Domain wall skew scattering in ferromagnetic Weyl metals

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We study transport in the presence of magnetic domain walls (DWs) in a lattice model of ferromagnetic type-I Weyl metals. We compute the diagonal and Hall conductivities in the presence of a DW, using both Kubo and Landauer formalisms, and uncover the effect of DW scattering. When the Fermi level lies near Weyl points, we find a strong skew scattering at the DW which leads to a significant additional Hall effect. We estimate the average Hall resistivity for multi-domain configurations and identify the limit where the DW scattering contribution becomes significant. We show that a continuum model obtained by linearizing the lattice dispersion around the Weyl points does not correctly capture this DW physics. Going beyond the linearized theory, and incorporating leading curvature terms, leads to a semi-quantitative agreement with our lattice model results. Our results are relevant for experiments on the Hall resistivity of spin-orbit coupled ferromagnets, which can have Weyl points near the Fermi energy.

I. INTRODUCTION

The anomalous Hall effect (AHE), a spontaneous deflection of electronic currents in magnetic solids, is now well-understood to result from two mechanisms: an intrinsic effect due to the Berry curvature of electronic bands, and an extrinsic effect arising from impurity scattering of electrons near the Fermi level [1]. The intrinsic Berry curvature is also intimately tied to band topology and topological invariants [2], as known from the two-dimensional (2D) quantum Hall effect, where the Hall conductivity $\sigma_{xy}$ takes on a quantized value determined by the Chern number $\mathcal{C}$ [3, 5]. In 3D, a layered quantum Hall state with a full bulk gap can undergo a transition into a topological Weyl semimetal as we increase the interlayer hopping [6]. The simplest inversion-symmetric and time-reversal broken Weyl semimetal features electronic bands which touch at two Weyl points [7], around which the dispersion is approximately linear. Such a pair of Weyl points cannot be removed by any small perturbations, and they act as a source and a sink of the Berry curvature. When the Fermi level coincides with the energy of the Weyl points, it leads to an intrinsic Hall conductivity $\sigma_{xy} = e^2Q/2\hbar$ where $Q$ is the momentum-space separation between the Weyl points [8]. In fact, as a result of the linear dispersion around the Weyl points, $\sigma_{xy}$ is pinned to this value for a finite range of the Fermi energy around the Weyl point energy $\mathcal{E}_0$. In this regime, the system is a Weyl metal with Fermi surfaces enclosing the individual Weyl points.

A large AHE arising from such Weyl points has been observed in several magnetic materials including ferromagnets such as Co$_3$Sn$_2$S$_2$ [9, 10] and Co$_2$MnGa [11], and antiferromagnets such as Mn$_2$X (X = Sn, Ge) [12, 13]. Among oxide ferromagnets, SrRuO$_3$ [14] hosts Weyl points near the Fermi level [15–18], which has been shown to account for its unusual nonmonotonic dependence of the AHE on magnetization, including a sign-change at a certain temperature below $T_c$. This non-monotonic AHE may be understood as the effect of the magnetization dependence of the band structure, with the Weyl points and Berry curvature being tuned by the temperature-dependent magnetization [11, 15, 16].

Recent Hall resistivity measurements of SrRuO$_3$ thin films have discovered unusual hysteresis loops, with bump-like anomalies in $\rho_{xy}$ near the coercive field where the magnetization begins to reverse direction as we go through the hysteresis loop [19]. The origin of these anomalies is still debated. Early proposals regarded these bumps as an extra Hall effect induced by chiral magnetic skyrmions [19–23] which can nucleate during the magnetization reversal and can be stabilized by the interfacial Dzyaloshinskii-Moriya (DM) interactions stemming from the strong spin-orbit coupling and the inversion-breaking substrate-film interfaces [19]. An alternative proposal argued that these anomalies emerged from imperfections in the thin films due to thickness inhomogeneities or site vacancies [24–28], leading to multiple regions in space with distinct electronic and magnetic properties. Simply adding up contributions to $\rho_{xy}$ from distinct regions was argued to qualitatively reproduce the Hall anomalies [24–28]. Strikingly, measurements of the magneto-optical Kerr effect in SrRuO$_3$ films [29] discovered similar bump-like anomalies, but in films which were hundreds of unit cells thick, so that interfacial DM interactions and skyrmions play no role. In previous theoretical work, we showed that magnetic domains play an important role, and these Kerr anomalies can be captured by locally averaging the Kerr effect over these domains [29], an approach justified by the locality of the high frequency response.

