

Aharonov-Anandan effect induced by spin-orbit interaction and charge-density waves in mesoscopic rings

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We study the spin-dependent geometric phase effect in mesoscopic rings of charge-density-wave (CDW) materials. When electron spin is explicitly taken into account, we show that the spin-dependent Aharonov-Casher phase can have pronounced frustration effects on such CDW materials with appropriate electron filling. We show that this frustration has observable consequences for transport experiments. We identify a phase transition from a Peierls insulator to metal, which is induced by spin-dependent phase interference effects. Mesoscopic CDW materials and spin-dependent geometric phase effects, and their interplay, are becoming attractive opportunities for exploitation with the rapid development of modern fabrication technology. [S0163-1829(98)01831-1]

Since Berry identified the importance of a “geometric phase” in adiabatic cyclic evolution,¹ there have been numerous theoretical and experimental studies of this homology phenomenon termed the Berry phase.² A fundamental generalization of the Berry phase was given by Aharonov and Anandan (AA).³ They removed the adiabatic condition and demonstrated the existence of the geometric phase in generic cyclic evolution. As is well known, the Aharonov-Bohm (AB) effect has led to a number of remarkable interference phenomena in mesoscopic systems, especially in rings.⁴ Based on the discovery of the geometric phase, it has been predicted that analogous interference effects can be induced by the geometric phases that originate from the interplay between an electron’s *spin* and *orbital* degrees of freedom. Such an interplay can be maintained by an external electric field, which leads to a spin-orbit (SO) interaction.

Loss *et al.* first studied a textured ring in an inhomogeneous magnetic field.⁵ They found that the inhomogeneity of the field can result in a Berry phase, which can result in persistent currents. The effects of this Berry phase on conductivity were then discussed.⁶ On the other hand, the Aharonov-Casher (AC) effect⁷ in mesoscopic systems has also attracted much attention, since it specifically includes the spin degree of freedom. Meir *et al.* showed that SO interaction in one-dimensional rings results in an effective magnetic flux.⁸ Mathur and Stone then pointed out that observable phenomena induced by SO interactions are essentially the manifestation of the AC effect and proposed an observation of the AC oscillation of the conductance on semiconductor samples.⁹ Balatsky and Altshuler¹⁰ and Choi¹¹ studied the persistent current produced by the AC effect. Inspired by these studies of textured rings, the AC effect has also been analyzed in connection with the spin geometric phase. Aronov and Lyanda-Geller considered the spin evolution in conducting rings, and found that SO interaction results in a spin-orbit Berry phase, which plays an interesting role in the transmission probability.¹²

The charge-density-wave (CDW) broken-symmetry state induced by electron-phonon interaction has also been intensively investigated during the last decades. The dynamics of CDW’s in materials such as NbSe₃,¹³ as well as their collec-

tive excitations,¹⁴ have received detailed study. Recently, it has been found that an external magnetic field has a pronounced effect on the CDW ground state.^{15,16} In sufficiently small mesoscopic rings, the AB flux induced by an external magnetic field can even destroy the CDW ground state.¹⁶ We have shown the instability of the CDW ground state with respect to the AB effect. Recently, it is further emphasized that, for spinless electrons, the AB effect depends on the parity of the number N of electrons.¹⁷ Specifically, when the number of spinless electrons are even, the electronic polarizability, which in the absence of magnetic flux has a well-known divergence at $2k_F$, can be compensated by magnetic flux, which then has a similar effect to temperature, inducing a transition from Peierls distortion to metal.

