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Effect of electric field on the electronic spectrum and the persistent current of a quantum ring with two electrons*

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The effect of an electric field E on a narrow quantum ring that contains two electrons and is threaded by a magnetic flux B has been investigated. Localization of the electronic distribution and suppression of the Aharonov–Bohm oscillation (ABO) are found in the two-electron ring, which are similar to those found in a one-electron ring. However, the period of ABO in a two-electron ring is reduced by half compared with that in a one-electron ring. Furthermore, during the variation of B, the persistent current of the ground state may undergo a sudden change in sign. This change is associated with a singlet–triplet transition and has no counterpart in one-electron rings. For a given E, there exists a threshold of energy. When the energy of the excited state exceeds the threshold, the localization would disappear and the ABO would recover. The value of the threshold is proportional to the magnitude of E. Once the threshold is exceeded, the persistent current is much stronger than the current of the ground state at $E = 0$.

Keywords: quantum ring, electronic structure, effect of electric field

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The quantum rings as a member of artificial microsystems have unique features that can be characterized by the Aharonov–Bohm oscillation (ABO)[1] of the ground state energy and the persistent current. The ABO would occur when a variable magnetic field is perpendicularly applied to the plane of the ring. At present, quantum rings with radii of about 20 to 120 nm, containing only a few electrons, can be fabricated in laboratories,[2,3] and the ABO has already been experimentally observed.[4,5] Just as the quantum dots, quantum rings can potentially be used as elementary elements in micro-devices.[6] In addition to the magnetic field, one has suggested using an external adjustable electric field to control the physical properties of the quantum rings. For quantum rings containing a single electron, the effect of electric field on their physical properties has been reported in detail in Ref.[7]. In the present paper, we study quantum rings with two electrons and take the e–e correlations into consideration as a generalization of Ref.[7].

Let the ring with a radius R lie in the x-y plane. A magnetic field B is applied along the z-axis, and an electric field E is along the x-axis. The Hamiltonian reads

$$H = \sum_{i=1}^{2} \left[\frac{1}{2m^*} (P_i + \frac{e}{c} A_i)^2 + eEx_i \right] + V_{\rm ee} + H_{\rm Zeeman}, \tag{1}$$

where m^* is the effective mass and $V_{\rm ee}$ is the e–e interaction. $A = B(-y, x, 0)/2$ is the vector potential and $H_{\rm Zeeman} = g\mu_B B S_Z$ is the Zeeman energy, where S_Z is the z-component of the total spin S. The ring is assumed to be so narrow that one-dimensional approximation can be adopted. In this approximation, the expression (1) can be rewritten as

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$$H=\sum_{i=1}^{2}\left[\frac{\hbar^2}{2m^*R^2}\left(-\mathrm{i}\frac{\partial}{\partial\theta_i}+\frac{\Phi}{\Phi_0}\right)^2+eER\cos\theta_i\right]+\frac{e^2}{2\varepsilon\sqrt{d^2+R^2\sin^2(\theta_1-\theta_2)/2)}}+H_{\mathrm{Zeeman}}, \tag{2}$$

where the radial degrees of freedom have been omitted, θ_i is the azimuthal angle of the ith electron, $\Phi=\pi R^2B$ the magnetic flux, $\Phi_0=hc/e$ the fundamental flux quantum, ε the dielectric constant, and the parameter d is introduced in V_{ee} to account for the effect of finite thickness of the ring.[8]

To diagonalize the Hamiltonian, we introduce the spatial functions

$$\varphi_{K_1,K_2}=\frac{1}{2\pi}\mathrm{e}^{\mathrm{i}(K_1\theta_1+K_2\theta_2)}, \tag{3}$$

where k_1 and k_2 are integers to assure the periodicity. From $\varphi_{K_1K_2}$ we further introduce the basis functions

$$\phi_{K_1K_2}=(\varphi_{K_1K_2}+(-1)^S\varphi_{K_1K_2})/(\sqrt{2})^{(1+\delta_{K_1K_2})}. \tag{4}$$

