Five- and six-electron quantum rings in a magnetic field

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(Received 7 January 2007; published 10 March 2008)

We study five and six electrons confined in a two-dimensional quantum ring (QR) by the exact diagonalization approach. An external magnetic field B perpendicular to the ring plane is considered. The energy spectra of low-lying states of the QR as a function of B are obtained. A phase diagram is presented indicating a rich variety of ground states, especially, revealing a ground-state transition in which the total spin changes while the total angular momentum remains the same. By plotting the density functions of the QR, the ground-state configuration is found to be a regular polygon (RP), while some excited states do not possess a RP.

DOI: 10.1103/PhysRevB.77.115311 PACS number(s): 73.21.Hb, 71.27.+a

Advances in nanofabrication technology allow a certain number of electrons to be confined in quantum rings (QRs).[1,2] QRs are currently under intense study because they exhibit rich physics.[3–11] Recently, the problem of few electrons in QRs has been widely considered.[2,10,12–16] Wendler *et al.* reported optical properties of two interacting electrons in QRs,[12] while Hu *et al.* obtained energy levels and far-infrared spectroscopy for a two-electron ring.[13] In 2003, Keyser *et al.* investigated Kondo effect in a QR with less than ten electrons,[2] and Ref. 10 gave fractional oscillations of the ground-state energy for a four-electron ring. Later, the energy spectra of three- and four-electron QRs were found.[14,15] In 2007, ground-state properties of QRs with a few electrons were studied.[16] It is recalled that the effect of the magnetic field on QRs has been studied.[17–21] However, the combined effect of the magnetic field and the QR size has not yet been clarified. We have summarized and visualized the effect on two- and three-electron QRs via phase diagrams.[22] As a continuation of Ref. 22, this paper is dedicated to study further five- and six-electron QRs in a magnetic field. By diagonalizing the Hamiltonian with the basis functions constructed by a set of single-electron states, the eigenenergies and eigenfunctions of the QRs are calculated, then the combined effect containing features is exhibited.

Let an N-electron planar QR be lain on the x-y plane. A magnetic field B is applied perpendicular to the plane. The Hamiltonian of the QR reads

$$H=\frac{\hbar^2}{2m^*R^2}\sum_{j=1}^{N}\left(-i\frac{\partial}{\partial\theta_j}+\Phi\right)^2+\sum_{J<j}^{N}V_{jJ}-g^*\mu_B B S_z, \quad (1)$$

where m^*, R, and θ_j stand for the effective mass of the electrons, the radius of the QR, and the azimuthal angle of the jth electron, respectively. $\Phi=(eBR^2)/2\hbar$. The last term is the Zeeman energy with g^* being the effective g factor, μ_B the Bohr magneton, and S_z the z component of the total spin S. The Coulomb electron-electron potential is adjusted as

$$V_{jJ}=\frac{e^2}{8\pi\varepsilon\sqrt{d^2+R^2\sin^2[(\theta_j-\theta_J)/2]}}, \quad (2)$$

where ε is the dielectric constant of the material, and d is a small parameter that eliminates the singularity at $\theta_j-\theta_J=0$. One can think that d gives the effect of finite thickness of the ring. In this paper $\varepsilon=12.4\varepsilon_0$ and $m^*=0.067m_e$ with m_e the bare mass of single electron are assumed (for a GaAs ring). The meV, nm, and T are used as the units of energy, length, and magnetic field, respectively. In what follows, $d=15$ nm is adopted. We find that the qualitative result is not sensitive to d. Nonetheless a larger d leads to a weaker e-e repulsion, and therefore a lower eigenenergy.

The Hamiltonian is diagonalized to obtain the eigenenergies by using the methods as outlined in Ref. 22. Figure 1 shows the evolution of energy levels of low-lying states as a function of B at $R=50$ for a five-electron QR, where L and S denote total angular momentum and spin, respectively. From the figure, several qualitative features can be found as follows. (1) For a given L state, the energy curve is parabola. This arises from the fact that H in Eq. (1) is a quadratic function of B. (2) The increase of B leads to the transitions of the ground state. (3) Due to these transitions, the energy of the ground state oscillates along a zigzag curve with increasing B. (4) The energy of the state with $L\neq 5k$ and $S=5/2$ is particularly high, where k is an integer. This feature will be explained later.

For other values of R, we obtain the analogous figures. As a result, a ground-state phase diagram can be generated. Let the ground state be labeled by two quantum numbers: total angular momentum L_0 and total spin S_0. The evolution of (L_0,S_0) of the five-electron QR in accordance with B and R is shown in Fig. 2.