In contrast to our theory for the Kerr anomalies, it is far from clear that previous theories for the Hall anomalies, which simply add up $\rho_{xy}$ from spatially distinct regions, provide a meaningful way to account for d.c. transport. In particular, such approaches do not explicitly account for bulk states scattering off DWs. Given the large number of magnetic solids with Weyl points, and the ubiquity of magnetic domains in such systems, it is clearly important to understand how magnetic DWs impact the Hall response of Weyl semimetals and metals. This is the key goal of our paper.
In order to examine the impact of magnetic DWs on transport in a Weyl metal, we study a minimal cubic-lattice model of a ferromagnetic which supports two Weyl points in the bulk band structure. Fig. 1 shows a configuration with two magnetic domains having uniform vector magnetizations $M_L$ and $M_R$. We assume the magnetization in each domain is uniform and choose the DW to be in the $yz$-plane. For large domains with linear dimension much larger than the electron mean free path, we may also view such an idealized flat DW as a section of a realistic meandering DW. In this paper, we compute the diagonal and Hall conductivities in the presence of such a DW using a full real-space Kubo formula and compare this with a Landauer theory framework which focuses on the states near the Fermi level scattering off the DW. This comparison allows us to discover a strong skew-scattering contribution to the Hall transport arising at the DW, which is significant when the Fermi energy is not too far from the Weyl points.

Previous theoretical work on the AHE in antiferromagnetic Weyl metal MnSn/Ge [30] has studied Hall transport in the plane of a magnetic DW and shown that chiral Fermi arc modes localized on the DW can dominate this Hall effect. By contrast, our work here examines transport in the plane perpendicular to the DW and the DW scattering of bulk states at the Fermi level. We compare our lattice model result with a continuum theory where we linearize around the Weyl points and discover that our lattice model result with a continuum theory where we linearize around the Weyl points and discover that curvature terms lead to semi-quantitative agreement with beyond the linearized theory and incorporating leading order processes [31].

We consider a four-band ferromagnetic model on a cubic lattice with a uniform magnetization $M$ [32]:

$$\mathcal{H}(k, M) = t(\sin k_x \sigma_x + \sin k_y \sigma_y + \sin k_z \sigma_z) \tau_z + m(k) \tau_x - J \mathbf{M} \cdot \sigma, \quad (1)$$

where the Hamiltonian $H = \sum_{k} C_{k}^\dagger \mathcal{H}(k, M) C_{k}$ is defined in the basis of $C_{k} = (c_{kA}^\dagger, c_{kA}, c_{kB}^\dagger, c_{kB})$. The Pauli matrices $\tau$ act on the orbital index $A$ and $B$, while the Pauli matrices $\sigma$ act on spin ($\uparrow, \downarrow$). The mass term $m(k) = r(3 - \cos k_x - \cos k_y - \cos k_z)$. Time reversal symmetry is broken by the magnetization $M$. For $M = M \hat{z}$, the model has a four-fold rotation symmetry around the $z$-axis and the inversion symmetry $\tau_x \mathcal{H}(-k) \tau_x = \mathcal{H}(k)$.

The dispersion is then given by

$$E(k) = \pm \sqrt{t^2(\sin^2 k_x + \sin^2 k_y) + (JM \pm D(k))^2}, \quad (2)$$

$$D(k) \equiv \sqrt{m^2(k) + t^2 \sin^2 k_z}. \quad (3)$$

For $M = 0$, the band structure has a four-fold degenerate Dirac node at the $\Gamma$ point of the Brillouin zone (BZ). With a nonzero $M$, this Dirac point splits into two Weyl points, which are located at zero energy and momenta $k_{\text{dir}} = (0, 0, \pm k^*_z)$, where

$$\cos k^*_z = \frac{-r^2 - \sqrt{t^4 + (r^2 - t^2)J^2 M^2}}{r^2 - t^2}. \quad (4)$$

The Weyl point separation $2k^*_z$ depends on the magnetization $M$. Figure 2(a) shows the band structure for $M = 1$. In this plot, and the rest of the paper, we fix $r = 0.8t$, and $J = t$. As we increase $M$, the two Weyl points move away from each other and mutually annihilate at the BZ boundary. This results in a fully gapped quantum Hall insulator with a quantized $\sigma_{xy} = e^2 G/2\pi h$ at half filling, where $G = 2\pi/a_0$ is the reciprocal lattice constant, and $a_0$ is the lattice constant of the cubic crystal. In the rest of this work, we study this model in the Weyl metal regime.

### II. MODEL FOR WEYL METAL

We consider a four-band ferromagnetic model on a cubic lattice with a uniform magnetization $M$ [32]:

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For a spatially uniform magnetization, $\sigma_{xy}$ is obtained from the momentum-space integration of the Berry curvatures

$$
\sigma_{xy} = \frac{e^2}{\hbar} \int \frac{d^3k}{(2\pi)^3} \sum_n f(E_{kn})\Omega^z(kn),
$$

