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Berry phase and its induced charge and spin currents in a ring of a double-exchange system

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A ring of double-exchange system is investigated to explore the Berry phase acquired by the interplay of localized and conduction electrons. The competition between the double-exchange ferromagnetism and the superexchange antiferromagnetic coupling from the localized electrons leads to a phase transition from a ferromagnetic state to a spin spiral state. The spin spiral state acquires a nonzero Berry phase along the ring, and induces both charge and spin currents simultaneously. It is predicted that both the Aharonov-Bohm effect and Aharonov-Casher effect will be exhibited spontaneously in the system. [S0163-1829(99)01442-3]

Doped manganite perovskite, such as $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$, was the first metallic ferromagnetic oxide extensively studied in the 1950s and has renewed recent research interests since the discovery of colossal magnetoresistance (CMR) effect. In the system, usually called double-exchange system, conduction electrons move in the background of the spin configuration of localized electrons. Strong Hund's rule coupling between the conduction and localized electrons in the same Mn ion forces the electrons to form high spin states, and makes the conduction electrons more mobile between the pairs of sites where the two localized spins align to parallel.^{1,2} The hopping term t_{ij} between the two sites is determined by the two-spin configuration:

$$t_{ij} = -t \left(\cos \frac{\theta_i}{2} \cos \frac{\theta_j}{2} + \sin \frac{\theta_i}{2} \sin \frac{\theta_j}{2} e^{-i(\phi_i - \phi_j)} \right), \quad (1)$$

where the localized spins are parametrized by polar angles θ_i and ϕ_i . It is noted that the Berry phase is acquired when $\phi_i \neq \phi_j$.³ A lot of theoretical efforts are made on the mechanism of ferromagnetism and anomalous transport properties of the systems. However, a profound understanding of this phase is highly desirable.^{4,5} Since the Berry phase comes from the strong interplay of electrons, it is anticipated that it will play an important role in the double-exchange system, especially when the route of the electron motion is closed.

Accumulation of the quantum phase in multiconnected geometry produces a quantum interference effect via the Aharonov-Bohm (AB) and/or Aharonov-Casher (AC) effect.^{3,6,7} Persistent currents in connection with AB, AC, and Berry phases in one-dimensional rings have been studied extensively.⁸⁻¹⁵ In particular, the AC effect, which is induced by the conventional spin orbit (SO) in the presence of disorder¹¹ or external electric field,¹² on persistent currents in mesoscopic rings were elucidated. Besides, it was found that Zeeman interaction between the electron spin and the texture couples spin and orbital motion in textured mesoscopic rings, and results in a Berry phase; as a consequence, the system supports persistent charge and spin currents.¹³ To explore the physical consequences of the Berry phase in Eq. (1), we here consider a ring of double-exchange system. Starting from a Kondo-like Hamiltonian, we derive an effective Hamiltonian by utilizing the projection technique. We investigate the AB and AC effects and find that persistent spin and charge cur-

rents can be induced spontaneously in the spin spiral state, in which the nontrivial geometric phase is accumulated. We expect that the contemporary nanotechnology makes it possible to observe this quantum phase effect experimentally.

Consider a clean ring of double-exchange system consisting of N sites and N_e electrons in the absence of external electromagnetic field. The momentum of an electron in the ring is

$$\mathbf{P} + e\mathbf{A}/c + \mu\hat{\boldsymbol{\sigma}} \times \boldsymbol{\mathcal{E}}/c,$$

where \mathbf{A} is the vector potential induced by an electric current and $\boldsymbol{\mathcal{E}}$ is the electric field induced by a spin current. We point out that although the above term essentially represents spin-orbit coupling which had been addressed before,¹¹⁻¹³ being significantly different from Refs. 11-13, the spin-orbit interaction considered here is related to the electric field induced by the spin current, which is supported by the Berry phase resulted from the Hund's coupling between the conduction and localized electrons in the double-exchange system. Hence the Hamiltonian to describe the ring is written as

$$H = -t \sum_{n=1, \sigma}^N (e^{i(2\pi/N)(f_{AB} + f_{AC}^\sigma)} c_{n, \sigma}^\dagger c_{n+1, \sigma} + \text{H.c.}) - \frac{J_H}{2} \sum_{n, \sigma, \sigma'} \mathbf{S}_{dn} \cdot \boldsymbol{\sigma}_{\sigma, \sigma'} c_{n, \sigma}^\dagger c_{n, \sigma'} + j_{AF} \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}. \quad (2)$$

