Nonadiabatic Geometric Phase and Induced Persistent Current in Mesoscopic Square Circuit with Tilted Magnetic Field at Edges *

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We investigate the geometric phase produced by nonadiabatic transition of spin states at corners of mesoscopic square circuit with tilted magnetic field at its edges. From the Schrödinger equation, the transitions of electron spin state at corners are described by the transfer matrices. The eigenenergies and eigenstates are obtained from the cyclic condition and the multiplying of the transfer matrices. We show that there exist persistent charge and spin currents in such a system due to the lift of degeneracy between the opposite moving directions in the presence of the tilted magnetic field. The dependences of eigenenergies, geometric phase, charge and spin persistent currents on the tilting angles of magnetic field are analysed.

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Since the pioneering work of Berry,[1] the Berry phase and its effects have been a subject of numerous investigations in condensed matter physics. A Berry phase may be acquired by a wavefunction when the parameters of its Hamiltonian perform an adiabatic circular change. When the change of parameters is nonadiabatic, the adiabatic approximation for the evolution of wavefunctions cannot be applied, but a more general phase, called the geometric phase, can still be created during the circular change of parameters. As this geometrical phase emerges from the very basic laws of quantum mechanics, it has important implications for a broad range of physical phenomena.[2] A particle with spin 1/2 follows adiabatically a magnetic field whose direction varies in time is the simplest example of the Berry phase.[3] When the magnetic field returns to its initial direction, the spin wavefunction of the particle acquires an additional phase. Berry phase also results from the Rashba spin–orbit coupling effect[4] in a similar way as produced by an inhomogeneous field. Influences of the Berry phase or geometric phase on the magnetoconductance,[5−9] on the universal conductance fluctuations,[5,6] and on the persistent currents[10−12] are examples of its measurable effects.[13,14]

Besides the adiabatic processes considered in original investigations of the Berry phase, the nonadiabatic transition of levels and related geometric phase become another central problem of recent studies. In this aspect the nonadiabatic level crossing in two-level Landau–Zener model has been extensively investigated.[15−18] In the Landau–Zener model the adiabaticity of the transition is controlled by the adiabatic parameter δ which describes the velocity of the transition. It has been found that the acquired geometric phases in the adiabatic and nonadiabatic level crossings are different. In this Letter we investigate the nonadiabatic geometric phase in another model: the transition of spin states at corners of mesoscopic square circuit with tilted magnetic field at its edges. As described in Fig. 1, the field is only applied at edges. In an edge, the field is uniform and perpendicular to it. The tilting angles of the field with respect to the normal direction of the circuit are the same for all edges and denoted as θ, a parameter determining the transitions at corners. We assume that the corners are sharp so that the transitions of electron spins through corners are nonadiabatic. By using the Schrödinger equation, the transitions are described by the transfer matrices. From the obtained eigenenergies and eigenstates we calculate the nonadiabatic geometric phase and show that there exist persistent charge and spin currents in such a system although there is no flux through the circuit. From the variation of the geometric phase and the resultant charge and spin current in increasing the tilting angle θ, we can analyse the change from the adiabatic case to the nonadiabatic case.

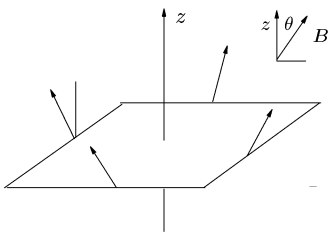

Fig. 1. A mesoscopic square circuit in the presence of magnetic field applied at edges with tilting angle θ with respect to the normal of the square.

We consider a one-dimensional square circuit with edges of length L. The square lies in the x–y plane, and its centre is in the origin. An effective magnetic field, which may be produced by internal magnetic moments of the circuit, is applied perpendicularly on every edge with tilting angle θ to the z axis as shown in Fig. 1. The strength of the field is the same in all the edges. The circuit is assumed to be metallic. We

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investigate the motion of non-interacting electrons. There is not magnetic flux through the loop.