In this paper, we focus on the role of the electron *spin* in a *cylindrical electrical* field, which is the source of the SO interaction. This induces an AC phase, as the electrical field is dual to the magnetic field. We concentrate on the condition that has a *destruction* effect on the mesoscopic CDW system. We found that, when *spin* degree of freedom is explicitly taken into account, the parity effect is more complicated and $4n$ (n is an integer) electrons have definite destruction effects, which is quite different from the spinless case. We will address the other filling case elsewhere. In the following, we focus on the $4n$ electron case, since our interest is mainly on the sector in which the spin-dependent geometric phase has a *destruction* effect. When the spin and the spin-dependent geometric phase are explicitly taken into account, we show that the Aharonov-Casher phase (comprised of the nonadiabatic AA phase and the dynamical phase by SO interaction) induced by the cylindrical electric field can have a pronounced destruction effect on the CDW. We further propose observable consequences on the transport properties of mesoscopic CDW rings.

In the presence of an electric field $\mathbf{E} = -\nabla V$, the one-particle Hamiltonian for noninteracting electrons confined to a mesoscopic ring is

$$H = \frac{1}{2m_e} \mathbf{p}^2 + eV - \frac{e\hbar}{4m_e^2 c^2} \boldsymbol{\sigma} \cdot \mathbf{E} \times \mathbf{p}, \quad (1)$$

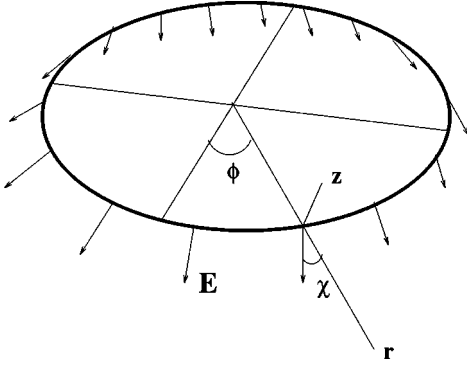


FIG. 1. The mesoscopic CDW ring in a cylindrically symmetric field with tilt angle χ .

where σ is the Pauli matrix, m_e is the effective mass of electrons, and \mathbf{p} represents the momentum of electrons. We consider a ring that is effectively one-dimensional and where the electric field that results in the SO interaction is cylindrically symmetric (see Fig. 1), i.e., $\mathbf{E} = E(\cos \chi \mathbf{e}_r - \sin \chi \mathbf{e}_z)$. For a ring lying in the xy plane with its center at the origin, the Hamiltonian reads

$$H = \frac{\hbar^2}{2m_e a^2} \left[-i \frac{\partial}{\partial \theta} + \alpha (\sin \chi \sigma_r + \cos \chi \sigma_z) \right]^2 - \frac{\alpha^2 \hbar^2}{2m_e a^2}, \quad (2)$$

with $\sigma_r = \sigma_x \cos \theta + \sigma_y \sin \theta$ and $\alpha = -eaE/4m_e c^2$, where a is the ring radius, and θ is the angular coordinate.

We adopt the geometric phase approach to identify the geometric and dynamical phases,³ which are responsible for the effects on the CDW broken-symmetry ground state in mesoscopic rings. The eigenstates of the Hamiltonian are of the form

$$\Psi_{n,\mu}(\theta) = \exp(in\theta) \tilde{\psi}_{n,\mu}(\theta) / \sqrt{2\pi}, \quad (3)$$

in which $\mu = \pm$, n are arbitrary integers, and the spin states are given by

$$\tilde{\psi}_{n,+}(\theta) = \begin{bmatrix} \cos \frac{\beta}{2} \\ e^{i\theta} \sin \frac{\beta}{2} \end{bmatrix}, \quad (4)$$

$$\tilde{\psi}_{n,-}(\theta) = \begin{bmatrix} -e^{-i\theta} \sin \frac{\beta}{2} \\ \cos \frac{\beta}{2} \end{bmatrix},$$

with $\tan \beta = 2\alpha \sin \chi / (2\alpha \cos \chi - 1)$. The geometrical phase (AA phase) is given by

$$\int_0^{2\pi} i \tilde{\psi}^{(\mu)\dagger}(\theta) d\tilde{\psi}^{(\mu)}(\theta) = -\mu \pi (1 - \cos \beta), \quad (5)$$

and the dynamical phase is

$$-\int_0^{2\pi} i \tilde{\psi}^{(\mu)\dagger}(\theta) H_s \tilde{\psi}^{(\mu)}(\theta) d\theta = -2\mu \pi \alpha \cos(\beta - \chi). \quad (6)$$