(5)

where $f$ is the Fermi-Dirac distribution at temperature $T$, and $\Omega^z(kn)$ is the z-component of the Berry curvature vector for a state with momentum $k$ and band index $n$. Figure 2(b) shows $\sigma_{xy}$ at $T = 0$ as a function of Fermi energy $E_F$ for a uniform z-magnetization $M = 1$. It exhibits a plateau-like behaviour in the window sandwiched between the two dashed lines, which has been studied in Ref. 8. This is referred to as the Weyl metal regime where the Fermi surface consists of two disjoint closed surfaces surrounding the individual Weyl points, and the dispersions are approximately linear near the Weyl points. The magnitude of $\sigma_{xy}$ for the plateau is determined by its value at $E_F = 0$, which is proportional to the momentum-space separation between the two Weyl points, $Q = 2k^*_z$. For $M = 1$, the separation $Q = 2.2a_0^{-1}$, and the plateau value is given by $\sigma_{xy} = e^2Q/2\pi\hbar \approx 0.35e^2/\hbar a_0$, which can also be seen from Fig. 2(b).

III. DOMAIN WALL AND HALL CONDUCTIVITY: KUBO FORMULA RESULT

We introduce a flat DW parallel to the $yz$-plane as shown in Fig. 1 which partitions the system into left and right domains whose magnetizations are respectively denoted by $M_L$ and $M_R$. Since the Weyl points in the minimal model Eq. 1 are always pinned to zero energy, completely independent of the magnetization, we supplement this model with a term $H_\Delta$ that also tunes the energy of the Weyl points in the right domain relative to those in the left domain.

$$
H_\Delta = \Delta \sum_i \Theta(i_x) C_i^\dagger C_i,
$$

(6)

where $\Theta(i_x)$ is the lattice Heaviside step function, namely $\Theta(i_x) = 0$ for $i_x < 0$ and 1 otherwise, and $i_x$ is the $x$-coordinate of the site $i$. The reason for including this term is that we envision that in a realistic setting and in material-specific models, there will be a relative energy shift of the Weyl points between the two domains. For instance, when domains are nucleated as we traverse the hysteresis loop, this energy shift $\Delta$ could reflect a difference in the magnitude of the magnetization between majority and minority domains in the presence of the external field, or it could reflect a local difference in the environment as minority magnetic domains are nucleated in regions with distinct strain fields or doping or site vacancies.

We compute the AHE of the above domain configuration using the Kubo formula (see also Appendix A) This full result contains contributions from bulk intrinsic Berry curvature as well as DW scattering effects. To study this, we consider a system with open boundary conditions in the $x$-direction and periodic boundary conditions along $y$- and $z$-directions. We choose the magnetizations to be $M_L = M \hat{z}$ and $M_R = -M \hat{z}$. Later, in Section IV E we will discuss the effect of tilting the magnetization vector. To obtain the AHE, which is time-reversal odd, we compute the transverse response for a magnetic configuration and its time-reversed counterpart and subtract one from the other in order to antisymmetrize.

Fig. 3 shows the anomalous Hall conductivity $\sigma_{yx}$ as a function of $\Delta$. Here, we have fixed the Hamiltonian parameters $M = 1$, $J = 1$ and $r = 0.8t$. We chose $E_F = 0.4t$, and used a system size $(L_x, L_y, L_z) = (150, 300, 300)a_0$.
with the DW in the center at \( x = L_x/2 \). As we vary \( \Delta \) within the window shown in Fig. [3] the bulk contribution \( \sigma_{yx}^{L,R} \) from deep within the interior of each domain stay roughly constant due to the plateau feature discussed in section [4] and they are opposite to each other \( \sigma_{yx}^{L} \approx -\sigma_{yx}^{R} \). We thus expect the bulk contributions to nearly cancel, leaving a DW contribution \( \sigma_{yx}^{DW} \) to dominate the Hall response. Interestingly, we observe a significant contribution from the DW scattering in the limit when the left domain is electron-like and the right domain is hole-like, i.e. \( \Delta > E_F = 0.4t \). It can even have a similar order of magnitude as the bulk value \( 0.35e^2/ha_0 \), e.g. at \( \Delta = 0.9t \). This implies a non-negligible DW scattering contribution to the AHE in the Weyl metal. We now turn to study the impact of DW scattering using Landauer theory and show that it indeed accounts for the \( \Delta \)-dependence of the Hall response.

IV. DOMAIN WALL SCATTERING

In this section, we focus on the DW scattering of bulk Bloch eigenstates, which will be used to later extract the Hall response using the Landauer formula [35, 36]. We show that the transmission and the reflection at the DW exhibit a skewness, similar to the impurity-induced skew scattering in a spin-orbit coupled ferromagnet. A notable feature is that the skewness is very pronounced when there are Weyl points near the Fermi level, which results in a significant Hall effect contribution. We later compare the DW scattering contribution to the bulk contribution. Finally, we will discuss the impact of tilting \( \mathbf{M}_R \) relative to \( \mathbf{M}_L \) on the Hall effect.

