Aharonov-Bohm oscillations in the local density of topological surface states

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We study Aharonov-Bohm (AB) oscillations in the local density of states (LDOS) for topological insulator (TI) and conventional metal Au(111) surfaces with spin-orbit interaction, which can be probed by spin-polarized scanning tunneling microscopy. We show that the spacial AB oscillation period in the total LDOS is a flux quantum $\Phi_0=\hbar c/e$ (weak localization) in both systems. Remarkably, an analogous weak antilocalization with $\Phi_0/2$ periodic spacial AB oscillations in spin components of LDOS for TI surface is observed, while it is absent in Au(111).

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Spin-orbit interaction (SOI) effects in semiconductors and metals have been an active theme in the modern condensed matter physics, but especially, the topological insulators (TI), which have been detected in series of two-dimensional [1–3] and three-dimensional [4–11] materials, suggest new directions for this field since the extraordinarily strong SOI exists in TI. The helical spin structure of electrons in TI acquire a spin-orbit induced nontrivial Berry phase of $\pi$ after a 2$\pi$ adiabatic rotation along the Fermi surface. This Berry phase corrects the quantum constructive interference between a closed trajectory that the electron passes and its time-reversal counterpart, and thus can give rise to the weak antilocalization (WAL) signature in the quantum coherent magneto-transport coefficients. Many efforts have been devoted to observing WAL in the HgTe quantum wells [12–13], Bi$_2$Te$_3$ [14–16], Bi$_2$Se$_3$ [17–23], and other materials. Very recently, for example, in a transport experiment [17] of Bi$_2$Se$_3$ nanowires, the Aharonov-Bohm (AB) oscillation with anomalous period $\Phi_0/2$ period was observed, while the WAL induced $\Phi_0/2$ period was absent. The period of these oscillations in conductance is determined by the doping level and the disorder of the TI nanowire [18, 19]. In addition, an energy gap at the Dirac cone opened by magnetic doping in TI films could also induce crossover from the WAL to the weak localization (WL), which is tunable by the Fermi energy and the gap [24].

In this letter, for exploring the analogous WAL in topological surface state, we consider an imaginary AB interferometer consisting of a spin-polarized scanning tunneling microscope (SP-STM) tip [25–27] and two identical nonmagnetic impurities apart tens of nanometers on the TI surface as shown in Fig. 1. When an electron travels along the clockwise and anticlockwise loops ($r_1=r_1\rightarrow r_2=r$) enclosing a finite area, the quantum interference phenomenon occurs. The interference contribution to the local density of states (LDOS) is affected by an external magnetic field $B$ via the AB effect arising from the threaded magnetic flux [28]. We will show that, on one hand, the AB oscillatory period of the total LDOS $\Delta N_L(r,\omega, B)$ (the subscription $L$ represents the loops enclosed by the scattering paths of the surface electrons) is a flux quantum $\Phi_0$, which is an analog of WL phenomenon. On the other hand, the strong SOI in TI materials can modify the electron AB interference effect via the chiral spin rotations during the non-collinear multiple scattering processes, and thereby the analogous WAL effect with $\Phi_0/2$ period in AB oscillations will be observed if the spin-resolved LDOS $[\Delta N_{\uparrow}(r,\omega, B)\text{ and }\Delta N_{\downarrow}(r,\omega, B)]$ are measured. Furthermore, for comparison, we briefly discuss the AB effect in the LDOS of conventional metal Au(111) surface with weak SOI, and find that the analogous WAL phenomenon is absent in Au(111) surface. Our finding may provide a useful method to characterize the topological surface states.

We describe the TI surface, on which two nonmagnetic impurities are adsorbed, by a low-energy effective Dirac Hamiltonian written as

$$H = v \sigma \cdot (\hat{z} \times \mathbf{q}) + V(\mathbf{r})$$

(1)

with the Fermi velocity $v=333$ (287) meV-nm in Bi$_2$Se$_3$ (Bi$_2$Te$_3$) [24]. $\mathbf{q}=(q_x,q_y)$ denotes the planar momentum operator, and $\sigma=(\sigma_1,\sigma_2,\sigma_3)$ is the Pauli spin matrix. $V(\mathbf{r})=\sum_{i=1}^N U_i \sigma_0 \delta(\mathbf{r}-\mathbf{r}_i)$ is the potential of two nonmagnetic impurities located at $\mathbf{r}_1=(-d/2,0)$ and $\mathbf{r}_2=(d/2,0)$ with strength $U_i$, $\sigma_0$ is the 2x2 unit matrix.