Then the AC phase is

$$\phi_{AC}^\mu = -\mu \pi (1 - \cos \beta) - 2\mu \pi \alpha \cos(\beta - \chi), \quad (7)$$

which satisfies $\sum_\mu \phi_{AC}^\mu = 0$, and the solution of the Hamiltonian in the mesoscopic system is

$$\varepsilon_{n,\mu} = \frac{\hbar \omega_0}{2} \left(n - \frac{\phi_{AC}^\mu}{2\pi} \right)^2 - \frac{\alpha^2 \hbar^2}{2m_e a^2}, \quad (8)$$

where $\omega_0 = \hbar / m a^2$.

The AC phase comprises the geometric AA phase and the dynamical phase, which is obtained by the spin cyclic evolution of the spin freedom of the electron. This AC phase will change the wave numbers of the two independent spin-polarized cyclic electron gases. Thus, when the spin degree of freedom is explicitly taken into account, the accumulated *spin*-dependent geometric phase will have pronounced effects in a CDW mesoscopic ring, and result in an interesting effect on the transport properties of the CDW system, as we discuss in the following.

As is well known, electron-phonon interaction treated adiabatically in a quasi-one-dimensional system leads to a CDW gap at wave vector $q = 2k_F$, so that the originally continuous energy band breaks into two bands: valence and conduction. Since Peierls first pointed out that a one-dimensional metal coupled to the lattice is unstable at low temperature, both theoretical and experimental studies have concentrated on the static and dynamical characters of charge-density waves, including the frequency- and electric-field-dependent conductivity, current oscillation, and pinning via defects or disorder.¹³ These studies focused on the conductivity character in direct external electrical fields for macroscopic quasi-one-dimensional CDW materials, such as $K_{0.3}MoO_3$, $NbSe_3$, etc. As fabrication techniques have become more mature, it is now promising that fabrication of mesoscopic CDW samples can be realized.¹⁸

The logarithmical singularity of the dielectric response function at wave vector $2k_F$ makes the corresponding phonon frequency soften drastically (Kohn anomaly). The modulated lattice structure also affects the electronic band structure. In second-quantized representation, with a cylindrical electric field in a CDW mesoscopic ring, we can use the Hamiltonian

$$H = \sum_{k,\mu} [\varepsilon_{k,\mu} C_{k,\mu}^\dagger C_{k,\mu} + \Delta (C_{k+2k_F,\mu}^\dagger C_{k,\mu} + \text{H.c.})]. \quad (9)$$

Here the CDW gap is $\Delta = 2\gamma u$, with γ the electron-lattice coupling constant and u the displacement after dimerization, and $\varepsilon_{k,\mu}$ the eigenenergies in an external cylindrical electric field [Eq. (8)]. We consider the half-filled case, but extension to other band fillings for many real quasi-one-dimensional CDW materials is straightforward. After diagonalizing the reduced 2×2 matrix

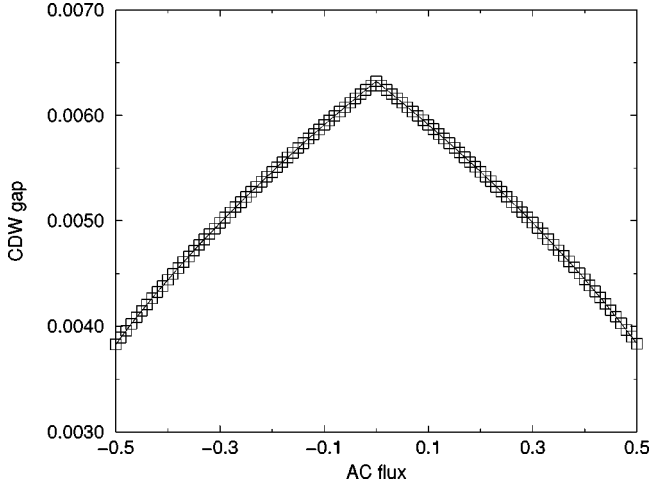


FIG. 2. The CDW gap dependence on the spin-dependent geometric phase, for the strength of effective e -ph interaction $g = 0.07$.

