Optical spectra and intensities of a magnetic quantum ring bound to an off-center neutral donor D^0

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In this paper, we study the effect of the position of a positively charged impurity, or so-called donor, in a single-electron two-dimensional (2D) magnetic quantum ring, where the magnetic field is zero within the ring and constant elsewhere, on the low-lying spectra of such a neutral donor D^0 system (involving a positively charged impurity surrounded by a single electron) under perpendicular magnetic fields. The optical absorption spectra with their corresponding intensities between the ground state and the first excited state are calculated. The donor is located at a distance d as measured vertically from the plane of the ring along the z direction. The ground-state orbital angular momentum (L) transitions induced by magnetic fields are overall presented in terms of a magnetic field versus donor position (B-d) phase diagram. Dependences of the absorption spectra and their intensities on the layer thickness for the quasi-two-dimensional (q2D) magnetic quantum ring are also discussed.

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In the past decade, there were considerable interests in the theoretical studies of impurity states in electrically confined quantum dots[1–5] since such impurity dopings on the systems can modify the energy levels and in turn affect both their electronic and optical properties. Recently, the studies of magnetic quantum dots' or magnetic quantum rings' systems[6–18] with and without on-center impurities arouse growing interests both theoretically and experimentally owing to the potential uses in high-density memory devices and spintronic materials.

In the presence of on-center impurities, either donor or acceptor, the low-lying spectra of two-dimensional (2D) magnetic quantum ring systems were calculated by numerical diagonalization, and the effects of both size and magnetic field were also discussed in detail.[17,18] One notable feature for the qualitative results showed that there exist ground-state L transitions induced by the external magnetic field for magnetic quantum ring bound to an acceptor but not for magnetic quantum dot except at very weak magnetic fields.[18] To our knowledge, the effects of the donor position on both the optical absorption spectra and their corresponding optical intensities of the magnetic quantum rings were not studied in the past, which are the part of the continuation of previous work[18] in the present paper. The case of quasi-two-dimensional (q2D) magnetic quantum ring with a finite layer thickness is also discussed with the assumption that the electron moves along the z direction in an one-dimensional infinite-depth quantum well.

We consider a neutral donor D^0 located at a distance d as measured from the plane of the magnetic quantum ring along the z-direction. Within the framework of the effective mass theory, the 2D Hamiltonian for such off-center D^0 system, when subjected to a perpendicular magnetic field B along the z direction, reads[18]

$$\hat{H}_{2D} = \frac{1}{2m}(\boldsymbol{P} + e\boldsymbol{A})^2 + \hat{H}_{\text{donor}}(d), \tag{1}$$

where m is the electron effective mass. The magnetic quantum ring of the inner radius r_{01} and the outer radius r_{02}, is formed by a spatially inhomogenous magnetic field, with zero field within the ring and constant field elsewhere, and the form of the corresponding magnetic vector potential $\boldsymbol{A}$ refers the previous work.[18] The donor Hamiltonian for the Coulomb attraction between the electron and the off-center donor, different from those of previous work,[18] reads

$$\hat{H}_{\text{donor}}(d) = -\frac{e^2}{4\pi\epsilon\sqrt{r^2 + d^2}}. \tag{2}$$

For the case of a q2D magnetic quantum ring with finite layer thickness d_z, the single electron Hamiltonian in Eq. (1) is expressed by

$$\hat{H}_{q2D} = \hat{H}_{2D} - \frac{\hbar^2}{2m}\frac{d^2}{dz^2}, \tag{3}$$

with the donor Hamiltonian in Eq. (2) replaced by the following:

$$\hat{H}_{\text{donor}}(d) = -\frac{e^2}{4\pi\epsilon\sqrt{r^2 + (d-z)^2}} \quad \text{for } |z| \leq d_z/2. \tag{4}$$