A. Scattering states

In the presence of a DW in the \( yz \)-plane, the eigenstates of the inhomogeneous problem \( H + H_\Delta \) consist of bound states and scattering states. Boundary states such as Fermi arc modes, originating from a change in topology across the DW when the magnetizations are opposite, exist as bound states at the DW [32, 37, 38]. Scattering states, on the other hand, are propagating waves and extend over the system. We will focus on the scattering states which are important for studying transport across the DW. The scattering states are divided into two groups: left-incident and right-incident, denoted by \( |\Psi_{D,E,k_\parallel\alpha}\rangle = \Psi_{D,E,k_\parallel\alpha}(0) \), where \( D = L, R \) are the label of left- or right-incident respectively. The energy \( E \) and the parallel momentum \( k_\parallel = (k_y, k_z) \) are conserved quantities for elastic scattering. \( \alpha \) is an additional label for multiple left(right)-incident channels. In the case that we will consider, there is a single incident channel once \( D, E, k_\parallel \) are fixed but we retain this label \( \alpha \) for generality.

We focus on states at the Fermi level \( E = E_F \). The creation operators \( \Psi_{D,E,k_\parallel\alpha}^\dagger \) can be expressed in terms of the basis \( C_{ia}^\dagger \) as the following,

\[
\Psi_{D,E,k_\parallel\alpha}^\dagger = \sum_{ia} \psi_{D,E,k_\parallel\alpha}(ia) C_{ia}^\dagger, \tag{7}
\]

where \( \psi_{D,E,k_\parallel\alpha}(ia) \) is the amplitude of the scattering state at site \( i \) and combined orbital-spin label \( a \). Similar to a continuum inhomogeneous problem, e.g. a potential-step problem, the amplitude can be expressed as a linear combination of the amplitudes of Bloch states of the homogeneous systems \( \mathcal{H}(k, M_L, R) \). The coefficients of the linear combination relation can be identified with the RC and TC of the incident mode upon scattering at the DW. For instance, the amplitude of the left-incident scattering state can be written as

\[
\psi_{L,E,F,k_\parallel\alpha}(ia) = \begin{cases} 
\varphi_{\alpha k_\parallel}(ia) + \sum_{\beta} r_{L,k_\parallel\beta}^{\alpha\beta} \varphi_{\beta k_\parallel}(ia) & (i_x < 0), \\
\sum_{\beta} r_{L,k_\parallel\beta}^{\alpha\beta} \varphi_{\beta k_\parallel}(ia) & (i_x \geq 0),
\end{cases} \tag{8}
\]

where \( \varphi_{\alpha k_\parallel}(ia) \) and \( \varphi_{\beta k_\parallel}(ia) \) are the amplitudes of the incident and reflected Bloch waves respectively, which are eigenstates of \( \mathcal{H}(k, M_L) \). \( \varphi_{\beta k_\parallel}(ia) \) is the amplitude of a transmitted Bloch wave, which is an eigenstate of \( \mathcal{H}(k, M_R) \). These are the states at the Fermi surfaces surrounding Weyl points as shown schematically in Fig. 4(a). The \( \beta \) summation is performed over all the reflected

![Diagram](image-url)
Similarly, TC is defined by $v$ to complex-valued problems as the following. Constructed from the eigenstates of the homogeneous states.

Similarly, the right-incident scattering states can be constructed from the eigenstates of the homogeneous problems $H$ on their Fermi surfaces are connected by RCs and TCs in the left-incident scattering states.

Such highly skew features result in a large Hall effect, which can be seen by considering any pair of left-incident scattering states whose $k_y$ momenta are opposite, i.e. $(k_y, k_z)$ and $(-k_y, k_z)$. The two incident Bloch states move with the opposite group velocities in the $y$-direction and get transmitted asymmetrically at the DW, as illustrated in Fig. 3(c). This produces a transverse Hall current when a bias voltage between the two domains is applied. This will be studied quantitatively in the next subsection by computing Hall conductance using Landauer formula. Such skewness is, in fact, expected in systems with strong spin-orbit couplings [40, 41]. However, our new result here is that the skewness is very pronounced when the Fermi level resides near the Weyl points. We have checked that when $E_F$ is far away from the Weyl points, such skewness is weaker, and TCs are many order of magnitude smaller (see Appendix B), which leads to a very small Hall contribution. Thus, DW scattering is significant when there are Weyl points near $E_F$.

**B. Skew reflection and skew transmission**

Figure 3 shows RCs and TCs for the left-incident scattering states as a function of their labels $k_i$, featuring a pronounced skewness between any pair of state with the same $k_x$ and opposite $k_y$. This implies that a pair of incident Bloch waves moving opposite to each other in the $y$-direction get transmitted asymmetrically at the DW, as illustrated in (c). This results in a transverse Hall current in the presence of a bias voltage between the two domains.

TCs and RCs for the left-incident scattering states are computed using a method described in great detail in Ref. [39].