$$\begin{vmatrix} E_{k,\mu} - \varepsilon_{k,\mu} & \Delta \\ \Delta & E_{k,\mu} - \varepsilon_{k+2k_F,\mu} \end{vmatrix} = 0, \quad (10)$$

we obtain the splitting into valence and conduction bands:

$$E_{k,\mu}^{val} = \frac{1}{2}(\varepsilon_{k,\mu} + \varepsilon_{k+2k_F,\mu}) - \frac{1}{2}\sqrt{(\varepsilon_{k,\mu} - \varepsilon_{k+2k_F,\mu})^2 + 4\Delta^2},$$

$$E_{k,\mu}^{con} = \frac{1}{2}(\varepsilon_{k,\mu} + \varepsilon_{k+2k_F,\mu}) + \frac{1}{2}\sqrt{(\varepsilon_{k,\mu} - \varepsilon_{k+2k_F,\mu})^2 + 4\Delta^2}. \quad (11)$$

From Eq. (11), we see that when the spin degree of freedom is taken into account, the spin-dependent geometric phase affects the CDW ground state. First, we concentrate on the effect on the CDW gap. We will turn to the effect on transport properties later. As the $2k_F$ mode is dominant in the electron-phonon interaction, we can obtain the following total effective potential:

$$E = \sum_{|k| \leq k_F} E_{k,\mu}^{val} + \frac{1}{2}\omega_{2k_F}^2 u_{2k_F}^2, \quad (12)$$

where $\Delta = \gamma u_{2k_F}$. Adopting a standard minimization procedure, we now find the effect on the CDW gap by the spin-dependent geometric phases for the electron numbers $4n$ is

$$\prod_{\mu} \frac{\left| \frac{\phi_{AC}^{\mu}}{2\pi} \right| + \sqrt{\left(\frac{\phi_{AC}^{\mu}}{2\pi} \right)^2 + \left(\frac{\Delta}{\hbar \omega_0 n_F} \right)^2}}{\left| \frac{\phi_{AC}^{\mu}}{2\pi} + 2n_F \right| + \sqrt{\left(\frac{\phi_{AC}^{\mu}}{2\pi} + 2n_F \right)^2 + \left(\frac{\Delta}{\hbar \omega_0 n_F} \right)^2}} = \exp\left(-\frac{1}{g}\right), \quad (13)$$

with g the dimensionless effective electron-lattice interaction, $g = \gamma^2 / \hbar \omega_0 n_F m \omega_{2k_F}^2$.

We have explored this AC phase effect on a CDW mesoscopic ring in various regions. We found that it is very sensitive to e -ph coupling, as illustrated in Figs. 2 and 3. The effects of the spin-dependent geometric phases for different

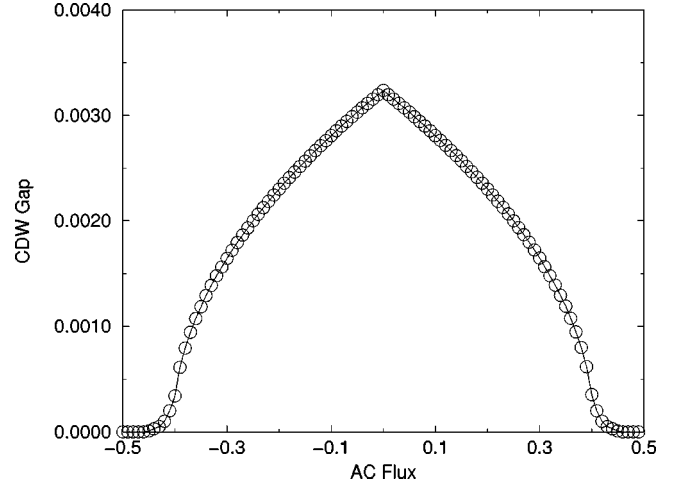


FIG. 3. The CDW gap dependence on the spin-dependent geometric phase, for the strength of effective e -ph interaction $g = 0.064$.

