

Competition between Weak Localization and Antilocalization in Topological Surface States

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A magnetoconductivity formula is presented for the surface states of a magnetically doped topological insulator. It reveals a competing effect of weak localization and weak antilocalization in quantum transport when an energy gap is opened at the Dirac point by magnetic doping. It is found that, while random magnetic scattering always drives the system from the symplectic to the unitary class, the gap could induce a crossover from weak antilocalization to weak localization, tunable by the Fermi energy or the gap. This crossover presents a unique feature characterizing the surface states of a topological insulator with the gap opened at the Dirac point in the quantum diffusion regime.

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Topological surface states, composed of an odd number of massless Dirac cones, are peculiar to three-dimensional (3D) topological insulators [1–3]. Electrons in these states have a helical spin structure in momentum space, and acquire a π Berry's phase after completing a closed trajectory adiabatically around the Fermi surface. The π Berry phase could lead to the absence of backscattering [4], weak antilocalization [5], and the absence of Anderson localization [6,7]. In the quantum diffusion regime (mean free path \ll system size \sim phase coherent length), an electron maintains its phase coherence after being scattered by static centers for many times. As a result, the destructive interference due to the π Berry phase can give a quantum enhancement to the classical electronic conductivity, leading to weak antilocalization (WAL) [8,9]. Applying a magnetic field tends to break the destructive interference, giving rise to negative magnetoconductivity (MC), a key signature of WAL. WAL is expected in systems with symplectic symmetry. Much effort has been devoted to observing WAL in graphene [5,10–13]. However, graphene has two valleys of gapless Dirac cones with opposite chiralities, and the intervalley scattering will inevitably suppress WAL [5,10–13]. In contrast, the surface states of recently discovered topological insulators Bi_2Te_3 and Bi_2Se_3 have only one helical Dirac cone [14–16], and WAL is intrinsic to them. Many observations of WAL in Bi_2Te_3 and Bi_2Se_3 have been reported recently [17–22]. In particular, there is great interest in the effect of magnetic doping, which is considered to be an efficient way to open an energy gap in the Dirac cone by breaking time reversal symmetry (TRS) [23–25]. This gap is expected to give rise to many interesting phenomena, such as Majorana fermion [26], topological magnetoelectric effect [27], and quantized anomalous Hall effect [28]. These developments call for a thorough theoretical investigation on WAL in topological insulators, in particular, in the presence of magnetic doping.

In this Letter, a MC formula is presented for the magnetically doped surface states of a topological insulator [Fig. 1(a)]. We assume that the mean field produced by magnetic doping may open a uniform gap at the Dirac point [24,25] [Fig. 1(b)], and the local fluctuation over the mean field can scatter conducting electrons in a random fashion [Fig. 1(c)]. With the help of the diagrammatic technique [5,8–10,29–35], we obtain the MC formula, which consists of two competing terms. Besides the WAL term due to the gapless Dirac fermion, an extra weak localization (WL) term arises as a result of the gap opening. We find that either the gap or the magnetic scattering can drive MC of the system from WAL to a parabolic dependence on the magnetic field ($\sim B^2$). Further increasing the gap/Fermi energy ratio may drive the system to WL after reaching the B^2 regime. A crossover from

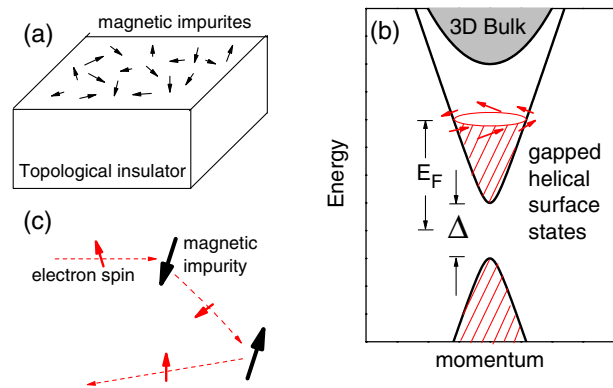


FIG. 1 (color online). (a) A topological insulator with magnetic doping on the top surface. (b) Magnetic doping may open a gap (Δ) at the Dirac point of the surface states [24,25]. E_F is the Fermi energy measured from the Dirac point. Δ tilts in-plane spin polarization of the massless Dirac fermion out of plane, leading to the deviation from the π Berry phase. (c) Scattering of an electron by random magnetic impurities. Dashed lines represent the trajectory of the electron.