The electron Hamiltonian is written as

$$H = \frac{p^2}{2m} - g\mu_B \boldsymbol{B}\cdot\boldsymbol{\sigma}, \tag{1}$$

where p is the momentum, m is the mass of electron, g is the gyromagnetic ratio, μ_B is the Bohr magneton, $\boldsymbol{B}$ is the magnetic field, and $\boldsymbol{\sigma}$ is the Pauli matrix for electron spin. By choosing the spin reference axis in the z direction, two spin states of electron in the ith edge ($i = 1, 2, 3, 4$ in the counterclockwise order), with spin parallel and antiparallel to the magnetic field there, can be expressed as two spinors,

$$|\uparrow\rangle_i = \begin{pmatrix} \cos\dfrac{\theta}{2} \\ -e^{-\mathrm{i}\varphi_i}\sin\dfrac{\theta}{2} \end{pmatrix}, \quad |\downarrow\rangle_i = \begin{pmatrix} e^{\mathrm{i}\varphi_i}\sin\dfrac{\theta}{2} \\ \cos\dfrac{\theta}{2} \end{pmatrix}, \tag{2}$$

where $\varphi_i = \dfrac{2(i-1)\pi}{M}$ is the azimuth angle of the field in the ith edge by choosing the in-plane component of the field in the first edge along the x direction. Together with the orbital part, an eigenstate of the electron, labelled by index l, can be expressed by the following linear combination:

$$\Psi_l(r) = A_{li}e^{\mathrm{i}k_l^+ r}\,|\uparrow\rangle_i + B_{li}e^{\mathrm{i}k_l^- r}\,|\downarrow\rangle_i + C_{li}e^{-\mathrm{i}k_l^+ r}\,|\uparrow\rangle_i + D_{li}e^{-\mathrm{i}k_l^- r}\,|\downarrow\rangle_i, \quad \text{for} \quad r \in i\text{th edge}, \tag{3}$$

where r is the linear coordinate along the square loop; A_{li}, B_{li}, C_{li}, and D_{li} are coefficients of wavefunction in the ith edge; and $k_l^\pm$ represents the wave vectors satisfying $\dfrac{(\hbar k_l^\pm)^2}{2m} = E_l \pm g\mu_B B$ with E_l being the corresponding eigen energy.

For an eigenstate there are 16 unknown coefficients. At the same time we can set up a 4×4 transfer matrix at every corner which connects the 8 coefficients in the two adjacent edges by using the continuity conditions for 2 spin components of the wavefunction and their corresponding currents:

$$\begin{pmatrix} A_{l,i+1} \\ B_{l,i+1} \\ C_{l,i+1} \\ D_{l,i+1} \end{pmatrix} = [T_{l,i+1}(r_{i+1}^{(S)})]^{-1} T_{l,i}(r_i^{(E)}) \begin{pmatrix} A_{l,i} \\ B_{l,i} \\ C_{l,i} \\ D_{l,i} \end{pmatrix}, \tag{4}$$

where $r_i^{(S)} = (i-1)L$ and $r_i^{(E)} = iL$ are the starting and ending linear coordinates of the ith edge, and

$$T_{l,i}(r) = \begin{pmatrix} e^{\mathrm{i}k_l^+ r}\cos\dfrac{\theta}{2} & -e^{\mathrm{i}(k_l^- r-\varphi_i)}\sin\dfrac{\theta}{2} & e^{-\mathrm{i}k_l^+ r}\cos\dfrac{\theta}{2} & -e^{\mathrm{i}(-\varphi_i-k_l^- r)}\sin\dfrac{\theta}{2} \\ e^{\mathrm{i}(k_l^+ r+\varphi_i)}\sin\dfrac{\theta}{2} & e^{\mathrm{i}k_l^- r}\cos\dfrac{\theta}{2} & e^{\mathrm{i}(\varphi_i-k_l^+ r)}\sin\dfrac{\theta}{2} & e^{-\mathrm{i}k_l^- r}\cos\dfrac{\theta}{2} \\ k_l^+ e^{\mathrm{i}k_l^+ r}\cos\dfrac{\theta}{2} & -k_l^- e^{\mathrm{i}(k_l^- r-\varphi_i)}\sin\dfrac{\theta}{2} & -k_l^+ e^{-\mathrm{i}k_l^+ r}\cos\dfrac{\theta}{2} & k_l^- e^{\mathrm{i}(-\varphi_i-k_l^- r)}\sin\dfrac{\theta}{2} \\ k_l^+ e^{\mathrm{i}(k_l^+ r+\varphi_i)}\sin\dfrac{\theta}{2} & k_l^- e^{\mathrm{i}k_l^- r}\cos\dfrac{\theta}{2} & -k_l^+ e^{\mathrm{i}(\varphi_i-k_l^+ r)}\sin\dfrac{\theta}{2} & -k_l^- e^{-\mathrm{i}k_l^- r}\cos\dfrac{\theta}{2} \end{pmatrix}. \tag{5}$$