e -ph coupling constants shows that only when the e -ph coupling is weak enough, is a breaking effect on the CDW observable: the stronger the e -ph coupling, the more stable is the CDW. We emphasize that the breaking effect ($4n$ electrons) by the AC phase is the result of the two spin-polarized electrons, which is produced by the external electric field, and these two spin-polarized electron gases accumulate a spin-dependent geometric phase through the SO interaction. Hence, we have identified a new mechanism, different from that due to an external magnetic field.

We have concluded that when the external electrical field reaches a critical strength, the CDW ground state in a mesoscopic ring can be destroyed with the appropriate electron fillings ($4n$ when spin is explicitly taken into account). Since the SO interaction is time-reversal invariant, we expect that the effect of the spin-dependent geometric phase on a CDW mesoscopic ring will be manifested in transport processes. Here, it is induced by the cylindrical electric field. This is different from previous studies in which the electrical field is parallel to the direction of the quasi-one-dimension of the CDW materials, and hence has no corresponding topological effect on the transport. We adopt the configuration with the

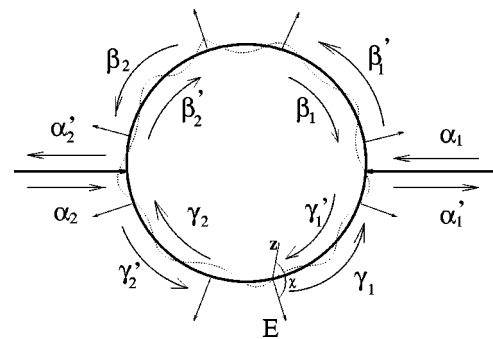


FIG. 4. Schematic illustration of the electronic waves propagating through a ring connected to current leads. The right junction is located at $\theta = 0$ and the left junction at $\theta = \pi$ with the upper branch lying within $(0, \pi)$ and the lower one within $(\pi, 2\pi)$. The dotted line illustrates the charge-density wave in the ring before the symmetry breaking.

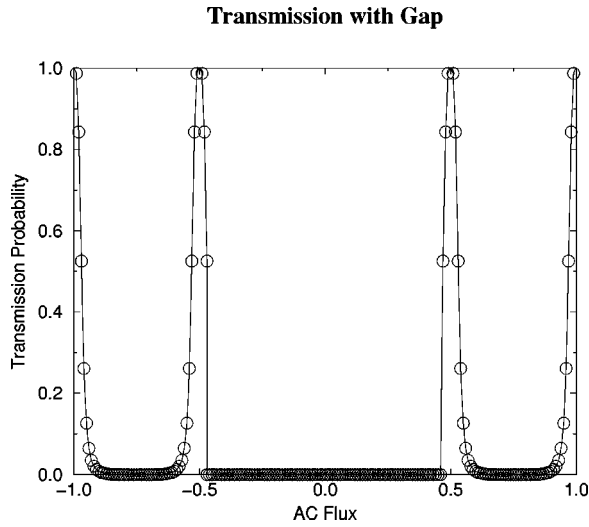


FIG. 5. The transmission probability with respect to the spin-dependent geometric phase, when the incident electron energy is within the CDW gap, and with $g = 0.064$.

ring connected to two current leads in opposite directions, which is the standard structure for transport studies and interference effects in a mesoscopic field (see Fig. 4).