WAL to WL is thus expected, tunable by the size of the TRS-breaking gap or the position of Fermi energy. Beyond the theories for non-Dirac systems with strong spin-orbit coupling [30] or strong ferromagnetism [36], the observation of the crossover will provide an important signature in transport experiments for the existence of a TRS-breaking gap in the topological surface states.

We describe the magnetically doped surface states of a 3D topological insulator by the massive Dirac model H in a random impurity potential $U(\mathbf{r})$. The Hamiltonian of the massive Dirac model is given by

$$H = \gamma(\sigma_x k_y - \sigma_y k_x) + h_z \sigma_z, \quad (1)$$

where $\sigma_{x,y,z}$ are the Pauli matrices. $\gamma = \hbar v_F$, with v_F the Fermi velocity. The σ_z term represents a gap opened by breaking TRS, with $h_z = \frac{1}{2}g\mu_B B + \frac{\Delta}{2}$, where the first term is the Zeeman energy of the out-of-plane magnetic field B , with g the g factor and μ_B the Bohr magneton. Δ is the gap opened at the Dirac point [24,25], it originates from the mean field produced by magnetic doping. The Hamiltonian describes two energy bands as shown in Fig. 1(b). In this work, we assume that the Fermi energy E_F is tuned into the gap of the 3D bulk bands, and intersects with the upper band of the surface states, which is the only band included in the calculation. Its band dispersion is given by $\epsilon_{\mathbf{k}} = \sqrt{\gamma^2 k^2 + h_z^2}$ and the wave function $\psi_{\mathbf{k}}(\mathbf{r}) = [a, -ie^{i\varphi}b]^T e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{S}$, where $\tan\varphi \equiv k_y/k_x$, \mathbf{k} is the wave vector, $a \equiv \cos\frac{\theta}{2}$, $b \equiv \sin\frac{\theta}{2}$, and $\cos\theta \equiv h_z/\sqrt{h_z^2 + \gamma^2 k^2}$, S is the area. In this work, all the physical quantities will be evaluated at the Fermi energy E_F at low temperatures. The density of states at E_F is $N_F = E_F/(2\pi\gamma^2)$. The scattering by nonmagnetic and magnetic impurities is modeled by the random potential

$$U(\mathbf{r}) = \sum_{i,\alpha} u_{\alpha}^i \sigma_{\alpha} \delta(\mathbf{r} - \mathbf{R}_i), \quad (2)$$

where α runs over 0, x , y , z . σ_0 is the 2×2 unit matrix. \mathbf{R}_i are the positions of the randomly distributed impurities. u_0^i depicts the potential at \mathbf{R}_i for nonmagnetic impurity, and $u_{x,y,z}^i$ for magnetic impurity. Note that $u_{x,y,z}^i$ do not represent the total local exchange field produced by the impurity at \mathbf{R}_i , but the local fluctuation over the mean field that gives the gap. Therefore, $\langle U(\mathbf{r}) \rangle_{\text{imp}} = 0$ and we can still assume the random potential is delta-correlated $\langle U(\mathbf{r})U(\mathbf{r}') \rangle_{\text{imp}} \sim \delta(\mathbf{r} - \mathbf{r}')$, where $\langle \cdots \rangle_{\text{imp}}$ means average over impurity configurations, and we follow the practical assumption that different types of impurity scattering are uncorrelated [10].

The quantum interference correction to conductivity of Dirac fermions can be calculated by the diagrams in Fig. 2, which are different from those for the usual two-dimensional electron gas (2DEG) [8,9,31,32] in several aspects [5,10,29]. (i) Besides the conventional maximally

crossed diagram (bare Hikami box) in Fig. 2(a), two dressed Hikami boxes in Fig. 2(b) are also needed; each gives $-1/4$ as the bare Hikami box for the gapless Dirac cone. (ii) The ladder diagram correction to the bare velocity $v_{\mathbf{k}}^x \equiv (1/\hbar)\partial\epsilon_{\mathbf{k}}/\partial k_x$ [Fig. 2(d)] must be taken into account, which corrects the velocity to $\tilde{v}_{\mathbf{k}}^x = 2v_{\mathbf{k}}^x$ for the gapless Dirac cone. We generalize these conclusions for the gapless case to the gapped Dirac cone as follows.