From the expressions (2) to (4) the matrix elements of the Hamiltonian can be obtained, thereby the eigenenergies $\varepsilon_{S,j}$ and eigenstates $\Psi_{S,j}$ can be further obtained via a numerical procedure of diagonalization, where j denotes the jth state of the series having the same S (energies in ascending order). $\Psi_{S,j}$ appears as a linear combination of the basis functions $\phi_{K_1K_2}$. In general, the appearance of the electric field might cause a number of consequences. The electrons might be close to the negative x-axis, resulting in a lower energy. The conservation of the total orbital angular momentum L would be broken, and accordingly each eigenstate is a mixture of different partial waves. The well-known ABO may, therefore, be affected. To study these possible effects, we calculate the average orbital angular momentum $\bar{L}=\langle\Psi_{S,j}|L|\Psi_{S,j}\rangle$, the fluctuation $\Delta L=\langle\Psi_{S,j}|(L-\bar{L})^2|\Psi_{S,j}\rangle^{12}$, and the current

$$J=\frac{\hbar}{m^*R^2}\int_0^{2\pi}\mathrm{d}\theta_2\left[\Psi^*_{S,j}\left(-\mathrm{i}\frac{\partial}{\partial\theta_1}+\frac{\Phi}{\Phi_0}\right)\Psi_{S,j}+\mathrm{c.c.}\right]. \tag{5}$$

All of them can be extracted from $\Psi_{S,j}$. We will also plot the wavefunctions as a function of θ_1 and θ_2 in order to visualize the electronic structure.

The following values are used throughout the paper: $m^*=0.067m_{\mathrm{e}}$, $\varepsilon=12.4$ (for a GaAs ring), $R=40$ nm, and $d=0.05$R. The qualitative result is not very sensitive to the values of R and d. Nevertheless, a greater value of R or d would lead to a weaker e–e repulsion, and therefore lower eigenenergies. The units of meV, nm, and Tesla are adopted, E is in units of e^{-1} meV/nm.

Let us first review the case of $E=0$ that has already been studied previously.[8,9] As B increases, the ABOs in the ground state energy ε_{g} and in the persistent current are clearly seen as shown in Fig.1(a) from which two conclusions can be drawn. (1) The adjacent minima of ε_{g} are separated from each other by 0.41Tesla, which is associated with a period $\Phi_0/2$ of magnetic flux. The normal ABO for a one-electron ring has a period Φ_0. Since the period for a two-electron ring is only half of that for the one-electron ring, the oscillation is termed fractional ABO.[3,9] (2) The ground state is alternately dominated by $S=0$ and 1 states. Furthermore, once the singlet-triplet transition occurs, the L of the ground state would increase by one, and it would be even if $S=0$, or odd if $S=1$.

To explain the two observations above, let us first introduce $\theta_{\mathrm{c}}=(\theta_1+\theta_2)/2$ and $\theta=\theta_1-\theta_2$ to describe the collective and relative motions, respectively. When $E=0$, the Hamiltonian can be exactly divided into two parts, namely the collective and relative parts:

$$H=H_{\mathrm{coll}}+H_{\mathrm{rel}}, \tag{6}$$

whereas θ_{C} is contained only in H_{coll}, which reads

$$H_{\mathrm{coll}}=\frac{\hbar^2}{4m^*R^2}\left(-\mathrm{i}\frac{\partial}{\partial\theta_{\mathrm{C}}}+2\frac{\Phi}{\Phi_0}\right)^2. \tag{7}$$

The eigenwavefunctions of H_{coll} are just $\mathrm{e}^{\mathrm{i}L\theta_{\mathrm{C}}}$, and the eigenvalues of H_{coll} are proportional to $(L+2\Phi/\Phi_0)^2$. Thus a decrease in L would be compensated by an increase in B (or Φ) to keep the collective energy small. As B increases, the L of the ground state would decrease step by step, each step by one. This leads to the oscillation of the ground state energy, similar to that in the one-electron ring. However, a comparison of H_{coll} with the Hamiltonian of the one-electron ring shows that Φ_0 is replaced by $\Phi_0/2$. This explains the origin of the fractional ABO, as it arises simply from the collective motion.[9,10]