Assume that only the lowest electronic subband in the z direction is occupied without coupling between the z direction and the xy plane, since the electron is more confined in the z direction than in the xy plane.[19] Then we can approximately consider the electron as moving in an one-dimensional infinite square-depth quantum well, and the eigenfunctions and the eigenvalues for the z motion are given, respectively, by

$$\phi_z = \begin{cases} \sqrt{\dfrac{2}{d_z}} \sin\left[\dfrac{\pi n_z}{d_z}\left(z + \dfrac{d_z}{2}\right)\right], & |z| \leq d_z/2, \\ 0, & \text{otherwise}, \end{cases} \tag{5}$$

TABLE I. Values of energy, distance, and magnetic field units for GaAs with characteristic material parameters $\epsilon=13.1\epsilon_0$, $m=0.067m_0$ (Ref. 20).

	Energy E_B	Distance a_B	Magnetic field $\hbar/a_B^2e$
Value	10.62 meV	10.36 nm	6.13 T

$$E_z=\frac{\hbar^2\pi^2n_z^2}{2md_z^2},\quad n_z=1,2,\ldots, \tag{6}$$

where n_z is the quantum number with the value of 1 for the lowest subband, and after integration over the z coordinate, Eq. (4) can be rewritten as the 2D donor Hamiltonian as follows:

$$\hat{H}'_{\text{donor}}(d)=-\frac{2e^2}{4\pi\epsilon d_z}\int_{-d_z/2}^{d_z/2}\frac{\sin^2\left[\frac{\pi n_z}{d_z}\left(z+\frac{d_z}{2}\right)\right]}{\sqrt{r^2+(d-z)^2}}dz. \tag{7}$$

The Hamiltonians in Eqs. (1) and (3) are simplified into 2D forms and then diagonalized, with the use of 2D harmonic product bases $\langle\vec{r}|\phi_{nl}\rangle=\frac{1}{\sqrt{2\pi}}e^{il\theta}R_{nl}(r)$, by the same method outlined in Ref. 18, which is no longer described here. Note that n and $l\hbar$ denote the radial quantum number and the orbital angular momentum, respectively, and $R_{nl}(r)$ is the radial function.

The aim of the present study is to calculate the intensity of the optical transition within the electric-dipole approximation or the probability of transition between two states defined as[3]

$$I=|\langle f|r\exp(\pm j\theta)|i\rangle|^2 \tag{8}$$

where $|i\rangle$ and $|f\rangle$ are the initial and the final states, respectively. The $\pm$ sign refers to circular left/right polarization of the light. Note that the presence of the phase factor $\exp(\pm j\theta)$ in Eq. (8) leads to the following selection rule: The matrix element $|\langle f|r\exp(\pm j\theta)|i\rangle|$ is different from zero only for transitions in which the angular momentum changes by one unit, i.e., $\Delta l=\pm1$, without any limit for the change of the quantum numbers n and n_z.

To what follows, we make numerical calculation for the magnetic quantum ring of inner radius $r_{01}=a_B$ and outer radius $r_{02}=2a_B$, and the magnetic field is presented in terms of $1/a_c^2$ for the figures of this paper. The numerical results are not specific for any materials since all parameters are presented in natural units for all figures of the paper. Using parameters appropriate for GaAs as an example, the values of the energy, the distance, and the magnetic field units are listed in Table I in order to get the grasp of the order of magnitude for the actual numerical results.

Consider the 2D case first, starting from the donor situated at $d=0.5a_B$ away from the magnetic quantum ring, shown in Fig. 1(a), the ground state transits from one orbital momentum to another higher one in the sequence $(0,-1)\rightarrow(0,-2)\rightarrow(0,-3)\rightarrow(0,-4)$, as the magnetic field increases. Such low-lying spectra are qualitatively the same as those of without on-center donor,[18] and very weak attraction