The arrowed lines in Fig. 2 stand for the impurity-averaged retarded (R) and advanced (A) Green's functions $G_{\mathbf{k}}^{R/A}(\omega) = 1/(\omega - \epsilon_{\mathbf{k}} \pm i\hbar/2\tau)$, where under the first-order Born approximation, the impurity-induced self-energy is given by the total scattering time τ , with $\hbar/\tau \equiv 2\pi \sum_{\mathbf{k}'} \langle |U_{\mathbf{k}'\mathbf{k}}|^2 \rangle_{\text{imp}} \delta(\omega - \epsilon_{\mathbf{k}'})$, where $U_{\mathbf{k},\mathbf{k}'} \equiv \langle \psi_{\mathbf{k}}(\mathbf{r}) | U(\mathbf{r}) | \psi_{\mathbf{k}'}(\mathbf{r}) \rangle$ is the scattering amplitude between two momenta. It can be separated into $1/\tau = 1/\tau_e + 1/\tau_m$, where the nonmagnetic elastic scattering time τ_e is given by $\hbar/\tau_e = 2\pi N_F n_0 u_0^2 (a^4 + b^4)$ and the total magnetic scattering time τ_m can be separated into $1/\tau_m = 2/\tau_x + 1/\tau_z$, with $\hbar/\tau_z = 2\pi N_F n_m u_z^2 (a^4 + b^4)$ and $\hbar/\tau_x = 2\pi N_F n_m u_x^2 (2a^2 b^2)$. In-plane isotropy ($u_x = u_y$) is assumed. u_0 depicts the average scattering strength for nonmagnetic impurities, while $u_{x,y,z}$ for magnetic impurities. n_0 and n_m are concentrations of nonmagnetic and magnetic impurities, respectively. τ_e and τ_m are related to the elastic scattering length ℓ_e and magnetic scattering length ℓ_m by $\ell_e = \sqrt{D\tau_e}$ and $\ell_m = \sqrt{D\tau_m}$, respectively. $D \equiv v_F^2 \tau / 2$ is the diffusion constant. Considering the poor

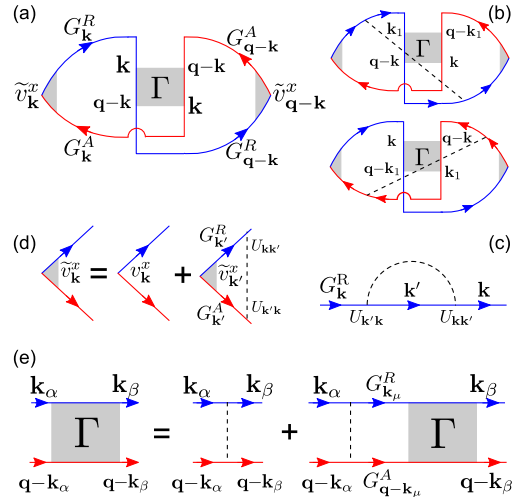


FIG. 2 (color online). The diagrams for the quantum interference correction to conductivity of Dirac fermions. The arrowed solid and dashed lines represent the Green's functions and impurity scattering, respectively. (a) The bare [31,32] and (b) two dressed [10] Hikami boxes give the quantum conductivity correction from the maximally crossed diagrams. (c) The retarded Green function with the first-order Born approximation to the impurity-averaged self-energy. (d) Ladder diagram vertex correction to velocity [29]. (e) The Bethe-Salpeter equation for the vertex of maximally crossed diagrams.

surface mobility [18–20], we assume that ℓ_e is much shorter than the phase coherence length ℓ_ϕ , as required by the quantum diffusion transport.

In the conductivity diagrams Figs. 2(a) and 2(b), the vertex function Γ from the maximally crossed diagrams usually is proportional to $1/q^2$, where \mathbf{q} is the summation of momenta before and after scattering. Since Γ diverges as $q \rightarrow 0$, it contributes mainly to backscattering. This allows us to sum \mathbf{k} and \mathbf{k}_1 for small q first, and write the zero-temperature conductivity correction from the bare and two dressed Hikami boxes as

$$\sigma^F = -\frac{e^2 N_F v_F^2 \tau^3 \sin^2 \theta}{\hbar^2} \eta_v^2 (1 + 2\eta_H) \sum_{\mathbf{q}} \Gamma(\mathbf{q}), \quad (3)$$

where η_v comes from the correction to velocity from the ladder diagrams in Fig. 2(d), with

$$\eta_v = \left[1 - \frac{1}{2} \left(\frac{\tau}{\tau_e} - \frac{\tau}{\tau_z} \right) \frac{2a^2 b^2}{a^4 + b^4} \right]^{-1}, \quad (4)$$

and each of the dressed Hikami boxes gives an extra η_H contribution as the bare Hikami box, with

$$\eta_H = -\frac{1}{2} \left(1 - \eta_v^{-1} - \frac{\tau}{\tau_x} \right). \quad (5)$$

η_v and η_H reduce to 2 and $-1/4$, respectively, in the absence of magnetic doping [5,10,29].