On the other hand, due to the e–e repulsion, a dumbbell shape for the electronic distribution (the

two electrons stay at the two ends of a diameter) is favourable for energy. However, for the dumbbell shape, a space inversion is equivalent to an interchange between particles. The former operation leads to the appearance of an additional factor $(-1)^L$ in the wavefunction, while the latter leads to $(-1)^S$. The states with $(-1)^L \neq (-1)^S$ would have zero wavefunctions at the dumbbell shape, and thus this shape is not accessible to these states. Consequently, the lower states always have even numbers of $L+S$. If the L of the ground state decreases by one each step, S has to be changed accordingly. This is the reason why $S=0$ and 1 states alternately appear in Fig.1(a). However, due to the Zeeman effect, $S=1$ states are increasingly benefited from an increase in B. Therefore, when B is sufficiently large, the ground state will be purely dominated by $S=1$ states, or purely polarized. In this case the ground state would have odd L only, and increasing B leads to decreasing L by two for each step. Thus the period of the ground state oscillation is changed to Φ_0 (refer to Eq.(7)) and the normal ABO recovers. Using the above parameters and with $E=0$, pure polarization would emerge if $B \geq 4.95$ (not shown in the figures).

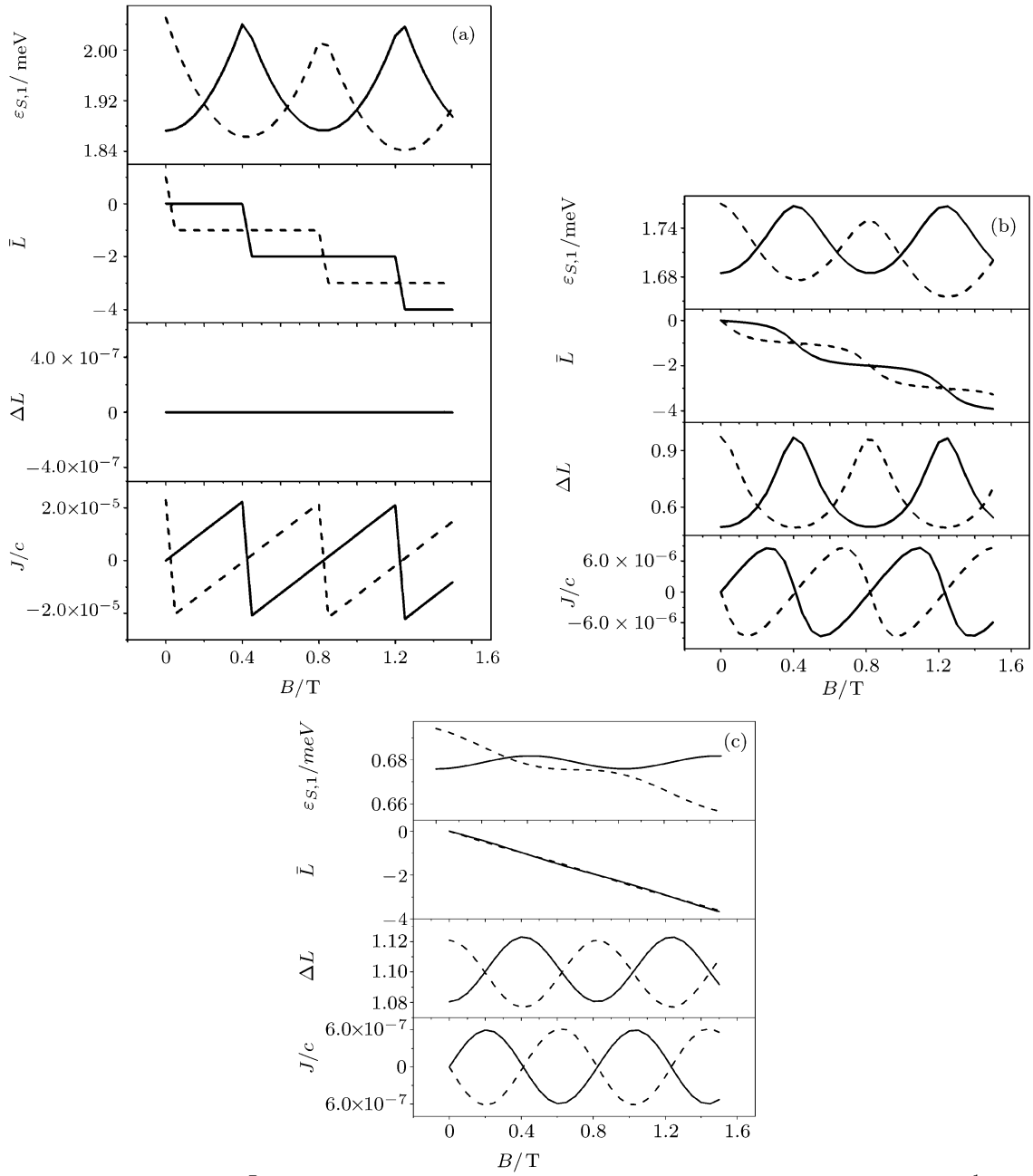