**C. Landauer theory of domain wall Hall conductance**

Hall conductance arising from DW scattering and longitudinal conductance across the DW can be computed within the Landauer formalism [35, 36] using TCs and RCs obtained above. In the presence of an applied bias voltage $\Delta V_x$, a current density along $x$-direction $j_x$ and $y$-direction $j_y$ are produced. These can be computed using the scattering states as derived in Appendix C (see also Ref. [40] and Ref. [41]). From these, we obtain the expressions for the conductance per unit cross section area...
\[
g_{xx} = j_x / \Delta V_x \quad \text{and} \quad g_{yx} = j_y / \Delta V_x
\]
as shown below

\[
g_{xx} = \frac{e^2}{\hbar} \int \frac{dk_y}{(2\pi)^2} \left[ T^{\alpha \rightarrow \beta}_{L_x k_1} \right]_{E=E_F};
\]

\[
g_{yx} = \frac{e^2}{2\hbar} \int \frac{dk_y}{(2\pi)^2} \left[ \frac{v_{y\alpha}}{|v_{x\alpha}|} + \frac{v_{y\beta}}{|v_{x\beta}|} + \frac{|v_{y\beta}|}{|v_{x\beta}|} T^{\alpha \rightarrow \beta}_{L_x k_1} \right]_{E=E_F}
\]

Summations over the incident channel \( \alpha \), reflected channel \( \beta \), and transmitted channel \( \beta \) are implicit. These expressions are valid at zero temperature where only states at \( E_F \) are important. To obtain anomalous Hall response which is time-reversal odd, we antisymmetrize \( g_{yx} \) as described in Section III for the Kubo Hall conductivity; we will continue to refer to the antisymmetrized version as \( g_{yx} \) in the rest of the paper.

Figure 6(a) and (b) show the \( \Delta \) dependence of \( g_{xx} \) and \( g_{yx} \) for the model parameters as in Section III. The ratio \( g_{yx}/g_{xx} \) shown in Fig 6(c) is rather large and is of the order of \( 10^{-1} \), which is a consequence of having highly skew TCs. We will show that the largeness of this ratio leads to an observable DW scattering contribution. Before that we first compare \( g_{yx} \) to the Hall conductivity obtained from Kubo formula in Section III.

We observe that the \( \Delta \) dependence of \( g_{yx} \) in Fig 6(b) and that of \( \sigma_{yx} \) in Fig 3 bear a strong resemblance. More importantly, they have the same sign at each \( \Delta \). These suggest that \( \sigma_{yx} \) in Fig 3 indeed tracks the DW scattering contribution which arises from skew scatterings at the DW. The connection between \( g_{yx} \) and \( \sigma_{yx} \) may be established by the following argument.

In the Kubo approach, we suppose that the Bloch electrons have a lifetime \( \hbar/\gamma \), where \( \gamma \) is an energy broadening used in the single-particle Green’s function. This translates to a mean free path \( \ell_0 = v_F \hbar/\gamma \), where \( v_F = \partial E/\hbar \partial k \) is the Fermi velocity. Only electrons at a distance less than \( \ell_0 \) from the DW can experience DW scattering, and they see a potential drop \( \Delta V_x \sim \ell_0 E_x \) across the DW, where \( E_x \) is the electric field. We thus infer from the Kubo calculation, a transverse current density due to DW scattering in this region, given by \( j_y = \sigma_{yx}^{\text{DW}} (\Delta V_x/\ell_0) = g_{yx}^{\text{DW}} \Delta V_x \). Thus, \( g_{yx}^{\text{DW}} = \sigma_{yx}^{\text{DW}} / \ell_0 \), which can be compared with \( g_{yx} \) in the Landauer formalism. Now, we have earlier argued that the Kubo response for our specific domain configuration is expected to have cancelling bulk contribution, so the entire result is expected to be dominated by \( \sigma_{yx}^{\text{DW}} \). We will thus use the computed curve in Fig. 3 as our estimate for \( \sigma_{yx}^{\text{DW}} \).

Our choice of \( \gamma = 0.01t \) used in the Kubo calculation, with \( v_F \approx a_0 t/\hbar \) from the band structure, where \( t \) is the hopping parameter and \( a_0 \) is the lattice constant, then leads to \( \ell_0 = 100 a_0 \). We thus expect \( g_{yx}^{\text{DW}} \approx \sigma_{yx}^{\text{DW}}/100 a_0 \). This is in reasonable agreement (within a factor of two) with the Landauer result shown in Fig. 6(b).

We have also checked that increasing \( \gamma \), which reduces \( \ell_0 \), leaves our estimated \( g_{yx}^{\text{DW}} \) to be nearly unchanged, so that this agreement between the Kubo and Landauer results is not sensitive to the choice of \( \gamma \) so long as it is not too small.