In Fig. 2, the total momentum is conserved on the incoming and outgoing sides of the vertex Γ , allowing the Bethe-Salpeter equation of the vertex to be written as [5] $\Gamma_{\mathbf{k}_\alpha \mathbf{k}_\beta} = \Gamma_{\mathbf{k}_\alpha \mathbf{k}_\beta}^0 + \sum_{\mathbf{k}_\mu} \Gamma_{\mathbf{k}_\alpha \mathbf{k}_\mu}^0 G_{\mathbf{k}_\mu}^R G_{\mathbf{q}-\mathbf{k}_\mu}^A \Gamma_{\mathbf{k}_\mu \mathbf{k}_\beta}$, where $\mathbf{k}_\alpha + \mathbf{k}_\beta = \mathbf{q}$, $\mathbf{k}_{\alpha,\beta}$ are the incoming and outgoing momenta, respectively. For small q , the bare vertex $\Gamma_{\mathbf{k}_\alpha \mathbf{k}_\beta}^0 \equiv \langle U_{\mathbf{k}_\alpha, \mathbf{k}_\alpha} U_{\mathbf{q}-\mathbf{k}_\beta, \mathbf{q}-\mathbf{k}_\alpha} \rangle_{\text{imp}}$ is found as $\Gamma_{\mathbf{k}_\alpha \mathbf{k}_\beta}^0 \approx \frac{\hbar}{2\pi N_F} [A + B e^{i(\varphi_\alpha - \varphi_\beta)} + C e^{i2(\varphi_\alpha - \varphi_\beta)}]$, with $A = (\tau_e^{-1} + \tau_z^{-1}) \frac{a^4}{a^4 + b^4}$, $B = [(\tau_e^{-1} - \tau_z^{-1}) \frac{2a^2 b^2}{(a^4 + b^4)} - 2\tau_x^{-1}]$, $C = (\tau_e^{-1} + \tau_z^{-1}) \frac{b^4}{a^4 + b^4}$. Different from the usual 2DEG, both the bare vertex $\Gamma_{\mathbf{k}_\alpha \mathbf{k}_\beta}^0$ and the advanced Green function $G_{\mathbf{q}-\mathbf{k}_\mu}^A$ are explicit functions of the momentum angle.

We propose an ansatz to the full vertex function

$$\Gamma_{\mathbf{k}_\alpha \mathbf{k}_\beta} = \frac{\hbar}{2\pi N_F \tau} \sum_{n,m \in 0,1,2} \gamma_{nm} e^{i(n\varphi_\alpha - m\varphi_\beta)}, \quad (6)$$

where γ_{nm} are the expansion coefficients independent of $\varphi_{\alpha,\beta}$. By putting the ansatz into the Bethe-Salpeter equation and expanding $G_{\mathbf{q}-\mathbf{k}_\mu}^A$ up to q^2 , we obtain the solution to the expansion coefficients

$$\gamma = 2 \begin{bmatrix} g_0 + Q^2 & iQ_+ & \frac{1}{2}Q_+^2 \\ iQ_- & g_1 + Q^2 & iQ_+ \\ \frac{1}{2}Q_-^2 & iQ_- & g_2 + Q^2 \end{bmatrix}^{-1}, \quad (7)$$

where $Q_\pm = Q_x \pm iQ_y$, $Q^2 = Q_x^2 + Q_y^2$, $\mathbf{Q} = v_F \tau \sin \theta (q_x, q_y)$, and the ‘‘Cooperon gaps’’

