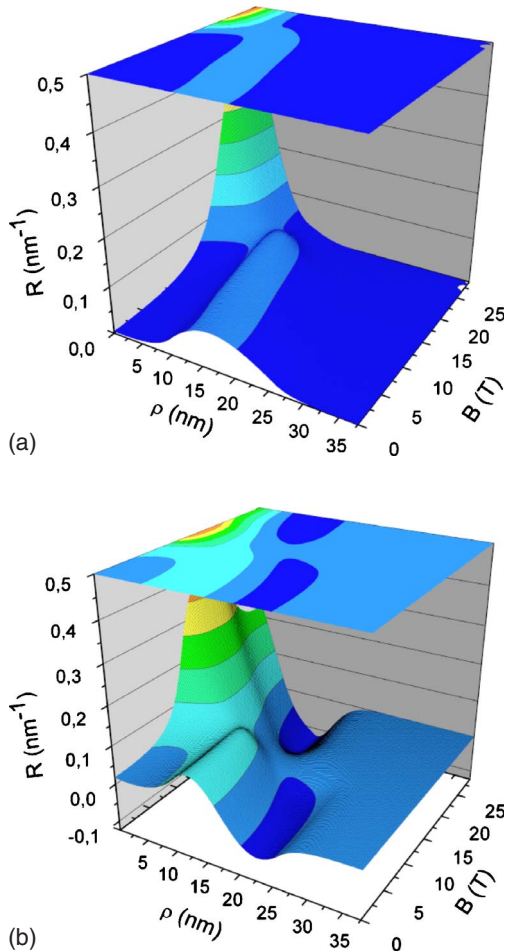


FIG. 2. (Color online) Envelope function of the (a) ground and (b) first excited states as a function of the applied magnetic field ($\ell=0$).

Increasing the magnetic field also yields a steeper increase of the energy (see solid lines in Fig. 1), as compared to the isolated 2D donor (see dashed lines in Fig. 1). This is to be expected since the spatial extent of the envelope function is larger in the former case, and the effects of the harmonic confining potential due the magnetic field are stronger. However, a careful inspection of Fig. 1 reveals a change of trend at some critical fields ($B_1 \approx 13$ T and $B_2 \approx 21$ T). We argue that anticrossing of levels of the donor and the potential well of the QR arises at these critical fields.

To provide support to this claim, in Fig. 2, we plot the radial envelope function $R(\rho)$ of the two low-lying states with $\ell=0$, for different values of the applied magnetic field. At low fields, the electron is localized within the potential well of the QR ($\rho_1 < \rho < \rho_2$). However, the electron localizes at the donor as the magnetic field is larger than $B_2 \approx 21$ T for the ground state [Fig. 2(a)] and $B_1 \approx 13$ T for the first excited state [Fig. 2(b)], respectively.

Absorption spectrum for in-plane polarization due to intraband bound-to-bound transitions is calculated as described earlier. The δ function in Eq. (6a) will be replaced by a Lorentzian of width $\Gamma=4$ meV. For the sake of clarity, we will focus on the transitions $|1,0\rangle \rightarrow |2,\pm 1\rangle$ hereafter. Figure

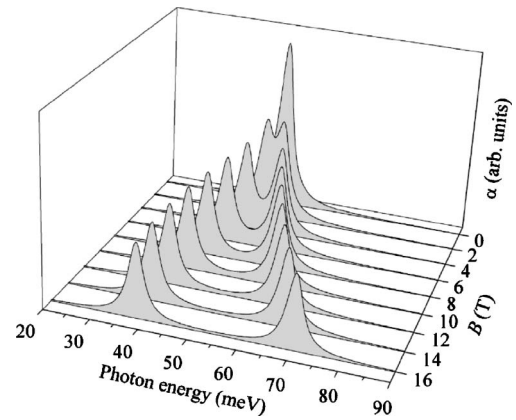


FIG. 3. Absorption spectra for in-plane polarization due to intraband $|1,0\rangle \rightarrow |2,\pm 1\rangle$ transitions as a function of the applied magnetic field, without on-center donor.

3 shows the evolution of the absorption coefficient as a function of the applied magnetic field, when no impurities are present in the QR. At zero magnetic field, both transitions are degenerated, as expected. Therefore, only one line arises in the absorption spectrum at zero applied field. The magnetic field splits the line into two peaks, one located at the low-energy side of the spectrum (corresponding to the transition $|1,0\rangle \rightarrow |2,1\rangle$) and the other at higher energy (corresponding to the transition $|1,0\rangle \rightarrow |2,-1\rangle$). The energy of the former line presents a minimum as a function of the magnetic field, while the latter one shifts superlinearly in the range of magnetic fields studied in this work, as shown in Fig. 4.