$c_{n, \sigma}^\dagger$ and $c_{n, \sigma}$ are the creation and annihilation operators of conduction electron at site n with spin $\sigma (= \pm 1)$, respectively. \mathbf{S}_{dn} is the localized spin operator at site n . The conduction and localized electrons are coupled strongly by J_H , which is positive according to the Hund's rule. $f_{AB} = \Phi^{AB}/\Phi_0$ and $f_{AC}^\sigma = \Phi_\sigma^{AC}/\Phi_0 = \sigma f_{AC}$ where $\Phi^{AB} = \oint \mathbf{A} \cdot d\mathbf{l}$ is the AB magnetic flux and $\Phi_\sigma^{AC} = (\sigma\mu/e)\oint (\boldsymbol{\varepsilon} \times d\mathbf{l}) \cdot \mathbf{z}$ is the AC flux with $\Phi_0 = hc/e$ as the flux quantum. The last term in Eq. (2) is a tiny antiferromagnetic interaction between localized electrons. Note that the energy eigenvalue is a periodic function of f_{AB} (or f_{AC}) with a period of 1.⁹ It is thus sufficient to consider only the range of 1 for f_{AB} (or f_{AC}).

In the double-exchange system, the exchange integral between conduction electrons and localized electrons is so strong that the spins of conduction electron and localized

electrons at the same site are parallel and form a state with spin- $(S+1/2)$. Mathematically a relevant effective Hamiltonian can be derived approximately from Eq. (2) by introducing the projection operator⁵

$$\mathbf{P}_n^+ = \sum_{\sigma, \sigma'} (P_n^+)_{\sigma\sigma'} \tilde{c}_{n,\sigma}^\dagger \tilde{c}_{n,\sigma'}, \quad (3)$$

where

$$(P_n^+)_{\sigma\sigma'} = \frac{\mathbf{S}_n \cdot \sigma_{\sigma\sigma'} + (S+1) \delta_{\sigma\sigma'}}{2S+1}$$

with $\tilde{c}_{n,\sigma} = (1 - c_{n,-\sigma}^\dagger c_{n,-\sigma}) c_{n,\sigma}$. To simplify our problem further, we parametrize \mathbf{S}_n by polar angles θ_n and ϕ_n , and take $S/(2S+1) \approx (S+1)/(2S+1) \approx 1/2$, which becomes exact in the large S limit. In this approximation, we obtain an effective Hamiltonian,⁵

$$\begin{aligned} H_{eff} = & - \sum_{n=1}^N (t_n \alpha_{n+1}^\dagger \alpha_n + \text{H.c.}) \\ & + J_{AF} \sum_n (\sin \theta_n \sin \theta_{n+1} \cos(\phi_n - \phi_{n+1}) \\ & + \cos \theta_n \cos \theta_{n+1}), \end{aligned} \quad (4)$$

of the ring with the periodic condition, where $J_{AF} = j_{AF} S^2$,

$$\alpha_n^\dagger = \cos \frac{\theta_n}{2} \tilde{c}_{n,\uparrow}^\dagger + \sin \frac{\theta_n}{2} e^{i\phi_n} \tilde{c}_{n,\downarrow}^\dagger$$

and

$$\begin{aligned} t_n = & t \left(\cos \frac{\theta_n}{2} \cos \frac{\theta_{n+1}}{2} e^{i(2\pi/N)(f_{AB} + f_{AC})} \right. \\ & \left. + \sin \frac{\theta_n}{2} \sin \frac{\theta_{n+1}}{2} e^{i[(2\pi/N)(f_{AB} - f_{AC}) + \Delta\phi_n]} \right). \end{aligned} \quad (5)$$

Here $\Delta\phi_n = \phi_n - \phi_{n+1}$. If we neglect the AB and AC phases in Eq. (4), the hopping terms go back to Eq. (1). α^\dagger and α operators satisfy the anticommutation relation and are of spinless fermion. Physically, the spin of conduction electrons is frozen to align to the localized spin, and α_i describes the charge degree of freedom of electrons. The cost of transformation from $c_{i,\sigma}^\dagger$ to α_i^\dagger is that the renormalized hopping matrix acquires a quantum phase $\Delta\phi$, which plays an important role in the present problem.