The features we discuss are expected to be seen in the change of the real-space LDOS owing to the influence of magnetic flux which passes through the area enclosed by the two scattering paths shown in Fig. 1. This quantity can directly reveal the WL or WAL effect in TI via AB oscillatory periods in LDOS. The real-space Green’s function involving the impurities scattering is given by...
The bare electron Green’s function \( G_0 \) for the TI surface states could be expressed in terms of a complex amplitude multiplied by a “complex” spin rotation:

\[
G_0(\mathbf{r}, \mathbf{r}'; \omega) = \frac{\omega^+}{4\pi} D_+ \hat{R}(\alpha, \beta, \eta),
\]

which is useful to gain more physical insight into the transport between \( \mathbf{r} \) and \( \mathbf{r}' \). Here, \( D_+ = \sqrt{g_0^2 + g_1^2} \), where \( g_{0/1} = \text{sgn}(\omega^+) Y_{0/1}(|k| \rho) \mp i Y_{0/1}(|k| \rho) \) with \( \rho = |\mathbf{r} - \mathbf{r}'| \), \( k = k_F (1 + \omega / E_F) \), and \( \omega^+ = \omega + E_F \), and \( E_F = v k_F \) the Fermi energy of TI. \( Y_{0/1} \) are the first (second) kind Bessel functions. \( \hat{R}(\alpha, \beta, \eta) = e^{i\alpha \sigma_3} e^{i\beta \sigma_2} e^{i\eta \sigma_1} \) is a spin rotation operator characterized by the three Euler angles \( \alpha = -\frac{\pi}{4} + \frac{\pi}{4} \) with \( e^{i\delta} = (\rho \times + i \rho \hat{y}) / \rho \), \( \beta = \tan^{-1}(\rho y / \rho x) \), and \( \eta = -\pi \). Equation (3) is exact under a high-energy cutoff [30, 31].

Following the perturbation approach, Eq. (2) can be expanded to any order in the impurity potential \( U_i \). Our effort will be concentrated on the scattering processes of surface electrons with the both impurities, in which the scattering paths enclose loops. Therefore, taking all this into account, after a long algebra calculation, we have

\[
\delta G_L = G_0(\mathbf{r} - \mathbf{r}_1) W_1 G_0(\mathbf{r}_1 - \mathbf{r}_2) T_2 G_0(\mathbf{r}_2 - \mathbf{r}') + G_0(\mathbf{r} - \mathbf{r}_2) W_2 G_0(\mathbf{r}_2 - \mathbf{r}_1) T_1 G_0(\mathbf{r}_1 - \mathbf{r}'),
\]

where

\[
W_{1/2} = \frac{T_{1/2}}{\sigma_0 - T_{1/2} G_0(\mathbf{r}_{1/2} - \mathbf{r}_2/1) T_{2/1} G_0(\mathbf{r}_{2/1} - \mathbf{r}_1/2)}
\]

is diagonal with \( T \)-matrices \( T_{1/2} = \frac{v_{1/2}}{1 - U_{1/2} G_0(0 \omega)} \). Equation (4) is a general formula describing the interference effect from the scattering with both two impurities participated. In the absence of SOI, the two terms in Eq. (4), i.e., the scattering amplitudes corresponding to the time-reversal processes, should be equal to each other and thereby give rise to the constructive quantum correction to the LDOS in the so-called WL theory. In the presence of a strong SOI, however, the electrons interference is affected remarkably due to the non-collinear multiple scattering trajectories that generate nontrivial spin rotations. The spin rotation leads to a destructive interference in LDOS by a phase change picked up during the clockwise and anticlockwise scattering processes, which is the origin of the WAL effect in systems with strong SOI. Explicitly, for collinear scattering paths between \( \mathbf{r}_1 \) and \( \mathbf{r}_2 \), there is no net spin rotation since \( G_0(\mathbf{r}_{1/2} - \mathbf{r}_2/1) G_0(\mathbf{r}_{2/1} - \mathbf{r}_1/2) \propto \sigma_0 \). Whereas for non-collinear multiple scattering trajectories, such as the loops shown in Fig. 1, \( G_0(\mathbf{r} - \mathbf{r}_{1/2}) G_0(\mathbf{r}_{1/2} - \mathbf{r}_{2/1}) G_0(\mathbf{r}_{2/1} - \mathbf{r}) \) is not a unit matrix which implies net spin rotations during scattering processes. As a result, in contrast to the collinear scattering process, the non-collinear multiple-impurity scattering on TI surface can induce dramatic modulations in the LDOS.