**D. Multidomain configurations: comparing bulk versus DW scattering contribution**

The DW scattering contribution in a transport experiment will clearly be sensitive to the number of minority domains and their domain sizes. For few and small minority domains, the measured Hall response will be dominated by the intrinsic bulk contribution. As we increase the number of minority domains, the DW contribution will increase, while the net bulk contribution will decrease due to partial cancellation between majority and minority domains. To gain a perspective on when the DW scattering contribution becomes significant relative to the bulk intrinsic contribution, we consider a simple multi-domain setting with a series of parallel yz-DWs. For simplicity, let us assume two types of domains with collinear magnetizations, \( \mathbf{M}_+ = M \hat{z} \) and \( \mathbf{M}_- = -M \hat{z} \), pointing along the \( z \)-direction, and \( N_{\text{DW}} \) DWs over the sample length \( L_x \), so that the average distance between two neighbouring DWs is \( L_x/N_{\text{DW}} \). Such a configuration has a \( z \)-mirror symmetry, under which \( (x, y) \rightarrow (-x, -y) \) but the magnetizations are left invariant. This enforces the conductances \( G_{yz} = G_{xz} = 0 \), thus simplifying the conductance tensor.

In the limit where the electron mean free path \( \ell_0 \ll L_x/N_{\text{DW}} \), we consider an \( x \)-interval \( (x_{\text{DW}} - \ell_0/2, x_{\text{DW}} + \ell_0/2) \), centered around a DW at \( x_{\text{DW}} \), where the Hall effect may be dominated by DW scattering. In the presence of a current density \( j_x \), the Hall voltage in this
The Hall effect here. Setting $\Delta$ to zero and setting the magnetization reversal process where magnetic domains proliferate and under an applied magnetic field in the $z$-direction, the magnetizations in the majority and the minority domains can become non-collinear. We study the impact of such non-collinearity on the DW Hall effect here. Setting $\Delta$ to zero and setting the norm of magnetization to unity, we consider two tilting cases: (1) $\mathbf{M}_L = \hat{z}$ and a tilting parallel to the $yz$ DW $\mathbf{M}_R = -(0, \sin \theta, \cos \theta)$ and (2) $\mathbf{M}_L = \hat{z}$ and a tilting out of the $yz$ DW $\mathbf{M}_R = -(\sin \theta, 0, \cos \theta)$. 

E. Impact of tilting the magnetization vectors

In a realistic system, there can be an easy-axis anisotropy along a certain low-symmetry direction. During a magnetization reversal process where magnetic domains proliferate and under an applied magnetic field in the $z$-direction, the magnetizations in the majority and the minority domains can become non-collinear. We study the impact of such non-collinearity on the DW Hall effect here. Setting $\Delta$ to zero and setting the norm of magnetization to unity, we consider two tilting cases: (1) $\mathbf{M}_L = \hat{z}$ and a tilting parallel to the $yz$ DW $\mathbf{M}_R = -(0, \sin \theta, \cos \theta)$ and (2) $\mathbf{M}_L = \hat{z}$ and a tilting out of the $yz$ DW $\mathbf{M}_R = -(\sin \theta, 0, \cos \theta)$.
Figure (a) and (b) show the impact of tilting in case (1) on the conductance per unit cross section area. $g_{yx}$ is nonzero due to the combination of (i) asymmetry of TCs as shown in Fig. (d) and (ii) the asymmetry of the magnitude of the group velocity $|v_y|$ which was absent in previous discussions and is now expected when the magnetization has a non-vanishing $y$-component. $g_{yx}$ is an even function of $\theta$, which can be understood by how the Hall conductivity transforms under the mirror $M_y$ followed by time reversal $T$. The magnitudes of both $g_{xx}$ and $g_{yx}$ are smaller than those in Fig. However, the $g_{yx}/g_{xx}$ ratio remains large and of the same order $\sim 10^{-1}$, so the DW scattering contribution to Hall effect is expected to be noticeable in experiment as inferred from Eq.\ref{eq:13} \cite{42}.

In case (2), $g_{yx}$ is zero for all the tilting angle $\theta$ (not shown). TCs are found to be symmetric ($|v_y|$ is also symmetric since the $y$-component of the magnetization vanishes.) It is unclear what protects TCs from being asymmetric. The net Hall conductivity (intrinsic + extrinsic) is non-zero in this case as allowed by symmetry, namely the broken $M_y$ and the broken $T$ are sufficient to allow a non-zero Hall effect in the $xy$-plane. However, the Hall contribution from the DW scattering vanishes. $g_{yx}$ becomes non-zero when $\Delta$ is set to non-zero. It is possible that a combination of particle-hole symmetry broken by a non-zero $\Delta$ and $M_y T$ broken by a non-zero $y$-component of the magnetization are responsible for the symmetric TCs. We have not done a full symmetry analysis of the TCs; we defer this to future work.

V. CONTINUUM MODEL OF WEYL METAL

In this section, we discuss the DW scattering within a continuum model obtained from Taylor expanding the lattice model dispersion around the Weyl points. We find that at linear order in momentum, the continuum model can lead to an incorrect result, while a qualitative agreement with the lattice model is obtained when we keep quadratic terms. This suggests that the higher order terms are important for studying DW scattering in Weyl metals.

