Magnetic-field dependence of low-lying spectra in magnetic quantum rings and dots

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In this paper, the magnetic-field dependence of low-lying spectra of a single-electron magnetic quantum ring and dot, formed by inhomogeneous magnetic fields, are calculated using the numerical diagonalization scheme. The effects of on-center acceptor and donor impurities are also considered. In the presence of an acceptor impurity, transitions in the orbital angular momentum, L, are found for both the magnetic quantum ring and the magnetic quantum dot when the magnetic field is varied.

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I. INTRODUCTION

In the past decade, the quantum dot was a subject of intense theoretical and experimental interest in nanotechnology areas[1–9] since the fabrication of quasi-zero-dimensional semiconductor heterostructures becomes reality to electrically confine few electrons in all spatial dimensions. The confining electrostatic potential of such quantum dots is well described by a parabolic shape theoretically. In recent years, owing to the potential uses in high density memory devices or spintronic materials, the studies of two-dimensional electron gas (2DEG) in the well-known magnetic quantum dot's and even the magnetic quantum ring's systems, which are different from the conventional quantum dot, address a lot of attention.[10–19] In case of the former one, the electrons are confined magnetically and the confining potential is inherently nonparabolic. Experimentally realistic examples for several magnetic structures were also proposed, e.g., type II superconducting materials deposited on conventional structures,[11] magnetic superlattices by the patterning of ferromagnetic materials integrated by semiconductors,[12] and nonplanar 2DEG systems by molecular beam epitaxy.[13] In Ref. 14, a chronological survey on the past experimental studies on such areas was also reviewed. One of the simple ways to experimentally realize the magnetic quantum dot or ring is that the same shape of thin superconducting material is placed on top of 2DEG. In this case, the magnetic fluxes are expelled from the superconducting material, resulting in inhomogeneous magnetic field profiles on 2DEG.

In the early theoretical studies, the magnetic quantum dot and ring were modeled by setting the magnetic field B to be zero within the dot and the ring regions, respectively, and constant B elsewhere. For magnetic dots, Sim *et al.*[16] studied the formation of the magnetic edge states along with the corresponding classical trajectories. The classical trajectories were obtained by using the general rule derived from the energy and angular momentum conservation laws.[20] Mallon and Maksym[17] generalized the above works to the case of two interacting electrons and discussed their stability. Reijniers *et al.*[18] calculated single electron low-lying spectra for two model systems in different magnetic profiles, with and without magnetic overshoot, respectively, at the edge of the dot. For the case of magnetic quantum rings, Kim *et al.*[19] investigated these electron structures and magnetic edge states, and found that the energy spectra critically depend on the number of missing magnetic flux quanta rather than the geometry of the structure or the field abruptness. Recently, in Ref. 14, based on the above models of both magnetic quantum dots and rings, Lee *et al.* modified the magnetic quantum dot and ring formed by two different magnetic fields, and analyzed interesting numerical results in great detail. The probability currents of the states are also calculated using the derivative of eigenvalue wrt angular momentum l, $I_{nl}=1/\hbar\ \partial E_{nl}/\partial l$. As a whole, the eigenvalues of the above systems were found by a traditional method via the continuity of the wave functions and their derivatives at the boundaries between regions of different magnetic fields. Note that all the past studies of above systems only focus on the impurity-free cases, and the impurities have to be considered in a real situation since it will modify the energy levels of the materials, and in turn largely affect their electronic and magnetic properties. To our knowledge, the magnetic dependence of quantum magnetic dots and rings involving impurity doping was not studied in the past, which is the novel part of the present work.

In the past decade, by using numerical diagonalization, low-lying spectra of few-electron or exciton quantum dots with and without impurity were calculated, for which electrons or holes are confined electrostatically by parabolic potentials in uniform magnetic fields.[2–4,7–9] Qualitative results for the ground state orbital and/or spin angular momenta transitions were taken that are in good agreement with those of experiments. In the present study, we apply the same computational technique on those systems of the magnetic quantum dot and ring. Here, starting from the Hamiltonian of the single electron magnetic quantum ring system in the presence of an on-center Coulomb acceptor or donor impurity, we rearrange the whole Hamiltonian and extract those terms as the unperturbed one such that its eigenvector is exactly the same as 2D harmonic product basis states in the model space. Note that the system will become the case of the magnetic dot when the inner radius of the ring is zero. The low-lying spectra of a single electron magnetic quantum ring and dot are then found by using numerical diagonalization. The magnetic moments are also found in order to get visible discontinuities at those points of orbital angular momentum L

transitions induced by magnetic fields. Finally, we compare and analyze our overall numerical results for such a system with and without acceptor or donor impurity.