Applying a magnetic field tends to destroy the destructive interference and may bring forth some key signatures of WAL effect, such as the \( \Phi_{0/2} \) periodic AB oscillations in the spin components of LDOS (similar to \( \Phi_{0/2} \) oscillations in the magneto-conductance due to WAL). In the presence of a low magnetic field, the Green’s function can be semiclassically approximated as [32],

\[
\hat{G}_0(\mathbf{r} - \mathbf{r}') = e^{i \frac{2\pi}{B} \Phi_{0/1}(\mathbf{r}') \cdot A(1) \cdot d} G_0(\mathbf{r} - \mathbf{r}'),
\]

where \( A = (-By, 0, 0) \) represents the vector potential. This approximation is exact so long as the magnetic length is much greater than the Fermi wave length \( l_B = (\Phi_0 / 2 B) / \lambda_F \). For magnetic field \( B = 5 \sim 10 \) T, the corresponding magnetic length \( l_B \approx 11.63 \sim 8.22 \) nm, while the Fermi wave length \( \lambda_F = 7.21 \sim 5.3 \) nm for TI with \( E_F = 250 \sim 340 \) meV [6]. Accordingly, the condition in Eq. (5) for the semiclassical approximation is valid for these low magnetic field and low energy ranges. Also, the Zeeman splitting is negligibly small (typically of 1.0 meV at \( B = 10 \) T for Bi2Se3 film) compared to the strong SOI, and thus is not taken into account in the following discussion.

The correction of the LDOS due to the magnetic flux is given by

\[
\Delta N_L(\mathbf{r}, \omega, B) = -\frac{1}{\pi} \text{STr} \left[ \delta \hat{G}_L(\mathbf{r}, \omega) - \delta G_L(\mathbf{r}, \omega) \right],
\]

where \( \delta \hat{G}_L \) is calculated from Eq. (4) with \( \hat{G}_0 \). For large distances \( (|k| \rho \gg 1) \), \( J_{0/1} \approx \pm \sqrt{2 / (\pi |k| \rho) \cos \left[ \pi / 4 \mp |k| \rho \right]} \) and \( Y_{0/1} \approx \pm \sqrt{2 / (\pi |k| \rho) \sin \left[ |k| \rho \mp \pi / 4 \right]} \). Combining Eqs.
strong spin interference effect deviates the real-space AB oscillations from $d_0$ period when a SP-STM tip scans on the TI surface in the presence of a fixed $B$, which is our concentration in the present paper. We can easily find that the spacial AB oscillation period of $\Delta N_L^{1/4}$ is determined by the factor $F^{1/4}=\sin(\frac{2\pi\Phi}{\Phi_0}) \pm \sin \phi$. Taking $\Delta N_L^{1/4}$ as an example (Similar analysis can be done on $\Delta N_T^{1/4}$) to find the AB period, we consider the roots of $F^1=0$ as an equation of $y$, which can be rewritten as $F^1=\sin \phi [\cos(\frac{2\pi\Phi}{\Phi_0})-1]\cos \phi \sin(\frac{2\pi\Phi}{\Phi_0})=0$. There are two cases that result in $F^1=0$: (i) First, it is easy to get that $y_1=\frac{2\Phi_0}{Bd}\Phi_0$ $(n=0, \pm 1, \cdots)$ are the roots of $F^1=0$; (ii) Second, expanding $F^1$ at point $y_2=(\frac{2n+1}{2Bd})\Phi_0$, a simple equation for $y$ can be obtained $M(y-(\frac{2n+1}{2Bd})\Phi_0)-P=0$, which gives out other asymptotic roots $y=\frac{(2n+1)\Phi_0}{Bd}+\frac{P}{M}$ ($M$ and $P$ are the expanding coefficients). These roots lie near $y_2$ and become better for the limit of small $B$ [see following Figs. 2(b) and 2(c)]. Combining with case (i), the AB oscillation signals for $\Delta N_L^{1/4}$ occur at $\frac{(2n+1)\Phi_0}{Bd}$ with a spacial period of $\frac{2\Phi_0}{Bd}$ (i.e., $\frac{2\Phi_0}{Bd}$ in the scale of flux), the half of $\Delta N_L$. This half period could be understood as an analog of WAL effect in the spin-polarized LDOS since strong SOI in TI can result in the two-dimensional WAL effect in the magneto-conductance, which can be represented as the AB oscillation phenomenon with period of $\frac{2\Phi_0}{Bd}$. 