Fig.1. The evolutions of $\varepsilon_{S,1}, \bar{L}, \Delta L$ and J/c of Ψ_{01} and Ψ_{11} the states against B at $E=0$, 0.02, and 0.05 e^{-1}meV/nm, respectively, for (a) to (c). Solid (dash) lines are for the $S=0(S=1)$ state. $R=40$ nm, energy is in meV and B is in Tesla. J is in units of $c=C/R$ (where C is the speed of light in vacuum). These units are also used in the following.

When $E \neq 0$, it has been found in Ref.[7] that the electronic distribution would be more or less localized, i.e. close to the negative x-axis. This is believed to be true also for two-electron rings. Apart from the similarities between one- and two-electron rings, their differences have also been found due to the introduction of the e–e correlation. Comparing Fig.1(a) with Figs.1(b) and 1(c), we find the following points:

(1) An increase in E leads to a remarkable decrease in eigenenergy. This fact is further shown in Fig.2.

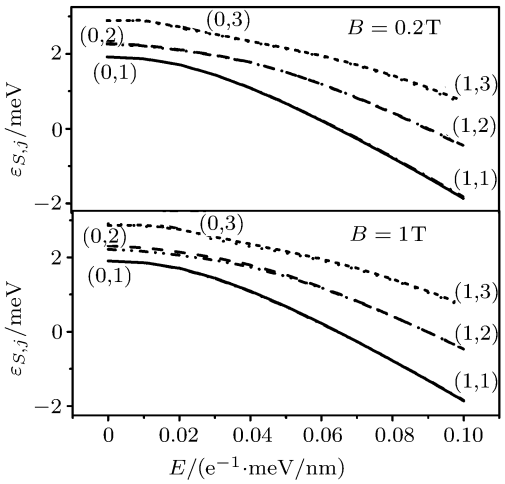


Fig.2. The low-lying spectra ($\varepsilon_{S,j}$) against E when B is fixed. The (S, j) labels are marked on the curves. The two curves having the same j nearly overlap.

(2) An increase in E leads to a reduction in the amplitude of the oscillation of the ground state energy. However, the period is not changed, as shown in Fig.1(b).

(3) An increase in E leads to the stronger mixing of partial waves (measured by the fluctuation ΔL) and leads to a smoother variation of $\bar{L}$ against B. When E is sufficiently large ($E \geq 0.05$), $\bar{L}$ of the ground state depends linearly on B as shown in Fig.1(c), where the slope of the straight line is independent of E. This implies that, while the magnitude of ΔL is determined by E, the magnitude of $\bar{L}$ is essentially determined by B.