II. THEORY

In the effective mass approximation, the Hamiltonian describing a single electron bound to an on-center Coulomb impurity, either acceptor or donor, in a 2D magnetic quantum ring subjected to a magnetic field, is given by

$$\hat{H} = \frac{1}{2m}(\vec{P} + e\vec{A})^2 + \eta\frac{e^2}{4\pi\epsilon r}, \tag{1}$$

where m is the effective mass of the electron, e is the absolute value of the electron charge, and ϵ is the dielectric constant of the medium the electron is moving in. Note that the electron-electron interactions are not considered for mathematical simplicity and the Zeeman energy for the coupling of the electron spin and the magnetic field can therefore be neglected without loss of physical significance. The last term is the Coulomb interaction between the electron and the on-center impurity. The parameter η is 1 for an acceptor impurity and -1 for a donor impurity.

In a real situation for experiments, the magnetic quantum ring is formed by inhomogeneous magnetic fields: the magnetic field perpendicular to the xy plane within the ring region is zero, $B=0$ for $r_{01} \leqslant r \leqslant r_{02}$, and constant B outside it, $B=B\hat{e}_z$, where $\hat{e}_z$ is the unit vector in the z direction, and r_{01} and r_{02} are the inner and the outer radii of the magnetic ring, respectively. In the representation of a polar coordinate, the corresponding vector potential $\vec{A}$ is then given by the following:[14,19]

$$\vec{A} = \begin{cases} \dfrac{B}{2}\hat{e}_z \times \vec{r}, & \text{for } 0 \leqslant r < r_{01}, \\ \dfrac{Br_{01}^2}{2r^2}\hat{e}_z \times \vec{r}, & \text{for } r_{01} \leqslant r \leqslant r_{02}, \\ \dfrac{B(r^2 - (r_{02}^2 - r_{01}^2))}{2r^2}\hat{e}_z \times \vec{r}, & \text{for } r > r_{02}. \end{cases} \tag{2}$$

When the inner radius r_{01} goes to zero, the resulting vector potential can be reduced to the case of a magnetic dot with the radius r_{02}. After rearrangement, Eq. (1) can be rewritten as

$$\hat{H} = \hat{H}_0 + \hat{V}_{\text{imp}} + \hat{V}_{l-B}. \tag{3}$$

In order to calculate the eigenenergy of the whole system by numerical diagonalization, the unperturbed Hamiltonian can be extracted from Eq. (1) as

$$\hat{H}_0 = \frac{1}{2m}P^2 + \frac{m\omega_c^2}{8}r^2 + \frac{\omega_c}{2}\hat{L}_z, \tag{4}$$

such that its eigenfunction can be chosen as the well-known 2D harmonic product basis states $\langle\vec{r}|\phi_{nl}\rangle = (1/\sqrt{2\pi})e^{il\theta}R_{nl}(r)$, that is similar to the case of a parabolic quantum dot,[2] where n and $l\hbar$ denote the radial quantum number and the orbital angular momentum, respectively. The symbol $\hat{L}_z$ in Eq. (4) is the orbital angular momentum operator in the z direction. The radial function $R_{nl}(r)$ is given by the following equation:

$$R_{nl}(r) = \left[\frac{2n!}{(n+|l|)!}\right]^{1/2} r^{|l|}L_n^{|l|}(r^2)e^{-r^2/2}, \tag{5}$$

where $L_n^{|l|}(r^2)$ is the associated Laguerre polynomial. For a succinct representation, r, r_{01}, and r_{02}, as measured from the center of the magnetic ring, are all in units of the magnetic length $a_c(=\sqrt{\hbar/m\omega_c})$ with the cyclotron frequency $\omega_c = eB/m$. Also hereafter the energies are in units of $\hbar\omega_c$.