Moreover, the interference signature of LDOS decays by a factor of $[d \rho_1 \rho_2]^{-1/2}$ in the asymptotic representations, Eqs. [8] and [10]. Actually, however, dephasing processes have been observed in transport investigations in Bi$_2$Se$_3$ and Bi$_2$Te$_3$ films [15, 21–23] as well as in AB-effect studies of Bi$_2$Se$_3$ nanowires [17, 19]. The phase coherence length $l_\phi$ of Bi$_2$Se$_3$ and Bi$_2$Te$_3$ can be as large as hundreds of nanometers, which is tens times of the Fermi wave length. The characteristic distance in our setup must be much smaller than the phase coherence length ($d \ll l_\phi$), so that we choose $d=20 \text{nm} \ll l_\phi$ without taking into account the dephasing processes in the following numerical calculations.

To supplement the above analytical results, typically, we present our numerically calculated data in Fig. 2, where the upper (lower) panels correspond to $B=5 \text{ T}$ ($10 \text{ T}$). The blue horizontal strips are the AB oscillation signals in the real-space LDOS, while the oscillatory ellipse features are the interference signals arising from the contributions of $N_L(r, \omega, B=0)$. It is obvious that in the case of $B=5 \text{ T}$ ($10 \text{ T}$), the interstrip distance is $d_0=85 \text{ nm}$ ($42 \text{ nm}$) in the total LDOS as shown in Fig. 2(a), corresponding to the $\Phi_0$ period of AB oscillations. The numerical data in Fig. 2(a) are exact while Eq. [8] is approximate.

However, differing from the $\Phi_0$ periodic AB oscillations in the total LDOS, Fig. 2(b) and 2(c) show that the interstrip distance in the spin-resolved LDOS is $\frac{2\Phi_0}{Bd}$, corresponding a $\Phi_0$ period. This analogous phenomenon of WAL with a period of $\frac{2\Phi_0}{Bd}$ in $\Delta N_L^{1/4}$ ($r, \omega, B$) found from the numerical calculation are accord well with our analytical result given by Eq. [10]. As addressed above, the present analogous WAL phenomenon
Hamiltonian of TI surface with $\tan \theta$.  

**FIG. 2**: (Color online) Simulations of the AB oscillations of the electronic LDOS in Bi$_2$Te$_3$(111) surface with fixed magnetic field $B$=5 T (upper panels) and $B$=10 T (lower panels). (a) the total LDOS pattern; (b) the spin-up component; (c) the spin-down component. The parameters are chosen as $v=287$ meV·nm, $E_F=250$ meV ($\lambda_F=7.21$ nm) and $d=20$ nm. The white dots denote the positions of adatoms. The periodic horizontal blue strips in patterns are signature of AB oscillations in LDOS.