From the cyclic condition at the beginning corner, one has

$$\begin{pmatrix} A_{l,1} \\ B_{l,1} \\ C_{l,1} \\ D_{l,1} \end{pmatrix} = \prod_{i=1}^{M} \left\{ [T_{l,i+1}(r_{i+1}^{(S)})]^{-1} T_{l,i}(r_i^{(E)}) \right\} \begin{pmatrix} A_{l,1} \\ B_{l,1} \\ C_{l,1} \\ D_{l,1} \end{pmatrix}, \tag{6}$$

where $T_{l,M+1}(r_{M+1}^{(S)}) \equiv T_{l,1}(r_1^{(S)})$. This is a complete set of linear homogeneous equations for 4 unknowns $A_{l,1}$, $B_{l,1}$, $C_{l,1}$, and $D_{l,1}$. From the condition of existence of non-zero solutions we can solve the eigen energies E_l from the following equation:

$$\det\left(\prod_{i=1}^{M} \left\{ [T_{l,i+1}(r_{i+1}^{(S)})]^{-1} T_{l,i}(r_i^{(E)}) \right\} - \hat{1} \right) = 0, \tag{7}$$

where $\hat{1}$ is 4×4 unit matrix. After obtaining the eigen energies, the corresponding wavefunctions can be calculated from the linear equations for the coefficients and the normalization.

To reduce the number of parameters we adopt the same tilting angle θ for all edges and the magnetic field at an edge is perpendicular to it. Thus we have $\varphi_i = \dfrac{(i-1)\pi}{2}$. The calculated lowest 8 eigen energies E_l, $l = 1, 2, \ldots, 8$ as functions of θ are shown in Fig. 2. They can be divided into two groups: group 1 with E_l, $l = 1, \ldots, 4$ and group 2 with E_l, $l = 5, \ldots, 8$, separated by an energy $\sim 2.8\,\mathrm{meV}$, corresponding to the energy discretization due to the quantum size effect. Within every group, the 4 levels represent 2 spins and two moving directions (clockwise and counterclockwise motions around the ring). At $\theta = 0$ or π, the magnetic field is perpendicular to the plane at four edges and the two directions for the motion are symmetric. In this case the energies for two spins are separated by the Zeeman energy of about $0.1\,\mathrm{meV}$, and the energies for two moving directions are degenerate. This is reflected by the coincidences of solid with dashed lines and dotted with dot-dashed lines at $\theta = 0$ or $\theta = \pi$ in both the panels. By increasing θ from 0 or decreasing θ from π, the angle of the magnetic field is tilting from the normal direction. This leads to the mixing of two spins at the corners. As a result the level spacings due to the Zeeman energy are decreased towards zero and the degeneracy of two moving directions is lifted due to the different orders of azimuth angles for them. Near $\theta = \pi/2$, the mixture of two spins reaches the maximum and the 4 levels in

a group become nearly degenerate. The detailed patterns of the degeneracy for groups 1 and 2 are different. For group 1, the degeneracy appears at $\theta = \pi/2$ and $\theta = \pi/2 \pm \delta$ with $\delta \sim 0.015\pi$, and there is no energy gap. For group 2, the degeneracy occurs only at $\theta = \pi/2$, and there is a gap of about 0.001 meV between two degenerate levels. The appearance of a gap in group 2 implies stronger effect of the order of the azimuth angles which produce additional phases. As we will see in the following, this effect can lead to larger geometric phase and larger persistent current in higher levels. The inhomogeneous magnetic fields at 4 edges may be regarded as effective fields produced by local moments in the mesoscopic loop. The result implies that the electron states moving in this loop can be changed by the inconsistence of directions of these moments.

When an electron is travelling around the ring, its spin undergoes the action of the magnetic field with varying tilting angles. This situation is similar to a localized spin in magnetic field with its direction moving around a circle. Now the argument which determines the tilting angle of the magnetic field is the spatial coordinate r around the ring, rather than time t in the case of localized spin. For a given r the electron situates in a straight edge with a magnetic field in a given direction. In the adiabatic approximation the wavefunction of the electron at this point is an eigenfunction of the Hamiltonian with the given magnetic field and can be written as $\Phi(r) = |\uparrow\rangle_i$ or $\Phi(r) = |\downarrow\rangle_i$, with i being the index of the edge where r is located. From such 'local' eigenfunctions one can reconstruct the r dependent wavefunction as

$$\overline{\Psi}(r) = e^{\mathrm{i}\int_0^r k_{r'}dr'} e^{\mathrm{i}\gamma_r}\Phi(r), \tag{8}$$

where the phase in the first exponent is the so-called dynamical phase and the phase γ_r is the adiabatic geometric phase called Berry phase; γ_r is determined by the requirement that $\overline{\Psi}(r)$ should satisfy the whole Schrödinger equation. Since in a circle of the motion the magnetic field felt by the electron performs a cyclic tilting, the Berry phase in this circle should be $\gamma_B = \pi$ in accord with the Berry theorem. The motion of electron, however, is not adiabatic at the corners, and the non-adiabatic treatment leads to the Aharonov–Anandan (AA) phase γ_A given by[19]