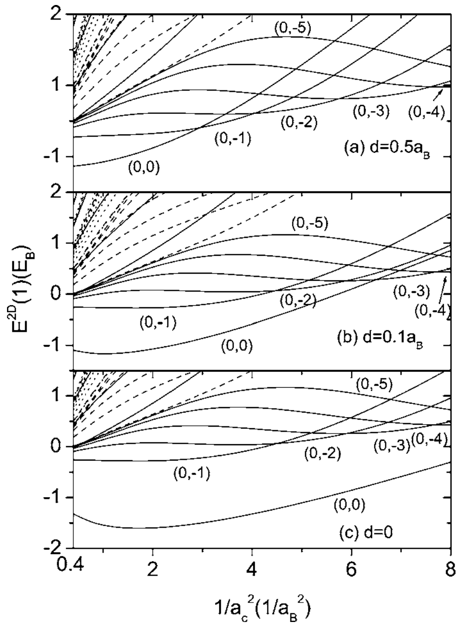

FIG. 1. Low-lying spectra of an electron 2D magnetic quantum ring as a function of $1/a_c^2(\propto B)$ for a donor at a distance from the plane of the ring along z direction (a) $d=0.5a_B$, (b) $d=0.1a_B$, and (c) $d=0$. Note that $E_B=m\alpha^2/\hbar^2$ with $\alpha=e^2/4\pi\epsilon$, the magnetic length $a_c=\sqrt{\hbar/m\omega_c}$ with $\omega_c=eB/m$, and a_B is the Bohr radius. All states are labeled by the quantum numbers (n,l) and those with $n=0,1,2$ are denoted by the curved solid, dashed, and dotted lines, respectively.

between the electron and the donor is expected. The qualitative aspect of the spectra can hence be explained by the same argument as that of impurity-free case:[18] At very weak magnetic fields, the states with angular momentum $l<0$ are far away from the magnetic edge or the ring region, and the electron moves with an analogy to that in uniform magnetic fields. The smaller the angular momentum states $|l|$, the closer the electron is to the magnetic edge of the ring. An increase of magnetic field brings the electron much closer and enter to the ring region. The electron then likely moves in the absence of the magnetic field, leading to lower electron's eigenenergy. A further increase of magnetic field brings the electron much closer or approaches to the center of the ring. The electron returns to move in a uniform magnetic field and increase its eigenenergy by a certain amount comparing with that in the zero magnetic field. Overall, the electron in different possible states exists in the ring region at different magnetic fields, leading to the ground-state L transitions induced by magnetic fields. Furthermore, from the corresponding absorption spectra [Fig. 2(a)], some local spikes can be observed at the magnetic fields corresponding to those ground-state L transitions induced by magnetic fields [Fig. 1(a)], with the continuous decrease of their intensities [Fig. 3(a)]. However, at the magnetic fields that the cross-overs in the neighboring higher state exist, the absorption intensities show discontinuous behavior and it is unequally probable for the electron to jump to the first and the second excited states [Fig. 3(a)]. When the magnetic field increases further, the corresponding absorption lines [Fig. 2(a)] split into two, having opposite trend in magnitudes with

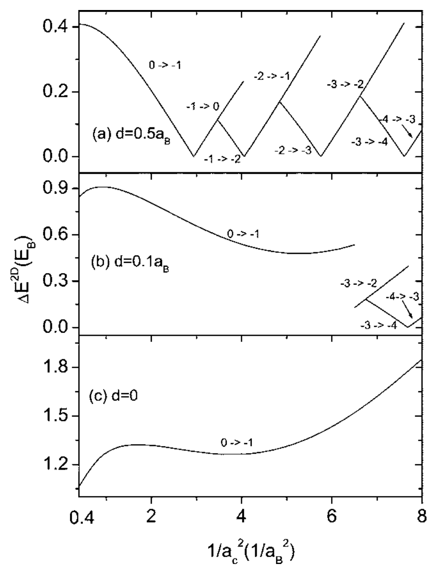

FIG. 2. Optical absorption spectra of an electron 2D magnetic quantum ring as a function of $1/a_c^2(\propto B)$. Note that the orbital angular momentum transitions between ground state and first excited state are denoted by $l \rightarrow l'$.