$g_0 \equiv 2 \left[\frac{a^4 + b^4}{a^4} \frac{1/\tau}{(1/\tau_e + 1/\tau_z)} - 1 \right]$, $g_1 \equiv 2 \left[\frac{1/\tau}{(1/\tau_e - 1/\tau_z) \frac{2a^2 b^2}{a^4 + b^4} - 2/\tau_x} - 1 \right]$, $g_2 \equiv 2 \left[\frac{a^4 + b^4}{b^4} \frac{1/\tau}{(1/\tau_e + 1/\tau_z)} - 1 \right]$. We note that it is crucial to include all the off-diagonal terms of γ in the calculation. Without them, the vertex will be 2 times larger [33,34] when going back to the gapless limit [5], and the derived MC formula cannot recover to that for 1/4 of graphene [10]. $\Gamma(\mathbf{q})$ in Eq. (3) can be obtained by letting $\mathbf{k}_\alpha = \mathbf{k}$ and $\mathbf{k}_\beta = \mathbf{q} - \mathbf{k}$ in $\Gamma_{\mathbf{k}_\alpha \mathbf{k}_\beta}$, and for $q \rightarrow 0$, $\varphi_{\mathbf{k}} - \varphi_{\mathbf{q}-\mathbf{k}} \approx \pi$. Finally, we collect the most divergent terms of the vertex

$$\Gamma(\mathbf{q}) \approx \frac{\hbar/(\pi N_F \tau)}{g_0 + (1 + \frac{1}{g_1})Q^2} - \frac{\hbar/(\pi N_F \tau)}{g_1 + (1 + \frac{1}{g_0} + \frac{1}{g_2})Q^2}. \quad (8)$$

Zero-field conductivity correction $\sigma^F(0)$ can be calculated by performing the integral over q in Eq. (3) between $1/\ell_e$ and $1/\ell_\phi$, respectively [5]. In the presence of the perpendicular magnetic field B , q^2 will be quantized into $q_n^2 = (n + 1/2)(4eB/\hbar) \equiv (n + 1/2)/\ell_B^2$, where n labels the Landau levels. Summation over n gives the conductivity correction $\sigma^F(B)$ at finite field [8]. The magnetoconductivity $\Delta\sigma(B) \equiv \sigma^F(B) - \sigma^F(0)$ is found for $\ell_B^2/\ell_e^2 \gg 1$ as

$$\Delta\sigma(B) = \sum_{i=0,1} \frac{\alpha_i e^2}{\pi h} \left[\Psi \left(\frac{\ell_B^2}{\ell_\phi^2} + \frac{\ell_B^2}{\ell_i^2} + \frac{1}{2} \right) - \ln \left(\frac{\ell_B^2}{\ell_\phi^2} + \frac{\ell_B^2}{\ell_i^2} \right) \right], \quad (9)$$

with Ψ the digamma function,

$$\alpha_1 = -\frac{\eta_v^2 (1 + 2\eta_H)}{2(1 + \frac{1}{g_0} + \frac{1}{g_2})}, \quad \ell_1^{-2} = \frac{g_1}{2\ell^2 \sin^2 \theta (1 + \frac{1}{g_0} + \frac{1}{g_2})}, \quad (10)$$

$$\alpha_0 = \frac{\eta_v^2 (1 + 2\eta_H)}{2(\frac{1}{g_1} + 1)}, \quad \ell_0^{-2} = \frac{g_0}{2\ell^2 \sin^2 \theta (\frac{1}{g_1} + 1)},$$

and $1/\ell^2 \equiv 1/\ell_e^2 + 1/\ell_m^2$. In the absence of magnetic impurities, $\alpha_0 = 0$, $\alpha_1 = -1/2$, one predicts WAL with a prefactor $-1/2$, consistent with the experimental observations [18–20]. For a finite gap, because α_0 and α_1 have opposite signs, the MC formula has two competing contributions, α_1 leads to WAL, α_0 to WL. ℓ_0 and ℓ_1 give corrections to ℓ_ϕ , in particular, when they are much shorter than ℓ_ϕ . This formula is the key result of this work.

We first examine the limit of weak magnetic scattering, i.e., $\ell_m \gg \ell_\phi$ [17–20]. We plot MC for different $\Delta/2E_F$ in Fig. 3(c). For $\Delta/2E_F = 0$, MC shows a positive cusp, which is the signature of WAL. As $\Delta/2E_F$ increases, MC gradually develops a B^2 dependence, and the system evolves into the unitary regime. Further increasing $\Delta/2E_F$ will change the sign of MC from negative to positive, i.e., a WL-like MC. Different from the usual 2DEG, the WL-like MC here has a prefactor $\sim 1/2$, instead of 1 [31]. This can be seen in Fig. 3(a), where we show the weight factors of the competing WL and WAL terms in the MC formula. In the limit of small $\Delta/2E_F$, α_1 overweighs