The perturbed Hamiltonian, including the electron-impurity Coulomb term $\hat{V}_{\text{imp}}$ and the interaction term between the electron and the inhomogeneous fields $\hat{V}_{l-B}$, can be expressed, respectively, in units of $\hbar\omega_c$, by

$$\hat{V}_{\text{imp}} = \eta\frac{a_c}{a_B}\frac{1}{r}, \tag{6}$$

$$\hat{V}_{l-B} = \begin{cases} 0, \quad \text{for } 0 \leqslant r < r_{01}, \\ -\frac{1}{2r^2}(r^2 - r_{01}^2)l - \frac{1}{8r^2}(r^4 - r_{01}^4), \quad \text{for } r_{01} \leqslant r \leqslant r_{02}, \\ -\frac{1}{2r^2}(r_{02}^2 - r_{01}^2)l - \frac{1}{8r^2}[2r^2(r_{02}^2 - r_{01}^2) - (r_{02}^2 - r_{01}^2)^2], \\ \quad \text{for } r > r_{02}. \end{cases} \tag{7}$$

The matrix elements used for numerical diagonalization are expressed by

$$\langle\phi_{nl}|\hat{H}_0|\phi_{n'l'}\rangle = \left\{n + \frac{1}{2}(|l| + l) + \frac{1}{2}\right\}\delta_{n,n'}\delta_{l,l'}, \tag{8}$$

$$\langle\phi_{nl}|\hat{V}_{\text{imp}}|\phi_{n'l'}\rangle = \eta\frac{a_c}{a_B}\int_0^\infty R_{nl}(r)\frac{1}{r}R_{n'l'}(r)r\,dr\,\delta_{l,l'}, \tag{9}$$

$$\langle\phi_{nl}|\hat{V}_{l-B}|\phi_{n'l'}\rangle = \int_0^\infty R_{nl}(r)\hat{V}_{l-B}R_{n'l'}(r)r\,dr\,\delta_{l,l'}. \tag{10}$$

One note worth mentioning here is that, in Eq. (8), the unperturbed energies give discrete values corresponding to the electron motion on the xy plane under a uniform field, and such an energy value can be written as the non-negative integer or Landau energy level index, $N_r = n + \frac{1}{2}(|l| + l)$. Finally, the lowest three Landau levels of the single electron magnetic quantum dot and ring, with and without on-center Coulomb impurity, are calculated for several lowest angular momenta ($l = 0, \pm 1, \ldots, \pm 5$) as a function of the magnetic field.

III. DISCUSSION AND CONCLUSIONS

In what follows, in order to illustrate the magnetic-field dependence of the low-lying spectra of the electron quantum dot or ring, we set the square of magnetic length (which is inversely proportional to B), as the independent variable for the figures of this paper. Also, the natural units are used in all