$$\gamma_A = \gamma_0 - \gamma_D, \tag{9}$$

where γ_0 is the total phase acquired by wavefunction $\Psi_l(r)$ during a cyclic motion, and γ_D is the dynamical phase. From the cyclic condition in solving $\Psi_l(r)$, we have $\gamma_0 = 0$. In this case the momentum is no longer a good quantum number, the dynamical phase is calculated by

$$\gamma_D^{(l)} = -\mathrm{i}\int \langle\Psi_l(r)\Big|\frac{\partial}{\partial r}\Big|\Psi_l(r)\rangle, \tag{10}$$

and the AA phase is $\gamma_A^{(l)} = -\gamma_D^{(l)}$. Here we use the eigen states to calculate the AA phase, so it is dependent on the index l of the states. In Fig. 3 we plot the AA phase as a function of the tilting angle θ for the lowest 8 levels. It can be seen that the AA phase is zero for the first 4 states ($l = 1, \ldots, 4$) and becomes nonzero for $l = 5, \ldots, 8$. The origin of different AA phases for these two groups is due to the different structures of degenerate points of levels shown in Fig. 2: For group of levels $l = 1, \ldots, 4$, the degeneracy occurs between any two levels near $\theta = \pi/2$, while for the group of levels $l = 5, \ldots, 8$, the degeneracy occurs only between levels $l = 5, 6$ and between levels $l = 7, 8$ at $\theta = \pi/2$. The latter corresponds to the diabolic point with two degenerate levels, while the former does not. We can also see that the AA phase for group of $l = 5, \ldots, 8$ has absolute value $\sim 1.4\pi$ greater than that of the adiabatic Berry phase, implying a certainly large modification due to the non-adiabatic behaviour at the corners.

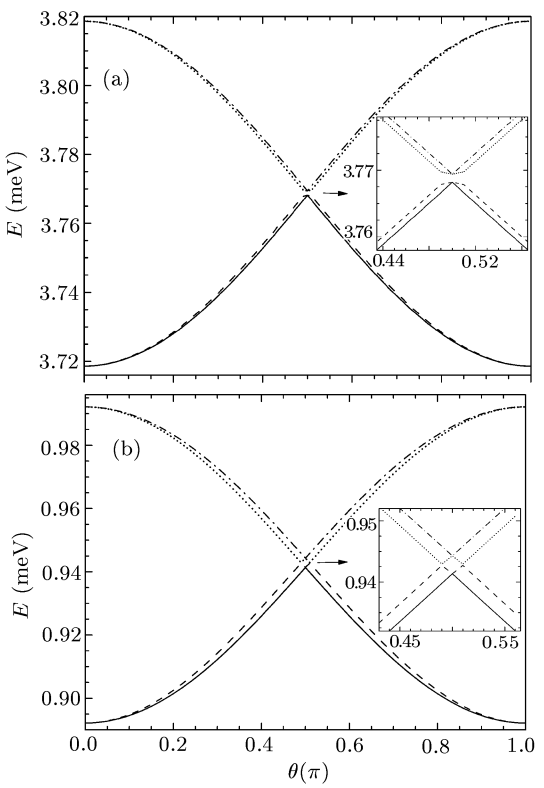

Fig. 2. Eigen energies $E_l (l = 1, \ldots, 4)$ (lower panel) and E_l $(l = 5, \ldots, 8)$ (upper panel) as functions of the tilting angle of magnetic field in 4 edges of the square ring. The length of square edges is $L = 10$ nm, and the strength of the magnetic fields at edges is $B = 1$ Tesla.

Owing to the removal of the degeneracy between two momentum directions, the persistent charge and spin currents may appear if the number of electrons is odd. When an electron is in state Ψ_l, its charge current can be calculated from the expectation value of the current operator:

$$I_e^{(l)} = \frac{\mathrm{i}e\hbar}{2m}\Big(\frac{\partial\Psi_l^\dagger(r)}{\partial r}\Psi_l(r) - \Psi_l^\dagger(r)\frac{\partial\Psi_l(r)}{\partial r}\Big). \tag{11}$$

The conventional definition of the spin current density

is

$$I_s^{(l)} = \mathrm{Re}\,\Psi_l^\dagger(r)\frac{1}{2}\{\hat{v},\hat{s}_z\}\Psi_l(r), \qquad (12)$$

where $\hat{v}$ is the velocity operator, $\hat{s}_z$ is the spin operator, and $\{\hat{v},\hat{s}_z\}$ denotes the anticommutator. This definition, however, can not meet the requirement of spin conservation. A new definition of the spin current is given by[20]

$$I_s^{(l)} = \Psi_l^\dagger(r)\frac{d(\boldsymbol{r}\hat{s}_z)}{dt}\Psi_l(r), \qquad (13)$$

where $\boldsymbol{r}$ is the position vector from an origin of the coordinates. Here we use Eq. (13) to calculate the spin current.