For a homogeneous system we take $\theta_i = \theta$ and $\Delta\phi_n = \phi$. The eigenvalues of Eq. (4) are obtained as

$$\begin{aligned} E_l = & -2t \left[\cos^2 \frac{\theta}{2} \cos \left(\frac{2\pi}{N} (l + F_+) \right) \right. \\ & \left. + \sin^2 \frac{\theta}{2} \cos \left(\frac{2\pi}{N} (l + F_- + \phi) \right) \right] \\ & + J_{AF} (\sin^2 \theta \cos \phi + \cos^2 \theta), \end{aligned} \quad (6)$$

where $F_\pm = f_{AB} \pm f_{AC}$ and $l = 0, \pm 1, \pm 2, \dots$

The ground energy of the effective Hamiltonian with N_e electrons [Eq. (4)] is obtained,

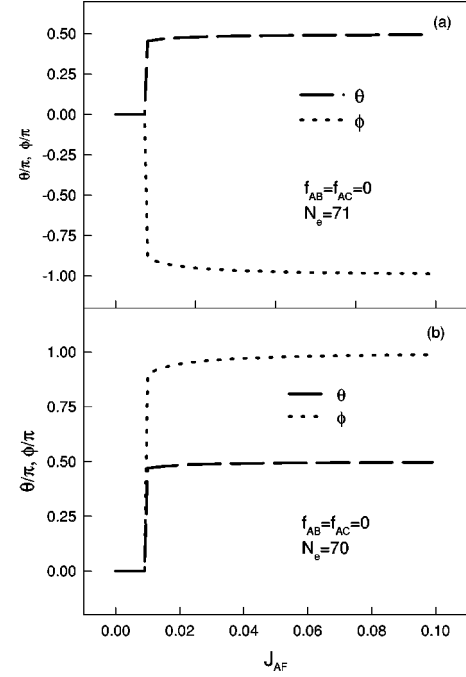


FIG. 1. Order parameters θ and ϕ versus the strength of the antiferromagnetic exchange interaction J_{AF} in the cases of (a) $N_e = 71$ and (b) $N_e = 70$.

$$\begin{aligned} E_g = & -\epsilon_0 \left[\cos^2 \frac{\theta}{2} \cos \left(\frac{2\pi}{N} (F_+ - \lambda) \right) \right. \\ & \left. + \sin^2 \frac{\theta}{2} \cos \left(\frac{2\pi}{N} (F_- + \phi - \lambda) \right) \right] \\ & + J_{AF} N_e (\sin^2 \theta \cos \phi + \cos^2 \theta), \end{aligned} \quad (7)$$

where $\epsilon_0 = 2t \sin(N_e \pi/N) / \sin(\pi/N)$, $f_{AB} \in (f_{AB}^{(0)} - \frac{1}{2}, f_{AB}^{(0)} + \frac{1}{2})$, and $f_{AC} \in (f_{AC}^{(0)} - \frac{1}{2}, f_{AC}^{(0)} + \frac{1}{2})$, with $f_{AB}^{(0)}$ and $f_{AC}^{(0)}$ being determined by minimizing the energy in Eq. (7) for given θ and ϕ . In Eq. (7), $\lambda = 0, 1/2$ correspond to the *odd* and *even* number of electron N_e , respectively. The energy unit is set to t in this paper. Physically, θ and ϕ characterize the orientation of the spin for localized electrons, and depend on the AB and AC fluxes. Different θ and ϕ characterize different spin orders of the system. $\theta=0$ represents a ferromagnetic state; $\theta \neq 0$ and $0 < \phi < \pi$ a spin spiral state; $\theta = \pi/2$ and $\phi = \pm \pi$ an antiferromagnetic state; $\theta \neq 0$ or $\pi/2$ and $\phi = \pm \pi$ a canted ferromagnetic state.