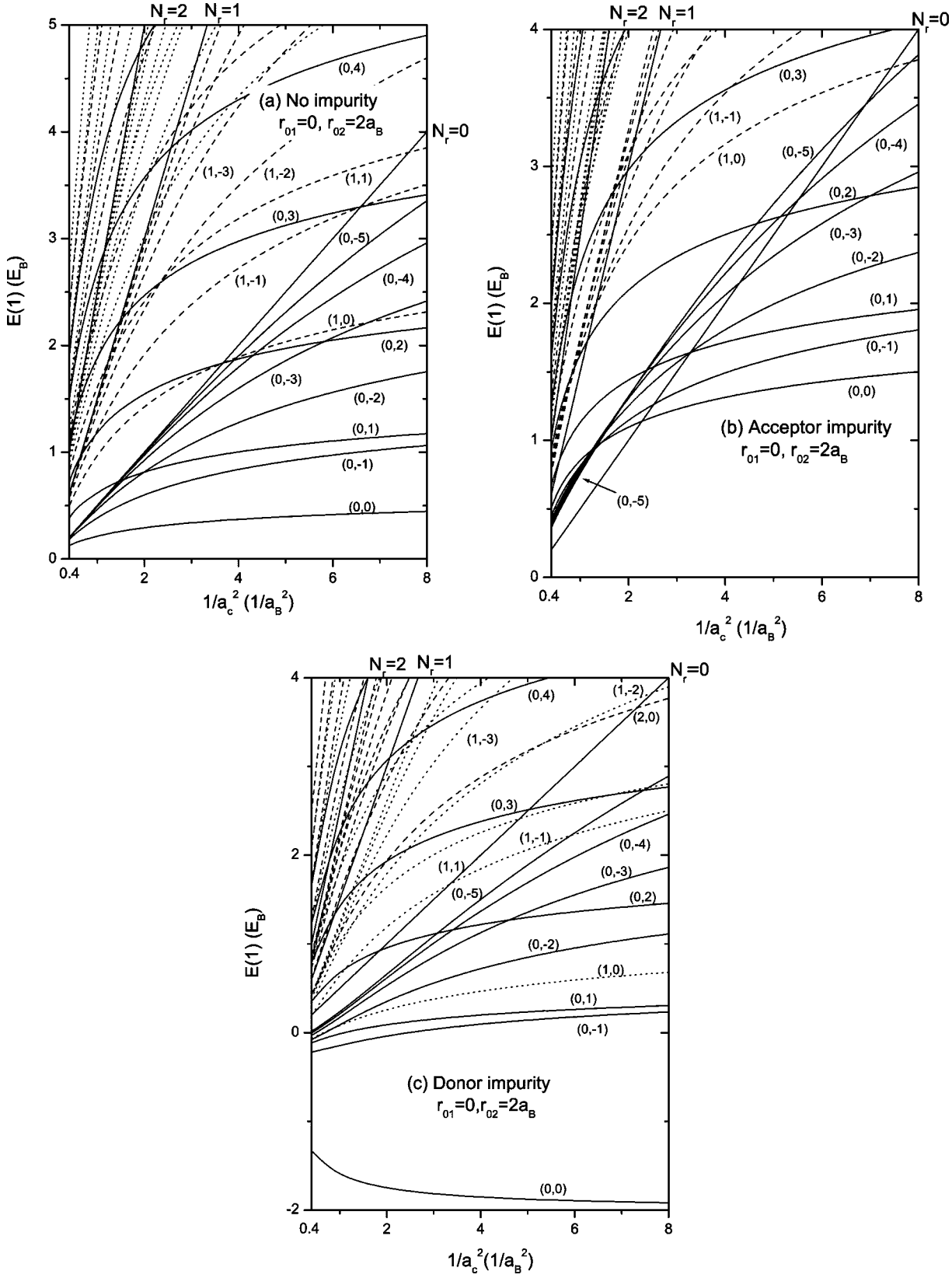

FIG. 1. Low-lying spectra of a magnetic quantum dot as a function of $1/a_c^2(\propto B)$, (a) no impurity, (b) acceptor, and (c) donor. Note that all states are labeled by the quantum numbers (n,l) and the states $n=0$, $n=1$, and $n=2$ are denoted by the curved solid, dashed, and dotted lines, respectively. The lowest three Landau levels ($N_r=0$, 1, 2) are denoted by solid straight lines.