increasing magnetic field. When the separation d between the donor and the ring decreases to $0.1a_B$ [Fig. 1(b)], the orbit radius of the electron shrinks much to the center of the ring due to the electron-donor attraction. Higher magnetic field is, therefore, required for the electron to jump to the orbits of higher angular momentum states. Together with the energy decrease by an appreciate amount in $(0,0)$ state comparing with neighboring angular momentum states, the $(0,0)$ is kept as the ground state up to the magnetic field $a_B^2/a_c^2=6.5$ and jumps to the $(0,-3)$ state as the magnetic field increases further, leaving $(0,-1)\rightarrow(0,-2)$ and $(0,-2)\rightarrow(0,-3)$ as the excited-state transitions at the magnetic fields $a_B^2/a_c^2<6.5$.

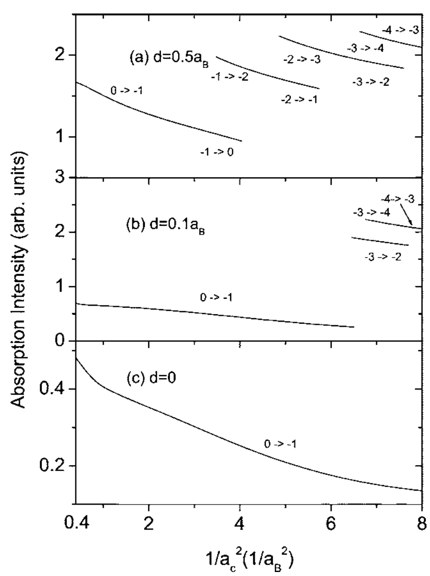

FIG. 3. Absorption intensities of an electron 2D magnetic quantum ring for the transitions from the ground state to the first excited state.

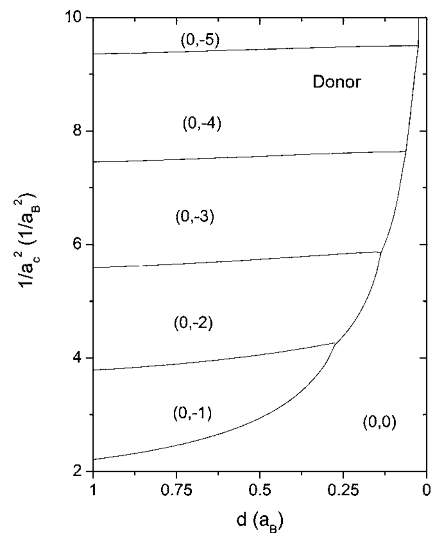

FIG. 4. $1/a_c^2(\propto B)$ vs donor position (B-d) phase diagram of the electron ground state in an electron 2D magnetic quantum ring, with the associated ground state within each domain as represented by the quantum number (n,l).

Note that the corresponding absorption line for the $(0,0)\rightarrow(0,-3)$ shows discontinuous behavior and decreases ΔE^{2D} by a certain amount [Fig. 2(b)].

When the donor moves closer and is placed exactly at the center of the ring [Fig. 1(c)], the electron in $l=0$ state has no centrifugal barrier, and approaches much closer or tends to be localized near the position of the donor in order to minimize its total energy. The electron no longer jumps to the higher orbits even in magnetic fields up to $a_B^2/a_c^2=8$ [see Fig. 1(c)]. Although the orbital angular momentum transitions, induced by magnetic fields, in the first excited states still occurs, owing to the selection rule $\Delta l=\pm 1$, the absorption line shows continuous behavior corresponding to $(0,0)\rightarrow(0,-1)$ ground-state transition. Overall, in order to show the dependence of the donor position on the ground state for the magnetic quantum ring, the B-d phase diagram are plotted in Fig. 4. Two remarkable points to be made here are as follows: (1) The ground-state L transitions no longer occur even for magnetic fields up to $a_B^2/a_c^2=10$, at small separation between the electron and the ring. (2) All transition lines between two neighboring L ground states shift to lower magnetic fields as the separation d increases, and such general trends are predicted to be extended to the cases without impurity and even with an acceptor.