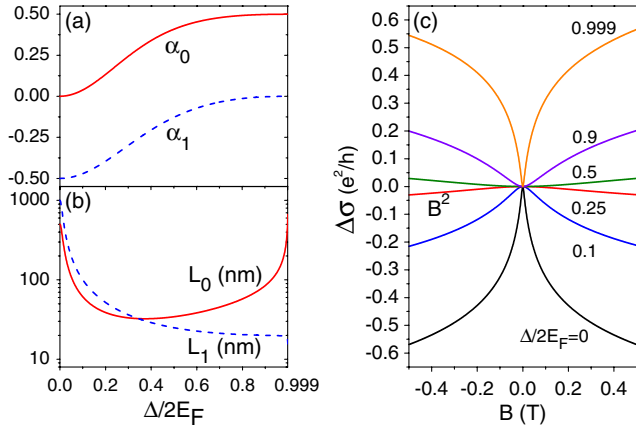


FIG. 3 (color online). (a) WL (α_0) and WAL (α_1) weight factors as functions of $\Delta/2E_F$, where Δ is the gap, E_F is the Fermi energy. (b) WL (ℓ_0) and WAL (ℓ_1) lengths as functions of $\Delta/2E_F$. (c) Magnetoconductivity $\Delta\sigma(B)$ for different $\Delta/2E_F$ in the limit of weak magnetic scattering. $\ell_\phi = 300$ nm. $\ell_m = 1000$ nm. $u_x = u_z$ is assumed.

α_0 , so MC is mainly contributed by WAL, with the maximal prefactor $-1/2$. In the limit of large $\Delta/2E_F$, α_1 vanishes and α_0 goes to $1/2$, then we have WL with the maximal prefactor $1/2$. As shown in Fig. 3(b), either ℓ_1 for small $\Delta/2E_F$ or ℓ_0 for large $\Delta/2E_F$ is much larger than ℓ_ϕ , this keeps the system well inside the quantum diffusion regime, and protects WAL or WL. For intermediate $\Delta/2E_F$, where both the WL and WAL terms contribute, the weak B^2 MC indicates that the system is driven from the quantum to classical diffusion regime due to the effective reduction of ℓ_ϕ by the much shorter ℓ_0 and ℓ_1 . The crossover from WAL to WL by changing $\Delta/2E_F$ can be understood with the Berry phase [4], which is readily evaluated for the surface band $\psi_{\mathbf{k}}(\mathbf{r})$ as

$$-i \int_0^{2\pi} d\varphi \left\langle \psi_{\mathbf{k}}(\mathbf{r}) \left| \frac{\partial}{\partial \varphi} \psi_{\mathbf{k}}(\mathbf{r}) \right. \right\rangle = \pi \left(1 - \frac{\Delta}{2E_F} \right). \quad (11)$$

It gives π for WAL when $\Delta/2E_F = 0$, and 0 for WL when $\Delta = 2E_F$. A similar argument was also given for the gap opened by the finite size effect [37]. In the limit of strong magnetic scattering $\ell_m \ll \ell_\phi$, both WAL and WL are suppressed, as shown in Fig. 4. On the other hand, because the Fermi energy in the ratio Δ/E_F can be controlled independently by gate voltage [18,19], it is possible to observe the transition from negative to positive MC by tuning the gate voltage even in this limit.

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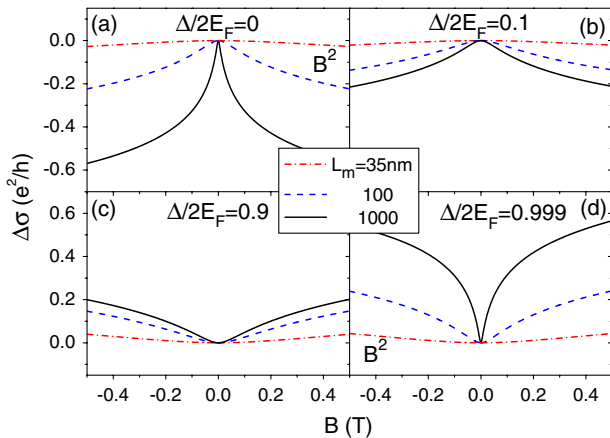


FIG. 4 (color online). Magnetoconductivity $\Delta\sigma(B)$ for different magnetic scattering lengths ℓ_m and $\Delta/2E_F$. $\ell_\phi = 300$ nm. $u_x = u_z$ is assumed. Shorter ℓ_m means stronger magnetic scattering.

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