Our formulation is standard for that developed in the study of quantum oscillations.¹⁹ We obtain the transmission probability in the presence of SO interactions (a detailed derivation is given elsewhere)²⁰ as

$$T = \frac{1}{2} \sum_{\mu} t \left(\frac{\phi_{AC}^{\mu}}{2\pi} \right), \quad (14)$$

with

$$t \left(\frac{\phi_{AC}^{\mu}}{2\pi} \right) = \frac{4\epsilon^2 \sin^2 \phi_s \cos^2 \phi_{AC}^{\mu}}{[a^2 + b^2 \cos 2\phi_{AC}^{\mu} - (1 - \epsilon) \cos 2\phi_s]^2 + \epsilon^2 \sin^2 2\phi_s}.$$

Here ϕ_s is the phase of the incident electron on the lead, where $a = \pm(\sqrt{1 - 2\epsilon} - 1)/2$ and $b = \pm(\sqrt{1 - 2\epsilon} + 1)/2$ with $0 \leq \epsilon \leq 1/2$.¹⁹

From Fig. 5, we see that the CDW breaking effect by the spin-dependent geometric phase is clearly manifested in electronic transport. When the CDW is absent, the transmission probability of the conducting ring should be periodic with respect to the AC phase, as illustrated in Fig. 6. When the e -ph coupling is turned on and the energy of the incident wave is within the CDW gap, a clear effect can be seen with the variation of the AC phase. Hence, there exists a critical

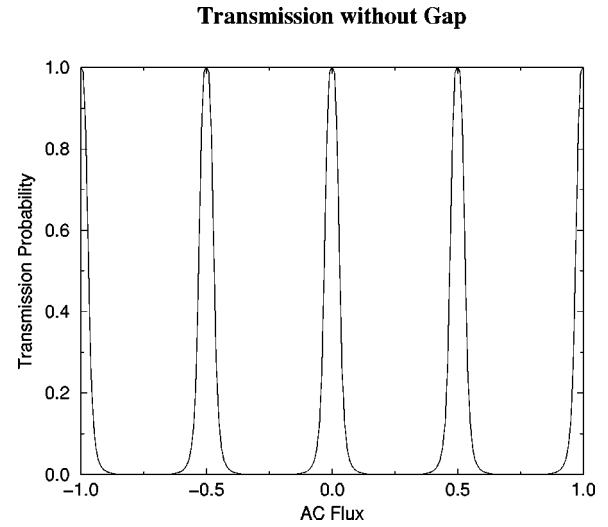


FIG. 6. The transmission probability with respect to the spin-dependent geometric phase in the absence of a CDW gap.

value of ϕ_{AC}^{μ} (± 0.43 for the effective e -ph coupling $g = 0.064$), where the transmission probability of the incident energy has a large jump, as illustrated in Fig. 5, a signature of the transition from Peierls insulator to metal. For experimental convenience, we can take the direction of the electrical field along the z axis (Fig. 1), i.e., $\chi = \pi/2$. In a mesoscopic ring with radius $a = 100 \mu\text{m}$, to make the above effect observable, an electrical field with strength $\sim 10^6 \text{ V/m}$ is necessary, so that the AC phase can be the order of unity.

In summary, we have investigated a spin-dependent geometric phase effect in mesoscopic CDW rings. When the electron spin is explicitly taken into account in the presence of a cylindrical external field and under appropriate filling electrons, the AC (AA) phase accumulated by the two independent spin-polarized electron gases can result in frustration of the CDW on a mesoscopic scale. We thus propose a mechanism with which to probe mesoscopic CDW materials, and associated spin-dependent geometric phase consequences. As a consequence, we suggest that a frustration effect of the spin-dependent geometric phase will be observable in transport experiments. There are natural extensions of our considerations to competing spin-density-wave and CDW situations, as well as the other filling electron case, which we will discuss elsewhere. These opportunities for studying mesoscopic systems are becoming increasingly attractive with the rapid progress of modern fabrication technology.

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