Let us now discuss a q2D magnetic quantum ring with finite thickness, three various magnetic fields a_B^2/a_c^2 are taken to be 2,4,6, for example, for an on-center donor's case. Dependences of the low-lying spectra, and absorption spectra together with their intensities on the layer thickness are presented in Figs. 5 and 6, respectively. Note that, the eigenenergies E_z for the z motion in Eq. (6) are not included in E^{q2D} (Fig. 5), for the sake of comparisons with those of 2D case, and the numerical results for $d_z=0$ are in fact equal to those of 2D case. From Fig. 5, it can be seen that as the ring is thicker, the eigenenergies generally increases in a finite amount mainly due to the decrease of the attraction between the electron and the donor [Eq. (7)]. This qualitative result

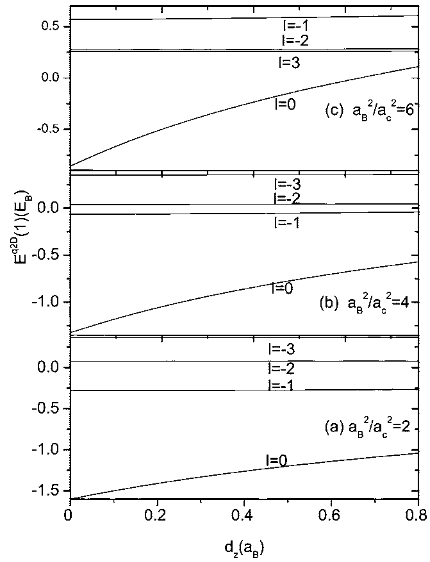

FIG. 5. Low-lying spectra of a q2D magnetic quantum ring as a function of layer thickness for an on-center donor under various magnetic fields, (a) $a_B^2/a_c^2=2$, (b) $a_B^2/a_c^2=4$, and (c) $a_B^2/a_c^2=6$.

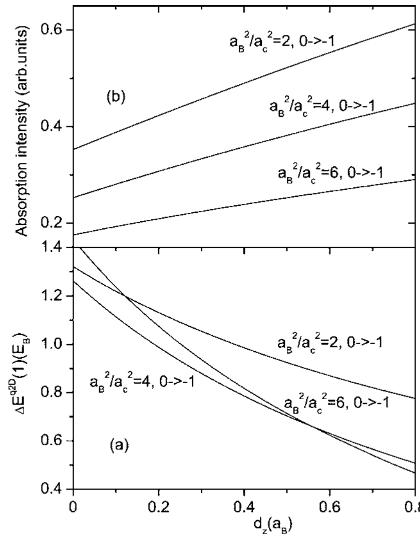

FIG. 6. (a) Optical absorption spectra and (b) their absorption intensities of a q2D magnetic quantum ring as a function of layer thickness for an on-center donor under various magnetic fields.

can be physically realized by the following: the thicker the ring, the much more space the electron can move, and the higher eigenvalue is to be expected. Especially for $l=0$ state, the electron has no centrifugal barrier with much smaller orbital radius, resulting in more contribution for the z motion, that can be obviously seen by the significant increase of $l=0$ eigenvalue comparing with those of neigboring states (Fig. 5). One more point worth mentioning here is that, as the layer thickness increases, ΔE^{q2D} decreases [Fig. 6(a)] with the increase of the absorption intensities [Fig. 6(b)] which are qualitatively the same as those effects of donor position (Figs. 2 and 3).

In summary, the dependences of both the donor position and the layer thickness on the low-lying spectra of a single electron 2D magnetic quantum ring are discussed. The optical absorption spectra and their intensities due to the transition between the ground state and the first excited state are calculated. The numerical results of the absorption spectra give good references awaiting actual experimental confirmation. These also motivate us to further study the effect of impurities on few-electron magnetic quantum ring without neglecting both electron-electron and spin-spin interactions and to see the stability of few-electron magnetic quantum ring only confined by magnetic fields.

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