The radial part of the envelope function $R(\rho)$ is distorted when an on-center donor is present in the system. To ascertain whether midinfrared absorption is sensitive to those changes, we have calculated the oscillator strength of the transition $|1,0\rangle \rightarrow |2,1\rangle$ as a function of the applied magnetic field. The oscillator strength is

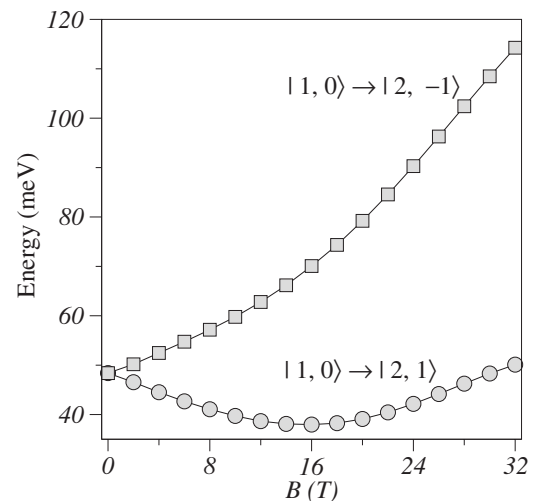


FIG. 4. Energy of the main lines in Fig. 3 as a function of the applied magnetic field.

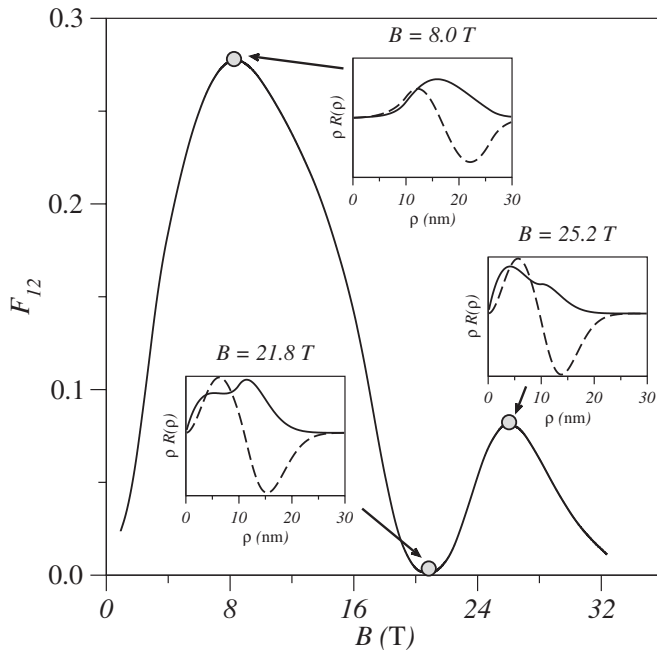


FIG. 5. Oscillator strength of the $|1,0\rangle \rightarrow |2,1\rangle$ transition as a function of the applied magnetic field when an on-center donor is present. The insets show $\rho R(\rho)$ corresponding to the ground (solid lined) and excited (dashed lines) states at three different values of the magnetic field.

$$F_{12} = \frac{2m_0}{\hbar^2} |\langle 1,0 | \rho | 2,1 \rangle|^2 (E_{21} - E_{10}), \quad (7)$$

m_0 being the free-electron mass. Notice that the oscillator strength is proportional to the square of the overlap integral of the two functions $\rho R_{10}(\rho)$ and $\rho R_{21}(\rho)$ given in Eq. (6b).

Figure 5 shows the oscillator strength as a function of the applied magnetic field when an ionized donor is located at the center of the QR. This magnitude changes noticeably upon minor distortions of radial envelope function. The in-

sets show $\rho R(\rho)$ of the ground and excited states at maxima and minimum of the oscillator strength. The latter state is not much distorted on increasing the magnetic field, as compared to the ground state. Consequently, the main contribution to the changes of the oscillator strength arises from distortions of the ground state which, however, are not too large. Therefore, we conclude that small changes in the ground state lead to large variations of the oscillator strength. Therefore, optical absorption is a reliable tool to detect those changes.

IV. CONCLUSIONS

We investigated the electronic states of a 2D QR with a perpendicular magnetic field under the influence of an ionized donor. Calculations were developed within a one-band envelope-function framework, which is suitable for wide gap semiconductors like those studied in this work. Finite-size effects of the QR were fully taken into account in the calculations.

The electron envelope functions of the lowest states are mainly localized at the well of the QR at low fields. An abrupt change of the localization properties appears at a critical magnetic field, since the electron is then mainly localized around the impurity. This transition gives rise to well-defined anticrossing of levels as a function of the magnetic field. Numerical results of the absorption spectrum in the mid-infrared are sensitive to minor changes in the envelope function when an ionized donor is located at the center of the QR. We conclude that optical techniques are suitable for characterizing the effects of ionized donors on the electron envelope functions.

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