In the absence of external AB and AC fluxes and the antiferromagnetic coupling J_{AF} , the ground state is ferromagnetic as expected by double-exchange mechanism. Order parameters θ and ϕ versus J_{AF} are plotted in Figs. 1(a) and (b) for $N = 100$ and $N_e = 71, 70$, respectively. The reason we choose $N_e/N \sim 0.7$ is that the metallic ferromagnetic phase of $R_{1-x}R_x\text{MnO}_3$ occurs in the range of interval $0.2 < x < 0.5$.¹⁶ With the increase of J_{AF} the ground state evolves from a ferromagnetic phase to a spiral phase, and further approaches to an antiferromagnetic phase. In particular, near $J_{AF} \approx 0.01$, θ and ϕ experience jumps, which indicate a phase transition from the ferromagnetic phase to the spiral phase. When J_{AF} increases further, ϕ approaches $\pm \pi$ and θ tends to be $\pi/2$, which indicates that the spin spiral state

evolves to an antiferromagnetic state. It is worth noting that there is no phase transition between these two states. Interestingly, $\phi < 0$ for $N_e = 71$ (odd number), while $\phi > 0$ for $N_e = 70$ (even number). Actually, for odd N_e and $F_- = 0$ the states with $\phi < 0$ and > 0 are degenerate for the energy in Eq. (7). For even N_e or $F_- \neq 0$ the states with different signs of ϕ are no longer degenerate. The sign of ϕ depends on the AB or AC flux F_- and λ . Consequently, $\phi > 0$ is expected for even N_e . Physically, the double-exchange ferromagnetism is predominant for a small antiferromagnetic coupling J_{AF} . With the increase of J_{AF} , the competition between the ferromagnetic double-exchange and the antiferromagnetic coupling drives electrons forming a spin spiral state, and an antiferromagnetic state eventually.

As is well known, the nonzero AB and/or AC fluxes induce charge and/or spin currents in a ring, which in turn stabilize the fluxes. The induced currents are given by

$$I_c = -\frac{e}{2\pi\hbar} \frac{\partial E_g}{\partial f_{AB}} = -\frac{I_0^c}{\sin(\pi/N)} \left[\cos^2 \frac{\theta}{2} \sin\left(\frac{2\pi}{N}(F_+ - \lambda)\right) + \sin^2 \frac{\theta}{2} \sin\left(\frac{2\pi}{N}(F_- + \phi - \lambda)\right) \right], \quad (8)$$

$$I_s = \frac{1}{4\pi} \frac{\partial E_g}{\partial f_{AC}} = \frac{I_0^s}{2\sin(\pi/N)} \left[\cos^2 \frac{\theta}{2} \sin\left(\frac{2\pi}{N}(F_+ - \lambda)\right) - \sin^2 \frac{\theta}{2} \sin\left(\frac{2\pi}{N}(F_- + \phi - \lambda)\right) \right], \quad (9)$$

respectively, where $I_0^c = [2et \sin(N_e \pi/N)/N\hbar]$ and $I_0^s = [2t \sin(N_e \pi/N)]/N$. If only the AB effect is considered

($f_{AC} = 0$) and $\phi = 0$, the charge current is independent of θ and reduces to the result of tight-binding model.⁹ If only the AC effect is considered ($f_{AB} = 0$) and $\phi = 0$, the spin current is also independent of θ . Actually, both θ and ϕ depend on the AB and AC fluxes and are determined by minimizing the total energy.

In reality, the ring is quasi-one-dimensional and the electromagnetic energies induced by the AB and AC fluxes should be taken into account.^{10,14,15} These electromagnetic energies can be written as $E_{AB} = (1/2B)f_{AB}^2$ and $E_{AC} = (1/2C)f_{AC}^2$, where $B = \mathcal{L}c^2/e^2\Phi_0^2$ and \mathcal{L} is the inductance of the ring and $C = \mu^2 LR/8\pi^2 a \hbar^2 c^2$.^{10,14,15} Thus the total energy of the ring is

$$E_T = E_g + E_{AB} + E_{AC}. \quad (10)$$

By minimizing the total energy E_T , we obtain a set of equations to determine θ_0 , ϕ_0 and the current-induced $f_{AB}^{(c)}$ and $f_{AC}^{(c)}$:

$$\frac{\epsilon}{2} \sin \theta_0 (\cos F_1 - \cos F_2) + J_{AF} N_e \sin(2\theta_0) (\cos \phi_0 - 1) = 0, \quad (11a)$$