(4) An increase in E leads to a great reduction in J. This fact is further illustrated in Fig.3. When $E > 0.08$, the lower states have nearly no persistent currents.

(5) When E is fixed ($\neq 0$) and B varies, the ground state would undergo transitions between the singlet and triplet states repeatedly as mentioned above. It is further found that the ground state is dominated by even (odd) L components if $S = 0$ (1) (e.g. when $E = 0.02$ and $B = 0.64$, the weight of even L component of the $\psi_{0,1}$ ($\psi_{1,1}$) state is 0.838 (0.169)). Thus the transition would cause a sudden change in composition of the partial waves. Consequently, this causes a sudden change in $\bar{L}$ as shown in Fig.1(b). In particular, we should emphasize that the persistent current undergoes a sudden change in sign (e.g. when $E = 0.02$ and B varies around 0.64, J/c would vary suddenly from about 7.5×10^{-6} to -6.5×10^{-6}).

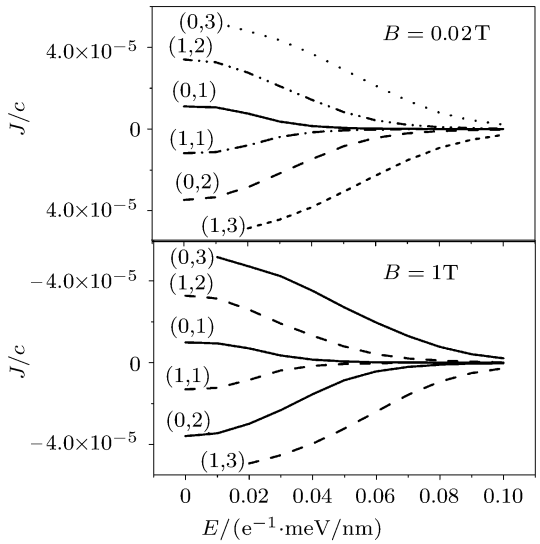


Fig.3. J/c of the $\Psi_{S,j}$ states against E when B is fixed. The (S, j) labels are marked on the curves.

The above points (1) to (4) are common for both one- and two-electron rings. However, point (5) holds only for two-electron rings, i.e. the sudden reversal of sign of J is related to the singlet-triplet transition and has no counterpart in one electron rings.

When E is sufficiently large, say $E \geq 0.08$, the fractional ABO would disappear from the low-lying spectrum due to the strong localization as shown in Fig.4 (this figure corresponds to Fig.2 in Ref.[7]).

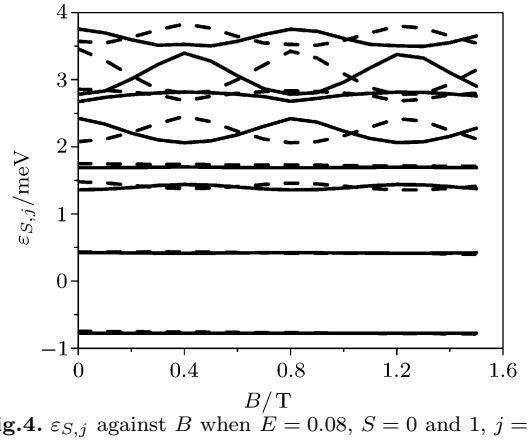


Fig.4. $\varepsilon_{S,j}$ against B when $E = 0.08$, $S = 0$ and 1, $j = 1$ to 8. For $j \leq 2$, solid ($S = 0$) and dash ($S = 1$) lines nearly overlap.