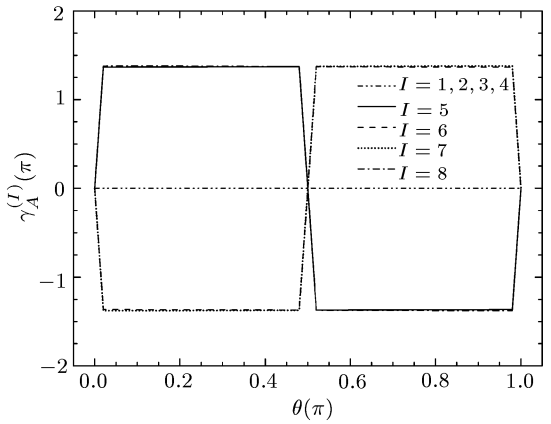

Fig. 3. The AA phase as a function of tilting angle θ of the magnetic field for the lowest 8 levels. Other parameters are the same as those in Fig. 2.

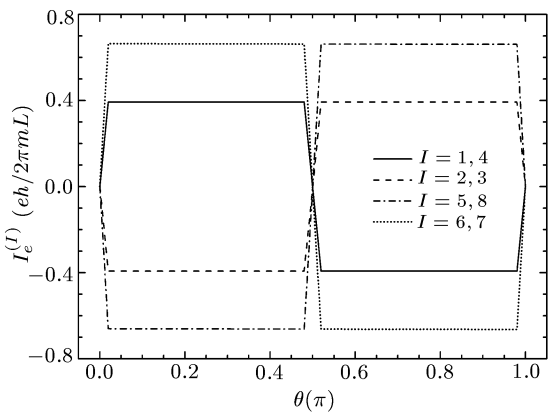

Fig. 4. Charge currents of the lowest 8 states as functions of θ. Other parameters are the same as those of Fig. 2.

In Fig. 4 we show the charge currents of the lowest 8 states as functions of the tilting angle θ of the magnetic field. It can be seen that the current vanishes at $\theta = 0$ and $\theta = \pi/2$, corresponding to the degeneracy of levels at these points. The odd and even levels have almost opposite currents, so the current happens only in the case of odd occupation. The spin current is shown in Fig. 5. Differently from the charge current shown in Fig. 4 which is almost unchanged in the ranges $0 < \theta < \pi/2$ and $\pi/2 < \theta < \pi$, the spin current is varying in changing θ from 0 to π. This implies that the spin current originates from the current of polarized particles whose polarization depends on the direction of the magnetic field.

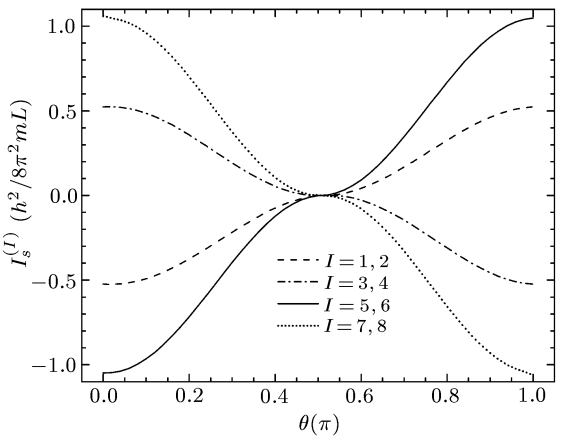

Fig. 5. Spin currents of the lowest 8 states as functions of θ. Other parameters are the same as those of Fig. 2.

In summary, we have investigated the geometric phase of electrons acquired in a cyclic motion around a square loop in which the magnetic field is applied on its edges with different tilting directions. The nonadiabatic transition of spin states at the corners of the square requires with tilted magnetic field at its edges. From the Schrödinger equation, and the transfer-matrix technique, we obtain the eigenenergies and eigenstates from the cyclic condition. We show that the geometric phase of the cyclic motion is much different from that of the adiabatic case. There exist persistent charge and spin currents in such a system due to the lift of degeneracy between the opposite moving directions.

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