$$\frac{2\pi}{N} \epsilon \sin^2 \frac{\theta_0}{2} \sin F_2 - J_{AF} N_e \sin^2 \theta_0 \sin \phi_0 = 0, \quad (11b)$$

$$\frac{2\pi}{N} \epsilon \left(\cos^2 \frac{\theta_0}{2} \sin F_1 + \sin^2 \frac{\theta_0}{2} \sin F_2 \right) + \frac{f_{AB}^{(c)}}{B} = 0, \quad (11c)$$

$$\frac{2\pi}{N} \epsilon \left(\cos^2 \frac{\theta_0}{2} \sin F_1 - \sin^2 \frac{\theta_0}{2} \sin F_2 \right) + \frac{f_{AC}^{(c)}}{C} = 0, \quad (11d)$$

where $F_1 = (2\pi/N)(f_{AB}^{(c)} + f_{AC}^{(c)} - \lambda)$ and $F_2 = (2\pi/N)(f_{AC}^{(c)} - f_{AB}^{(c)} + \phi_0 - \lambda)$. The AB and AC fluxes can be expressed approximately as

$$f_{AB}^{(c)} \approx \frac{(2\pi/N)^2 \epsilon_0 (\lambda - \phi_0/2) \sin^2 \theta_0 + (1/C)[\lambda - \phi_0 \sin^2(\theta_0/2)]}{(2\pi/N)^2 \epsilon_0 \sin^2 \theta_0 + (1/B + 1/C) + (1/BC \epsilon_0)(N/2\pi)^2}, \quad (12)$$

$$f_{AC}^{(c)} \approx \frac{(2\pi/N)^2 \epsilon_0 (\phi_0/2) \sin^2 \theta_0 + (1/B)[\lambda \cos(\theta_0/2) + (\phi_0 - \lambda) \sin^2(\theta_0/2)]}{(2\pi/N)^2 \epsilon_0 \sin^2 \theta_0 + (1/B + 1/C) + (1/BC \epsilon_0)(N/2\pi)^2}, \quad (13)$$

which indicates that the quantum phase ϕ can sustain both AB and AC effects. By ignoring the electromagnetic energies generated by the persistent current, i.e., $B = C \rightarrow \infty$, it is easy to obtain $f_{AB}^{(c)} \approx \lambda - \phi_0/2$ and $f_{AC}^{(c)} \approx \phi_0/2$. For general cases, we solve the set of Eq. (14) numerically.

Figure 2(a) presents both θ_0 and ϕ_0 dependence of J_{AF} in different cases. Their behaviors are almost independent of B and C in the interested range. With the increase of J_{AF} , the ground state evolves from the ferromagnetic phase to the spiral phase, and to the antiferromagnetic phase eventually. The current-induced AB and AC fluxes as a function of J_{AF}

are plotted in Fig. 2(b), from which it is seen that there is a competition between AB and AC effects ($f_{AB}^{(c)} > 0$ and $f_{AC}^{(c)} < 0$). When J_{AF} increases, $f_{AB}^{(c)}$ and $f_{AC}^{(c)}$ tend to saturation. The saturated values of $f_{AB}^{(c)}$ and $f_{AC}^{(c)}$ depend on different B and C . In a typical mesoscopic system, $C \ll B$, and therefore $f_{AC}^{(c)} \ll f_{AB}^{(c)}$.^{14,15}

The charge and spin persistent currents versus J_{AF} are plotted in Figs. 2(c) and (d). Both currents vanish for $J_{AF} < 0.01$, but jump to finite values for $J_{AF} > 0.01$. In the cases of $1/B = 1/C = 0$, I_c decreases with increasing of J_{AF} due to the competition between $f_{AB}^{(c)}$, $f_{AC}^{(c)}$, and ϕ_0 . I_s also shows a