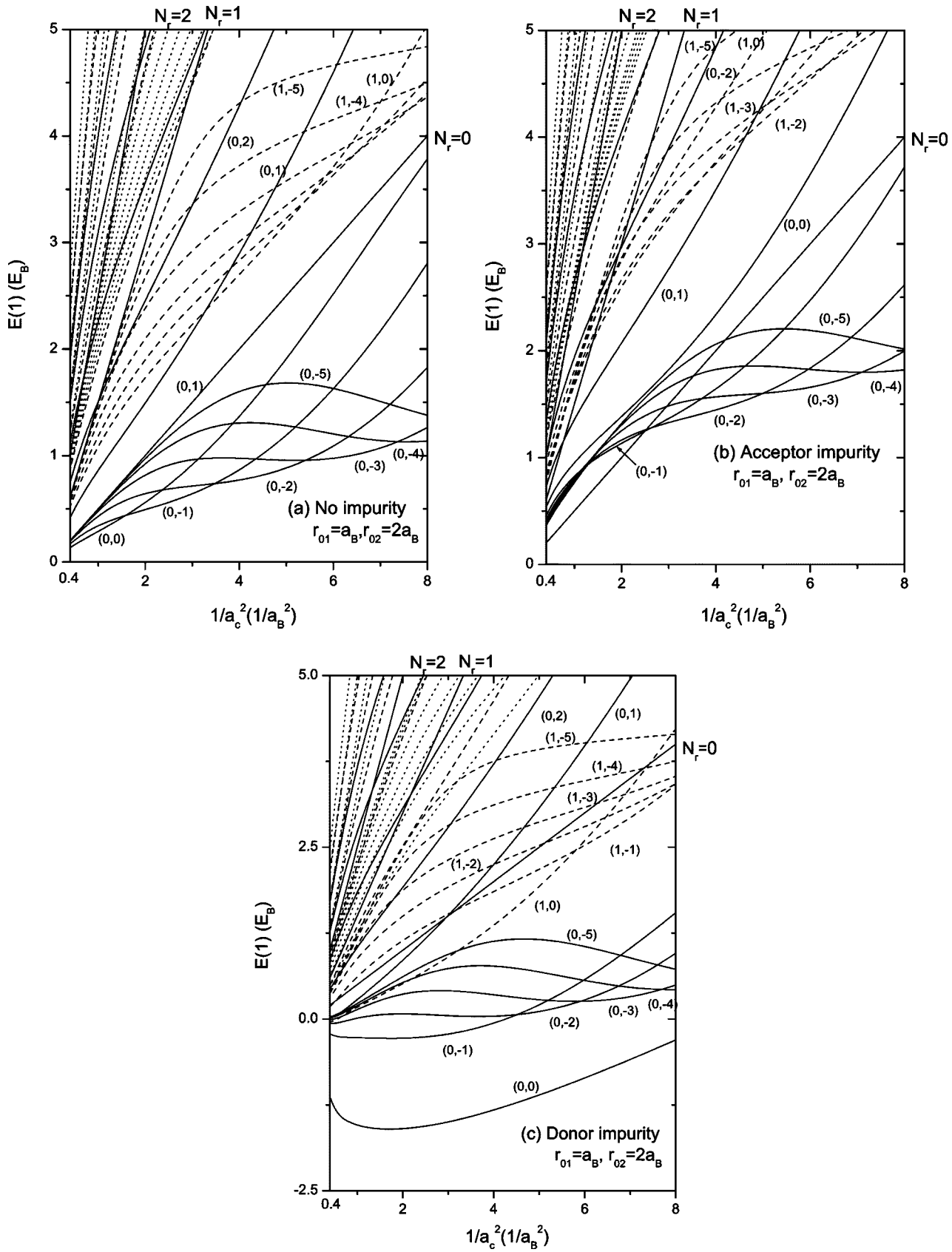

FIG. 2. Low-lying spectra of a magnetic quantum ring as a function of $1/a_c^2(\propto B)$, (a) no impurity, (b) acceptor, and (c) donor. The meanings of different line types are similar to those of Fig. 1.

TABLE I. Numerical results of the magnetic quantum dot with on-center acceptor impurity.

State	(0,0)	(0,−1)	(0,−2)	(0,−3)	(0,−4)	(0,−5)
Eigenenergy (E_B) at $a_B^2=0.4a_c^2$	0.785 71	0.726 75	0.702 95	0.679 03	0.657 24	0.638 89
Eigenenergy (E_B) at $a_B^2=2a_c^2$	1.314 27	1.492 79	1.808 11	2.061 99	2.217 03	2.296 58

the figures of the present paper: the Bohr radius ($a_B=\hbar^2/m\alpha$) as the magnetic length unit and $E_B=m\alpha^2/\hbar^2$ as the energy unit, where $\alpha=e^2/4\pi\epsilon$.[21] In our actual numerical diagonalization, the rate of convergence depends on the strength of the magnetic field. At sufficiently low or zero magnetic fields, the electron wave function is very extended, leading to the extremely slow convergence, and very large basis space is required to get reliable numerical results. Therefore, we calculate the eigenenergies of the systems starting from the magnetic field $a_B^2/a_c^2=0.4$, without affecting our discussion on the qualitative aspect of the magnetic dot or ring. In the present numerical work, ten basis states for each angular momentum $l\hbar$ are included, since the ratio of the difference in eigenenergy is less than 0.001% for the further increase of number of basis states. With better views, hereafter, we discuss the qualitative aspects of the energy spectra in Figs. 1 and 2 only for the lowest Landau level, since the same argument can be applied for higher ones.