For $M_L = M_R = 1$ corresponding to the magnetizations in the $z$-direction, the Weyl points reside at the same momentum positions for both domains $k_{wp} = (0, 0, \pm k_z^*)$ where $k_z^*$ is given in Eq.\ref{eq:4}. Let $q \equiv k - k_{wp}$. The linearized continuum model is given by

$$H(q)_{L/R} = t_{q_x} \sigma_x + t_{q_y} \sigma_y + J \sigma_z + \sigma_z \left[ t(\sin k_{z}^* + \cos k_{z}^* q_z) \tau_z + r(1 - \cos k_{z}^* + \sin k_{z}^* q_z) \tau_x \right],$$

where we have performed a unitary transformation $U = \text{diag}(1, 1, 1, -1)$ on Eq.\ref{eq:4} before the linearization. Here $q_x$ is viewed as an operator $q_x = -i d/dx$ since the translational invariance along the $x$-direction is broken. $q_y$ and $q_z$ are still good quantum numbers and can be treated as numbers. We can diagonalize the term in the square bracket for a given $k_z$. As a result, the two domains can be simultaneously block diagonalized into the following form.

$$H(q)_{L/R} = t_{q_x} \sigma_x + t_{q_y} \sigma_y + \sigma_z \left( \begin{array}{cc} Z_+ & J \\ 0 & Z_- \end{array} \right),$$

where $Z_{\pm}$ are the eigenvalues of the matrix in the square bracket in Eq.\ref{eq:14}. Let $Z_+ \geq 0$ and $Z_- \leq 0$. In the left domain with $-J$, all propagating-wave solutions at a small, positive Fermi level reside on the bands associated with the Weyl points and thus correspond to the upper block where the mass term $Z_+ - J$ can become zero. This means that the propagating-wave solutions in the left domain have zero weight in the lower-block entry. For the right domain, the mass term $Z_- + J$ in the lower block can instead become zero. Therefore, the propagating-wave solutions in the right domain have zero weight in the upper block. These result in a zero transmission for all $(q_y, q_z)$ since the incident modes from the left domain are orthogonal to the transmitted modes in the right domain. This result is robust against adding the energy shift term $H_{\Delta}$. Therefore, at linear order, the continuum model predicts a zero transmission and suggests an infinite DW resistance. This is obviously incorrect, for we have seen nonzero transmission and a rich $\Delta$ dependence of TC in the full lattice model. The orthogonality and the existence of a basis where $H_{L/R}$ can be simultaneously block diagonalized are an artefact of the linearized model and can be removed by keeping higher order terms.

Fig. 9 shows the comparison between the RCs and TCs obtained from the lattice model and the quadratic model, featuring their qualitative agreement in terms of their asymmetry in $k_y$.
Finally, we note that when $M_L \neq M_R$, the linear model predicts nonzero TCs like in the lattice model. However, they are a few orders of magnitude smaller. All these suggest that (1) the linear model is insufficient for studying the DW scattering and (2) higher order terms are responsible for the results discussed in the previous sections.

VI. CONCLUSION

We have shown that DW scattering in Weyl metals for states on the Fermi surfaces surrounding the Weyl points is highly skew. This can lead to a large, observable AHE contribution. For Fermi level away from Weyl points, the effect of DW scattering diminishes. Therefore, the DW scattering contribution must not be neglected when there are Weyl points near the Fermi level. A continuum model obtained from linearizing the Weyl metal lattice model around the Weyl points fails to capture this result. We show that curvature terms in momentum are needed to qualitatively reproduce the results of the lattice model. Our results call for a re-examination of AHE in SrRuO$_3$ thin films through a realistic model in the presence of DWs in order to understand the peculiar bumps features in the AHE hysteresis loops. Our results may also be tested in transport experiments on ferromagnetic Weyl metals Co$_3$Sn$_2$S$_2$ [9,10] and Co$_2$MnGa [11]. Our results also suggest that the extra AHE observed in the antiferromagnetic Weyl metal CeAlGe during a magnetic domain proliferation process could be attributed to DW scattering [31]. Another important message of our work is that a careful account of such DW scattering must be taken into consideration before one can attribute Hall resistivity anomalies to the topological Hall effect due to skyrmion spin textures.