However, all higher states can be freed from the localization, because their electrons have sufficient energy

to overcome the binding from the electric field. Thus the fractional ABO, including the oscillations in $\varepsilon_{S,j}$ and J, recovers in higher states. Taking $E = 0.08$ for example, the oscillations in $\varepsilon_{S,j}$ and J would suddenly appear if $j = 5$ as shown in Figs.4 and 5. In order to visualize directly the electronic structures, $|\Psi_{0,j}|^2$ is plotted in Fig.6. Although $\Psi_{1,j}$ and $\Psi_{0,j}$ may have different compositions of partial waves, their norms are found to be qualitatively similar. When E is small, the localization is not strong as shown in the upper part in Fig.6.

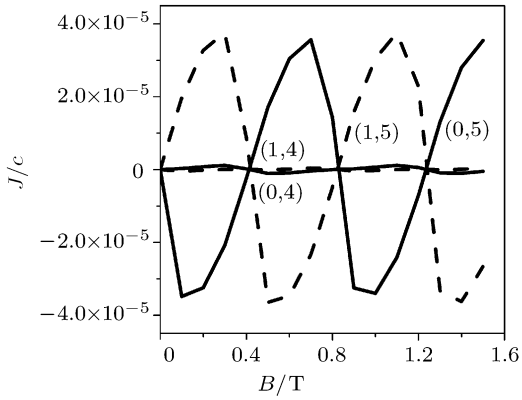


Fig.5. Persistent current J/c of higher states in the vicinity of the threshold against B when $E = 0.08$. The (S, j) labels are marked on the curves.