First of all, let us consider the low-lying spectra of an electron magnetic quantum dot with and without on-center acceptor and donor impurity as presented in Fig. 1. In Fig. 1(a), in the case of the impurity-free system, the eigenenergies deviate more significantly from the bulk Landau level as the magnetic field increases. Note that, when the magnetic field is weak, the radii of the orbits are large and the electron essentially moves around in a uniform magnetic field outside of the dot. As the magnetic field strength increases, the orbits contract toward the center of the dot and the effect of an inhomogeneous magnetic field becomes more evident. On the other hand, the smaller the quantum values $(2n+|l|)$, the more significant the eigenenergies deviate from the bulk Landau level. It can be physically explained by the following. As is well known, a single electron eigenstate $\langle\vec{r}|\phi_{nl}\rangle=(1/\sqrt{2\pi})e^{il\theta}R_{nl}(r)$ can be qualitatively regarded as the circular motion of the electron about the center with orbital angular momentum $l\hbar$, and the mean square orbit radius r can be expressed by[2]

$$\langle\phi_{nl}|r^2|\phi_{nl}\rangle \propto 2n+|l|+1=2N_r-l+1. \tag{11}$$

The smaller the quantum value of $2n+|l|$, the closer the electron is to the magnetic edge near the center of the dot. Since the interaction energy $\hat{V}_{l-B}$ is more negative, (0,0) is left as the ground state regardless of the magnetic field strength. And for our present calculation of angular momenta up to $l=-5$, the state labeled by $(0,-5)$ is closer to the bulk Landau level since the electron is far from the magnetic edge and moves with an analogy to that in a uniform field. The above argument is also applied for the rings. For convenience of presentation, all perturbed or excited states are labeled similarly to those of the unperturbed one.

In Fig. 1(b), in the presence of on-center acceptor impurity, there is a clear-cut ground state L transition at $a_B^2/a_c^2\approx1.38$. At fixed magnetic fields, the eigenstates in the increasing sequence are just in opposition between magnetic fields lower and higher than about such an a_B^2/a_c^2 value, and the eigenenergies for magnetic fields $a_B^2/a_c^2=0.4$ and 2, for example, are listed in Table I for comparison since the energy difference is very small below $a_B^2/a_c^2\approx1.38$. At magnetic fields below this transition point, the (0,0) state has no centrifugal barrier and the electron is closer to the center of the acceptor impurity comparing with other angular momentum states. The electron becomes most unstable and the (0,0) state has the highest energy for the lowest Landau level, while $(0,-5)$ is left as the ground state. At magnetic fields higher than $a_B^2/a_c^2\approx1.38$, the magnetic confinement, however, becomes more dominant than the effect of on-center acceptor impurity, and the sequence of the states will return to those cases without impurity. As a whole, all states shift to higher eigenenergies at nonzero magnetic fields owing to the net small repulsion between the electron and the on-center acceptor impurity. In the case of on-center donor impurity shown in Fig. 1(c), using the same argument of a Coulomb effect, the electron-donor attraction brings the electron much closer to the center of the dot. The states have the same sequence as those of the impurity-free case and the eigenenergies shift to lower values, and that of the (0,0) state is even negative for magnetic fields up to $a_B^2/a_c^2=8$.

In the case of magnetic quantum ring shown in Fig. 2, the qualitative aspects of low lying spectra is completely different from those of the magnetic quantum dot. In Fig. 2(a), it can be clearly seen that, for the impurity-free system, there are L ground state transitions in the sequence $(0,0)\rightarrow(0,-1)\rightarrow(0,-2)\rightarrow(0,-3)\rightarrow(0,-4)\cdots$ as the magnetic field increases, which is consistent with the results of Ref. 14. It can be explained physically by the following: For weak magnetic fields, the states with angular momenta $l<0$ is far away from the magnetic edge or the center of the ring, and the electron moves with an analogy to that in a uniform field, and the states therefore resemble the bulk Landau level. As the magnetic field increases, the field confinement brings the states much closer to the ring region, and the electron moves in the absence of a magnetic field, leading to deviation from the bulk Landau level. A further increase in the magnetic field brings the electron much closer or approaches the center of the ring, and the electron returns to move in a uniform magnetic field. In other words, the eigenenergy for each angular momentum state starts to deviate from the bulk Landau level and then approaches it, leading to the L ground state transitions. It is worth noting here that, in conventional electrostatically confined quantum dots, different from those of a single electron magnetic quantum ring, there are ground state transitions only for the cases of more than one electron[2] or

one electron with on-center acceptor impurity,[8] but no transitions for those systems with only one electron.