We first investigate the ground-state transitions with increasing B for a fixed R. At $R=50$, e.g., L_0 increases in steps of 1 as B increases from 0.0 to 1.0. The increase of L_0 is mainly due to the term Φ (proportional to B) in the Hamiltonian. Equation (1) demonstrates clearly that the Zeeman term lowers the energy of $S_0\neq 0$ state. Since the energy re-

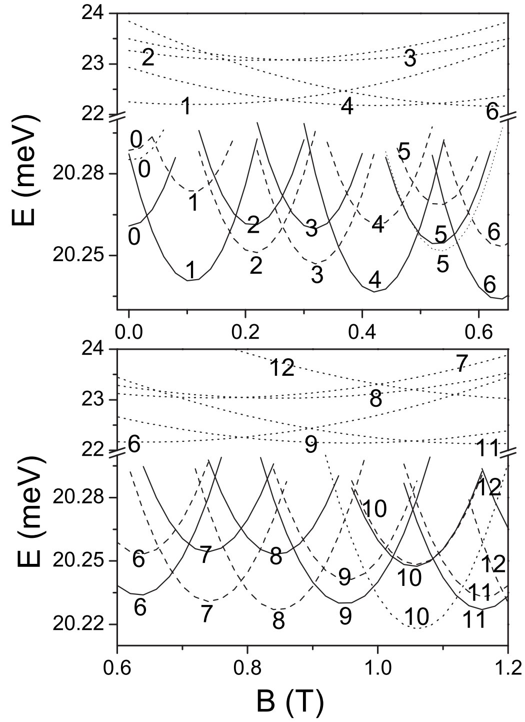

FIG. 1. The evolution of the low-lying levels of a five-electron QR with $R=50$ nm against B. The numbers inside the figure are L. $S=1/2$, $3/2$, and $5/2$ states are marked by solid, dash, and dot lines, respectively.

duction of the spin-polarized state is faster than that of the unpolarized state as B increases, the polarized state only survives at strong magnetic field. In the case of $N=5$ and $R=50$, when $B>1.196$, the unpolarized state ($S_0=1/2$) disappears (see Fig. 1). The partially polarized state ($S_0=3/2$) is squeezed out by the polarized state ($S_0=5/2$) at $B>11.342$

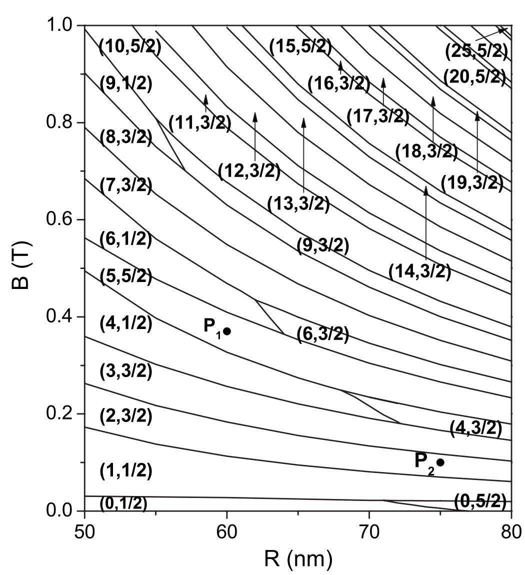

FIG. 2. The evolution of the ground state as a function of B and R for a five-electron QR. Angular momenta up to 25 are shown. The numbers inside the figure are (L_0,S_0) of each specified domain.

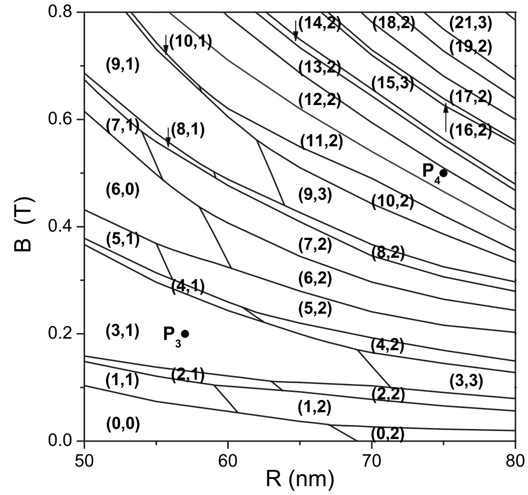

FIG. 3. Same as in Fig. 2, but for a six-electron QR.

(not yet plotted). At the same time, L_0 increases in steps of 5. Therefore, when B is sufficiently large, no spin transition occurs, and the ground state will be dominated by the polarized state. At a fixed B, the increase of R often leads to a bigger L_0. The reason for this is given in Ref. 22.