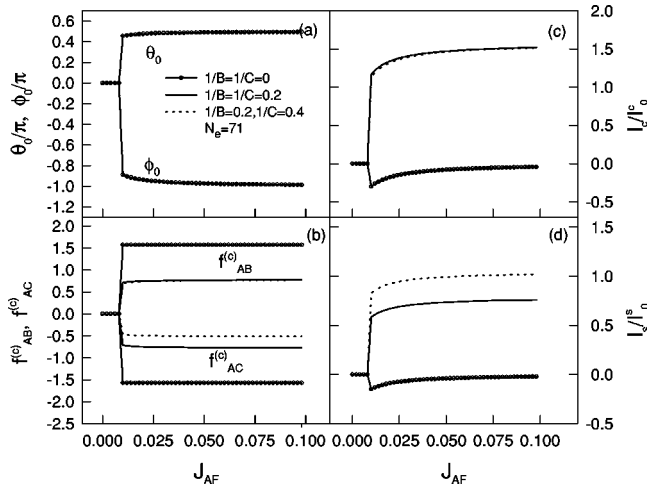


FIG. 2. For $N_e = 71$ (odd number), (a): Order parameter θ_0 and ϕ_0 versus J_{AF} ; (b): the current-induced AB and AC fluxes versus J_{AF} ; (c): the charge current versus J_{AF} ; (d): the spin current versus J_{AF} .

similar behavior in the cases of $1/B = 1/C = 0$. When the electromagnetic energy is taken into account ($1/B = 1/C = 0.2$ and $1/B = 0.2$ with $1/C = 0.4$), I_c and I_s increase quickly at $J_{AF} \approx 0.01$ and tend to saturation whose value depends on $1/B$ and $1/C$, respectively.

It is noted that, in the case of even N_e , the phase shifts a half flux quantum ($\lambda = 1/2$). As a result, the topological effect may change as shown in Figs. 3(a)–(d). Since the sign of ϕ is opposite to that for $N_e = 71$ (odd number), the current-induced AB and AC effects are affected, even though the ground state properties do not change. It can be seen from Fig. 3(b) that $f_{AB}^{(c)}$ and $f_{AC}^{(c)}$ change in opposite directions to those for $N_e = 71$. $f_{AB}^{(c)}$ and $f_{AC}^{(c)}$ may still be nonzero in the ferromagnetic state ($J_{AF} < 0.01$), which sustains the charge and spin currents as shown in Figs. 3(c) and (d).

In summary, we have addressed an effective Hamiltonian for a ring of double-exchange system from an electronic model by considering both the Aharonov-Bohm and Aharonov-Casher effects. The motion of conduction elec-

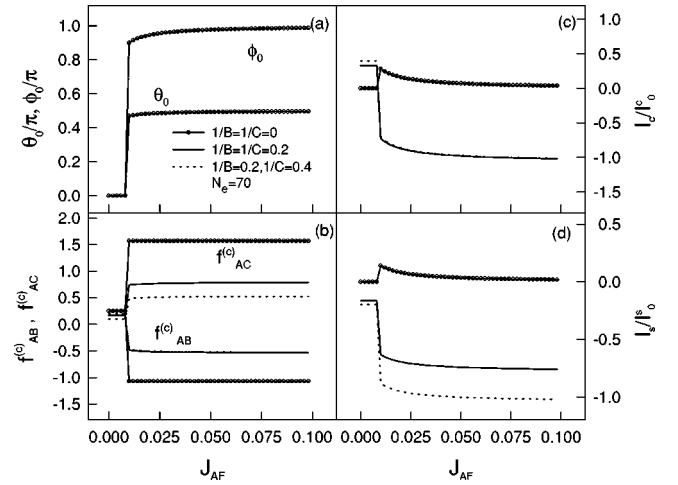


FIG. 3. For $N_e = 70$ (even number), (a): Order parameter θ_0 and ϕ_0 versus J_{AF} ; (b): the current-induced AB and AC fluxes versus J_{AF} ; (c): the charge current versus J_{AF} ; (d): the spin current versus J_{AF} .

trons in the system acquires a Berry phase via the Hund's coupling between these electrons and the localized electrons. This produces an observable quantum effect in a closed route of electron's motion. In the classical double-exchange model, the phase is neglected at all.¹ Apart from the double-exchange ferromagnetism in the system, the superexchange antiferromagnetic coupling from the localized spins also plays an important role in stabilizing the magnetic structure. A spin spiral state can be stabilized for a moderate antiferromagnetic coupling and both charge and spin currents can be induced simultaneously via the geometric Berry phase in this state, which is a piece of physics emerging from the present analysis. This current-induced topological effect is expected to be observable in mesoscopic systems, which might provide a new way to investigate the magnetic structure in such double-exchange materials.

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