For the case of on-center acceptor impurity, shown in Fig. 2(b), the low spectra are in general the same as those of impurity-free cases, except for very weak magnetic fields. Similar to the case of the magnetic quantum dot (Fig. 1(b)), $(0,-5)$ becomes the ground state for very weak magnetic fields. Furthermore, apart from the argument for the impurity-free case, there is another reason to explain such L ground state transitions: As the magnetic field increases, the magnetic confinement strength brings the states close to the position near the on-center acceptor impurity and the electron in turn has to jump to the orbit with higher states in order to avoid the increase of electron-acceptor repulsion. Hence, all ground state transitions shift to lower magnetic fields, comparing with those of the impurity-free case. In Fig. 2(c), for an on-center donor impurity magnetic ring, owing to the electron-donor attraction, the electron with the (0,0) state tends to localize near the position of the on-center donor impurity to minimize its interaction energy, and (0,0) is therefore left as the ground state for the magnetic fields up to $a_B^2/a_c^2=8$. For the neighboring higher states, there are still L ground state transitions, in the sequence $(0,-1)\rightarrow(0,-2)\rightarrow(0,-3)\rightarrow(0,-4)\cdots$, with all transition points shifting to higher magnetic fields.

The magnetic moment can be defined by the derivative of the lowest ground state eigenenergy with respect to the magnetic field, $-\partial E_{\text{ground}}(1)/\partial B$ at the absolute zero of temperature.[22] In order to get the visible discontinuities or spikes at the corresponding orbital angular momentum L ground state transitions for the overall results of Figs. 1 and 2, the magnetic moments of the electron magnetic quantum dot and ring with and without impurity are plotted in Fig. 3, and clearly shows that there is ground state L transition at $a_B^2/a_c^2\approx 1.38$ for a magnetic quantum dot with acceptor impurity. In the case of a magnetic quantum ring, regardless of the presence of acceptor impurity, both have ground state L transitions and the transition points all shift slightly to lower magnetic fields for those with acceptor impurity.

In summary, the magnetic-field dependence of low-lying spectra of an electron magnetic quantum dot and ring are calculated by using numerical diagonalization. The present interesting numerical results motivate us to further study not only on the effect of off-center impurity both inside and outside the magnetic quantum dot or ring, but also on those systems of few electrons without neglecting both electron-electron and spin-spin interactions.

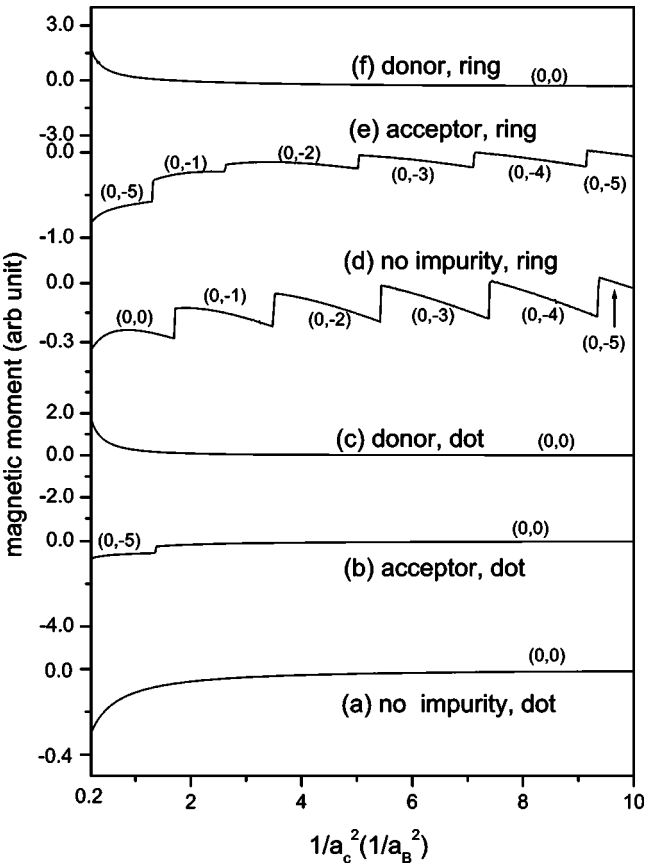

FIG. 3. Magnetic moments as a function of $1/a_c^2(\propto B)$. Note that, for a clear presentation, the magnetic moments for the curves are drawn in different scales.

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