In Fig. 2 we observe a peculiar phase boundary between the states (L_0,S_0) and (L_0,S_0') which is not seen for two- and three-electron QRs.[22] Through the boundary S_0 switches from one spin state to another unaccompanied by an angular-momentum transition. E.g., the transitions $(0,1/2)-(0,5/2)$, $(4,1/2)-(4,3/2)$, and $(6,1/2)-(6,3/2)$. The $(L_0,S_0)-(L_0,S_0')$ transition line shows that the increase of B and/or R lead to the increase of S_0. If R is made large enough, the $S_0=1/2$ state disappears. For example, the $(0,5/2)$ state replaces the $(0,1/2)$ state when $R>76.5$. At $R=68-72.2$ the transition from the $(4,1/2)$ state to the $(4,3/2)$ state is triggered by increasing B. Incidentally, if $R>99.9$, the $(1,1/2)$ state will be replaced by the $(1,3/2)$ state (not shown in Fig. 2). This behavior is readily understood by considering the size effect of the QR and the Zeeman term in Eq. (1). For larger R the electrons in the ring are more spatially separated and their spin direction becomes as identical as possible. This point is crucial to assure that the ground state is the lowest. Therefore, S_0 increases in accord with the increase of R. According to the Zeeman contribution, it can be explained that S_0 increases as B increases. Obviously, a large radius cannot cause elimination of the $S_0=3/2$ state, whereas a strong magnetic field may get rid of the state.

The ground-state phase diagram of a six-electron QR, i.e., Fig. 3, has similar above-mentioned features. Some of them are stressed as follows. (1) At strong magnetic field, the ground state is dominated by the $S_0=3$ polarized state. (2) As R increases, the $S_0=2$ and 3 states replace the $S_0=0$ and 1 states.

It is worthy to mention that the transition of L_0 and S_0 is matched. In the case of $N=5$, $L_0=5k$ if $S_0=5/2$, and $L_0\neq 5k$ if $S_0=3/2$, where k is an integer. When $N=6$, $L_0=6k+3$ if $S_0=3$, and $L_0\neq 6k+3$ if $S_0=2$. The match can be explained by "magic number" theory.[23,24] According to this

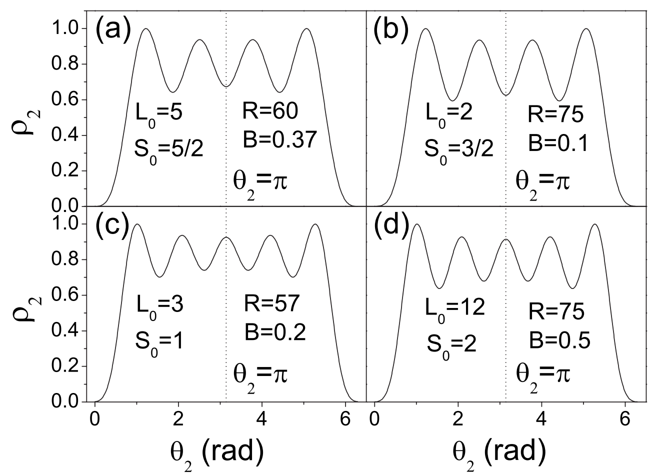

FIG. 4. The evolution of ρ_2 of the ground state in accord with θ_2. (a)–(d) correspond to the points P_1–P_4 in Figs. 2 and 3.

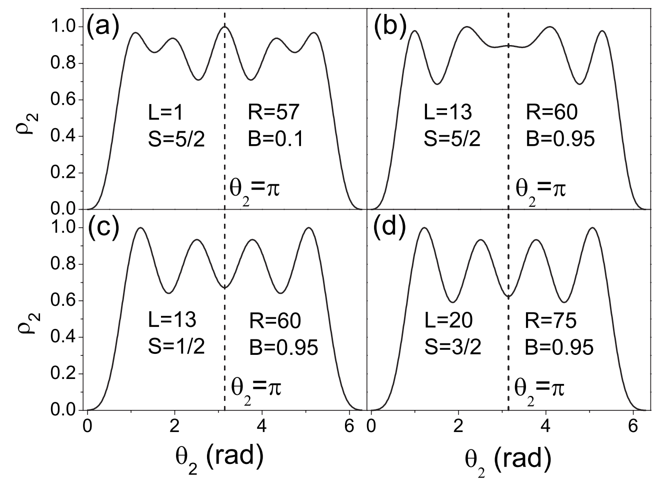

FIG. 5. Evolution of ρ_2 of the excited state against θ_2 for a five-electron QR.

theory, each regular polygon (RP) is accessible only to a specific group of states having specific L_0 and S_0. From dynamical consideration, if the N electrons in a QR form an N-side RP, the potential energy is minimized, thus the total energy is minimized. Such a match of L_0 and S_0 just assures that the ground state is RP accessible.[22–24] When the two cases $S_0=N/2$ and $S_0=N/2-1$ are considered, the allowed L_0 of the RP configuration are complementary,[24] they cover the whole range of L_0 as shown in Figs. 2 and 3. Therefore, there is a transition of spin state at fixed angular momentum for five- and six-electron QRs, while this transition does not occur in two- and three-electron QRs because they only have two spin states. Incidentally, a four-electron QR also has the transition.