can be understood via the Berry phase. Explicitly, the quantum phase difference between the closed loops in opposite directions in our setup corresponds to the Berry phase associated with spin rotation by $2\pi$, which is given by $\Delta \varphi = -i \int_{\hat{q}^0}^{\hat{q}^0+2\pi} d\theta \langle \psi_q | \partial_\theta | \psi_q \rangle = \pm \pi$. Here, $|\psi_q\rangle = \frac{1}{\sqrt{2}} \left( \pm e^{i\theta(q)}, 1 \right)^T$ are the eigenstates for the free Hamiltonian of TI surface with $\tan \theta(q) = \frac{2m}{\gamma}$. To experimentally verify our predicted AB interference strips with $\frac{\pi}{2}$-period in the spin-resolved LDOS shown in Fig. 2(b) and 2(c), the SP-STM tip and sufficiently strong scattering potentials are required, which we believe are achievable in current experimental capabilities. So we hope the present prediction can be directly observed by STM in situ measurement instead of the complicated low-temperature transport measurement.

For comparison, we also calculate the AB oscillations on the conventional metal surface with weak but observable SOI. We choose Au(111) as an example, in which the Rashba SOI is $\sim 40$ meV·nm and the Fermi wave length is $\sim 7.4$ nm. The consequence calculated results are shown in Fig. 3 for $B=10$ T. From Fig. 3 the SOI influence on the electron interference in Au(111) can be summarized as follows: (i) The AB interference strips in the spin-resolved LDOS display oscillatory behavior induced by non-colinear multiple scattering trajectories; (ii) The SOI destroys the elliptic features in the LDOS maps even if there is no applied magnetic field, see the longitudinal extending blue strips in Fig. 3. However, the AB oscillation period in the LDOS pattern is also $\Phi_0$ (the interstrip distance is $\sim 42$ nm); (iii) Especially, there is no $\Phi_0/2$ period in the spin-resolved LDOS in Fig. 3 because there is zero net Berry phase and no topological chirality in the Shockley surface state on Au(111), which is totally different from the case of TI surface. Analytically, the unperturbed spatial Green’s function for the conventional metal surface with weak Rashba SOI described by the Hamiltonian $H_0^{(c)} = (\hbar q)^2/2m - (\gamma/\hbar) (\sigma \times \mathbf{q}) \cdot \hat{z}$ is asymptotically expressed as $G_0(\mathbf{r}, \mathbf{r}', \omega) \approx \tau \left[ f_\mu(\rho, \omega) + f_\nu(\rho, \omega) (\sigma \cdot \hat{\rho}) \right]$, where $\tau = -\frac{m^* (\gamma/\hbar)}{2(\hbar^2 k^2 + \Delta_0^2)}$, $\rho = \mathbf{r} - \mathbf{r}'$, and $f_\mu/\nu(\rho, \omega) \approx \sqrt{\frac{\gamma}{\hbar^2 k^2}} \pm \sqrt{\frac{\gamma}{2\hbar^2 k^2}} e^{\pm 2i k_{\rho0} \rho}$ with $k_{\rho0} = \pm k_{\rho0} + \sqrt{k_{\rho0}^2 + \frac{\gamma}{\hbar^2}}$ and $k_{\rho0} = m^* \gamma/\hbar^2$. After a tedious derivation, we find that for the conventional metal surface with the same interferometer setup shown in Fig. 1, the correction in the spin-resolved LDOS due to the magnetic flux can be approximated by

$$\Delta N_k^0(r, \omega, B) \approx -2 \text{Im} \left[ \tilde{f}(\omega) \tau^3 \int \int f_\mu(\rho_1) f_\nu(\rho_2) d\rho_1 d\rho_2 \right] \times \left[ \cos (2\pi \Phi_0/\Phi_0) - 1 \right], \quad (11)$$

from which the absence of $\Phi_0$ AB oscillatory period becomes obvious.

In summary, we have performed a semiclassical analysis of the SP-STM probed AB oscillations in the LDOS induced by two impurities on a TI surface as well as on a conventional metal surface with spin splitting. We have found that the total LDOS in both systems present WL phenomenon with an oscillatory period $\Phi_0$ in the AB oscillations. Remarkably, the analogous WAL signified by a $\Phi_0/2$ oscillation period has been found in the spin-resolved LDOS in the TI system, while it was absent in the conventional metal surfaces. This phenomenon, which can be observed in the SP-STM experiments, may provide an important signature for the existence of the topological surface states and provide a useful criterion to distinguish the TI surface from other two-dimensional systems.

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