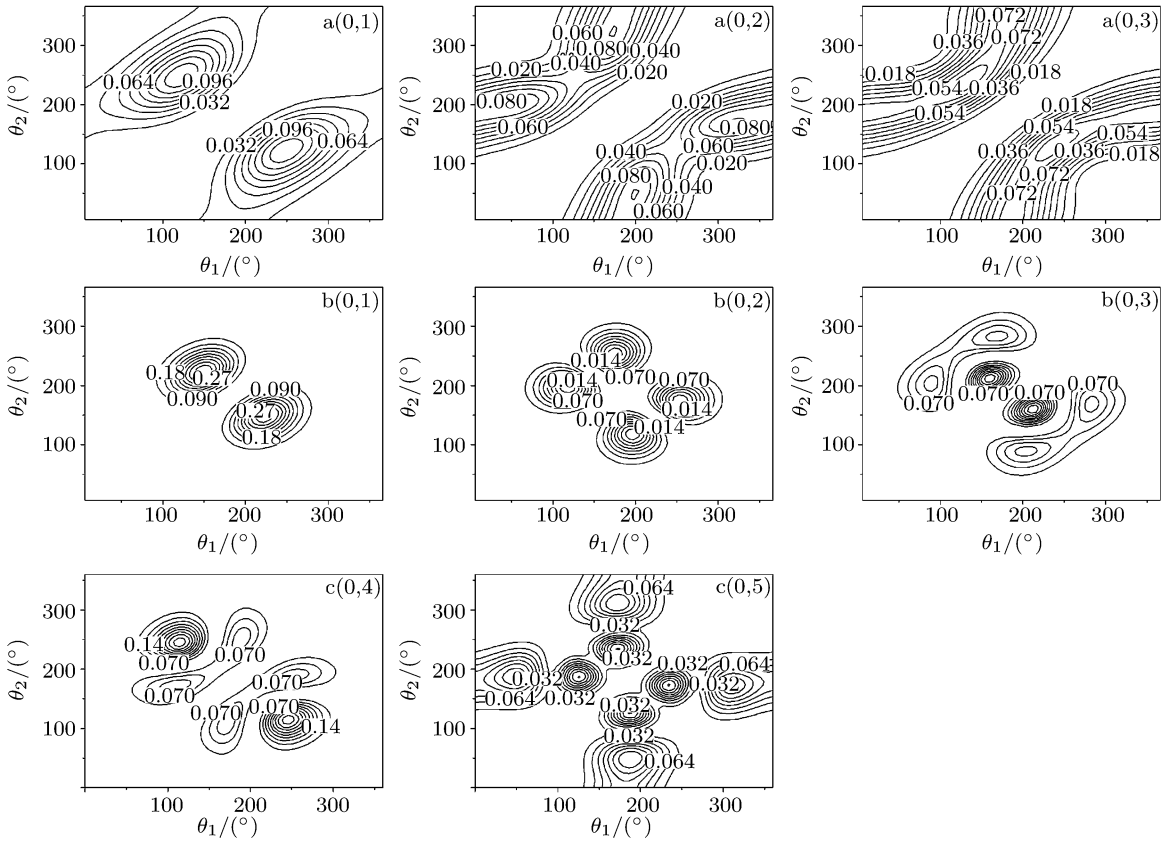


Fig.6. $|\Psi_{0,1}|$ as a function of θ_1 and θ_2. $B = 1$, $E = 0.02$ (upper), 0.1 (middle), and 0.08(lower). The labels (S, j) are marked in the corners.

For the $\Psi_{0,j}$ state, the norm is peaked at $\theta_1 = 117^0$ and $\theta_2 = 243^0$ (or reversely), $|\theta_2 - \theta_1| = 126^0$. If the electric field is removed, the electrons would prefer to be distributed in the dumbbell shape, i.e. $|\theta_2 - \theta_1| = 180^0$. If the e–e repulsion is removed, the electrons would prefer to lie on the negative x-axis, i.e. $|\theta_2 - \theta_1| = 180^0$. Thus the present configuration reflects a competition between the e–e repulsion and the attraction from the electric field. As a result, the electrons deviate from the dumbbell shape and are slightly close to the negative x-axis. For the two higher states ($j = 2$ and 3), the distribution becomes more extensive and the localization becomes weaker. When E is large as shown in the middle part of the figure, the localization is strong. The norm of the $\Psi_{0,1}$ state is now sharply peaked at $\theta_1 = 140^0$ and $\theta_2 = 220^0$ (or reversely), and is very close to the negative x-axis. For the two higher states ($j = 2$ and 3), the previous peaks become nodes, and internal oscillations have been excited back and forth around the

nodes as shown in the figures. When $E = 0.08$, $j \leq 4$ and $j \geq 5$ states have completely different structures, in that the former are localized while the latter have their wavefunctions spreading out along the ring. A great distinction between $j = 4$ and 5 states is shown in the lower part of Fig.6, while a great difference in J is shown in Fig.5. Incidentally, while the lower states have a negligible current, the higher states may suddenly have a strong current, e.g. the amplitudes of J of $j = 5$ states at $E = 0.08$ are nearly twice as large as those of the ground states at $E = 0$.

In summary, the effect of an electric field E on a two-electron ring has been investigated. It is found that the one- and two-electron rings are similarly affected by the field. For example, the field would lower the eigenenergies and mix different partial waves. It would also cause severe localization and thus spoil the ABO, i.e. the amplitudes of oscillation of energy and persistent current would be suppressed. The similarity results from the fact that the e–e repulsion affects mainly the relative motion while the ABO is mainly determined by the centre-of-mass motion (see Eqs.(7)). Nonetheless, an increase in particle number would change the period and cause a fractional ABO. Furthermore, the introduction of the e–e correlation causes the pursuit of favourable geometric configurations (e.g. a dumbbell shape for two-electron rings). These configurations are in general constrained by quantum mechanical symmetry, and the constraint depends on L and S as explained above. Consequently, an increase in B leads to a transition of S, and accordingly the persistent current of the ground state would change its sign abruptly. In contrast, when $E \neq 0$, the variation in J of one-electron rings is always continuous, and this kind of sudden reversal does not appear. It is noted that there exists a threshold of energy, associated with a given E. Above this threshold (e.g. above 1.8 meV in Fig.4), E has a negligible effect, and the persistent current suddenly becomes very strong. This finding is of particular importance when an electric field is used to control the behaviour of the ring as a micro-device.

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