The pursuit of the RP can be demonstrated via the density functions. Let us define the two-body density functions as

$$\rho_2(\theta_1,\theta_2) = \int |\Psi_0^2| d\theta_3 d\theta_4 \cdots d\theta_N, \tag{3}$$

satisfying

$$1 = \int \rho_2(\theta_1,\theta_2) d\theta_1 d\theta_2, \tag{4}$$

where Ψ_0 denotes the ground state of an N-electron QR. In what follows, the first electron e_1 is given at $\theta_1=0$ location, then ρ_2 as a function of θ_2 gives the distribution of the second electron e_2 and is plotted as a diagram. The electron correlation can be understood from the diagram, where the maximum of ρ_2 is associated with the most probable location of e_2.

Some examples of ρ_2 of the ground state are plotted in Fig. 4, where (a) and (b) correspond to the points P_1 to P_2 in Fig. 2. Each subfigure has four peaks which are at $\theta_2 = 2\pi/5$, $4\pi/5$, $6\pi/5$, and $8\pi/5$. This fact implies that, if e_1 is fixed at $\theta_1=0$, the four peaks are the most probable locations of e_2 to e_5 and form electronic configuration with e_1. Therefore, the ground-state configuration of a five-electron QR is a regular pentagon. In the case of a six-electron QR the ground state possesses a regular hexagon as shown in Figs. 4(c) and 4(d). The RP configuration can be understood as the formation of a Wigner crystal.

Incidentally, the configuration of the excited state might not be a RP. In Fig. 5 we plot the diagrams of ρ_2 of some excited states for a five-electron QR. One can notice that ρ_2 in Figs. 5(a) and 5(b) has four valleys and five peaks. Thus the wave functions of e_2–e_5 do not mainly distribute at the minimums of potential energy (i.e., $\theta_2=2\pi/5$, $4\pi/5$, $6\pi/5$, and $8\pi/5$). The fact implies that e_2–e_5 oscillate back and forth around the valleys as equilibrium points, which will cause a great increase in energy. This explains why the energy of the state with $L\neq 5k$ and $S=5/2$ is remarkably high. Figures 5(c) and 5(d) show that ρ_2 has four peaks. They together with e_1 form a regular pentagon. Therefore, the energy of the two excited states is lower. Other ρ_2 diagrams give the similar results. Consequently, the configuration of the excited state with $L\neq 5k$ and $S=5/2$ is not a RP, while other excited states possess a RP configuration.

In summary, a QR with five and six electrons subjected to an external magnetic field is studied. We obtain the energy spectra of low-lying states of the QR as a function of B for different R. As a result, the ground state can be determined, then the phase diagram, namely, the (L_0,S_0) diagram, can be generated. The diagram clearly shows how the ground-state properties in accord with B and R vary. Physical mechanism of the variation is clarified. Comparing with the phase diagram obtained in Ref. 22, we find a transition between the states (L_0,S_0) and (L_0,S_0') in which the total spin changes while the angular momentum remains the same. We have previously studied the case with $N=2$ and 3, all ground states were found to possess a RP configuration.[22] Here we see that the ground-state configuration of the five- and six-electron QRs is also a RP. Thus, we believe that the RP will exist in a wide range of N. Arising from the RP, L_0 and S_0 are matched with each other in a specific way when $S_0=N/2$ and $N/2-1$. Other S_0 will disappear if R and/or B are/is sufficiently large. Reference 22 did not investigate the excited state. In this paper, we find that some excited states (say, the state with $L\neq 5k$ and $S=5/2$ in the case of $N=5$) are not accessible to a RP configuration, which results in a remarkable increase of energy.

This work is supported by the National Natural Science Foundation of China under Grant Nos. 10747146 and 10674154, Natural Science Foundation of Hubei Province of China under Grant No. 2006ABA354, Natural Science Foundation of Guangdong Province of China under Grant Nos. 06300345 and 7007806, and the Foundation of the State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics of CAS under Grant No. T152615.

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