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Appendix A: Kubo formula

In linear response, the d.c. conductivity is given by

$$\sigma_{\alpha\beta} = \lim_{\omega \to 0} \frac{i2\pi e^2}{V} \sum_{k_i,m,n} \frac{f(E_{k_{1m}}) - f(E_{k_{1n}})}{E_{k_{1m}} - E_{k_{1n}}} \left[ \frac{\langle \hat{j}\rangle_{mn}}{\hbar\omega + i\gamma + E_{k_{1m}} - E_{k_{1n}}} \right] \right]_\alpha \left. \right|_{\beta},$$

(A1)

where $V$ is the volume, $f$ is the Fermi distribution function, $k_i = (k_x, k_z)$, $E_{k_{1m}}$ is an energy eigenvalue, $m,n$ are the band indices, $\langle \hat{j}\rangle_{mn} = \langle k_{1m} | \hat{j}_x | k_{1n} \rangle$, and $\gamma$ is a small broadening. The current operator is obtained from Peierls substitution in each hopping term $t_{ia,jb}c_{ia}^\dagger c_{jb}$ as the following.

$$t_{ia,jb}c_{ia}^\dagger c_{jb} \rightarrow t_{ia,jb}c_{ia}^\dagger c_{jb} \exp \left( i \int_{i}^{j} dr \cdot A \right),$$

(A2)

$$\approx t_{ia,jb}c_{ia}^\dagger c_{jb} \left( 1 + \frac{1}{2} \right) \left( 1 + \text{i} r_{ij} \frac{A(i) + A(j)}{2} \right),$$

(A3)

where $r_{ij} = r_j - r_i$, and $A$ is a vector potential corresponding to an electric field $E = -\partial A/\partial t$. The current operator at a site $i$ is given by

$$\hat{j}(i) = \frac{\delta H[A]}{\delta A(i)},$$

(A4)

where $H[A]$ is the Hamiltonian after the Peierls substitution. A real-space expression of the lattice model, Eq.(1) can be found in Ref.[32].

The current operator in Eq.(1) is defined by $\hat{j}_x = \sum_i \hat{j}_x(i)$. Since the system has translational invariance along $y$ and $z$, $\hat{j}_x$ can be Fourier transformed partially in $(y, z)$ space and becomes block diagonal in $k_i$. Each block corresponding to a $k_i$ is a $4L_x$ by $4L_y$ matrix, where $4$ is the number of band of the model in the homogeneous case. This matrix can be used to numerically evaluate $\langle \hat{j}\rangle_{mn}$. 

Appendix B: Transmission coefficient away from Weyl points

Figure 10 shows TCs at $E_F = 5t$ far away from Weyl points and for $\Delta = 0.1t$ and $M_L = M_R = 1$. The skewness of TCs is weaker than that when $E_F$ is near Weyl points in Fig.6. Meanwhile, TCs here are 4 order of magnitude smaller than TCs near Weyl points, leading to a very small $g_{xy}$ compared to that in Fig.4. In contrast, the bulk $\sigma_{xy}$ only reduces by 2 order of magnitude from $0.35e^2/ha_0$ when $E_F = 0$ to 0.0055e$^2/ha_0$ when $E_F = 5t$. These suggest that the impact of DW on Hall effect is small away from Weyl points and becomes significant when $E_F$ lies near Weyl points.
FIG. 10. Transmission coefficient at $E_F = 5t$, far away from the Weyl points and for $\Delta = 0.1t$ and $M_L = M_R = 1$. The transmission coefficients are orders of magnitude small than those where $E_F$ lies near Weyl points.

Appendix C: Computation of conductance

In a bias voltage $\Delta V_x$, the current density can be computed by using the scattering states. The left-incident states are associated with a Fermi distribution function $f_L(E) = f(E - (E_F - e\Delta V_x))$, while $f_R(E) = f(E - E_F)$ for the right-incident states. This is because the left-incident states are in equilibrium with a reservoir at a different potential energy due to $\Delta V_x$. The current density $j_\nu$ for $\nu = x,y$ is given by

$$j_\nu = -e \int \frac{dk_\| dE}{(2\pi)^3 h} \left[ \frac{1}{2} \hat{v}_{k_{\|} l, \alpha} \frac{1}{2} \hat{v}_{k_{\|} l, \beta} \right] \left[ f_L(E) - f_R(E) \right],$$

(C2) where we have identified $\frac{1}{V} \sum \langle k \rangle = \int \frac{dk_\| dE}{(2\pi)^3 h} \frac{1}{|E/E|\Delta k_x}$. The last identification is not strictly rigorous since the denominator $dE/dk_x$, i.e., the group velocity in the x-direction, is spatially dependent. The proper way is to have a normalization factor in the scattering states $\frac{1}{V}$, which is done by attaching a prefactor $\frac{1}{\sqrt{|E|}}$ to Eq. (1) and $\frac{1}{\sqrt{|E|}}$ to Eq. (9). It ensures the anticommutators of the creation and annihilation operators, $\{ \Psi_D; E k_\|, \alpha \}, \Psi_D^\dagger; E' k'_\|, \alpha' \} = \delta_{D D'} \delta(E - E') \delta(k_\| - k'_\|) \delta_{\alpha \alpha'}$, where $D, D' = L, R$ denote the left- or right-incident states. We have included this normalization factor in Eq. (C1). From these, we obtain

$$j_x = \frac{e^2 \Delta V_x}{2(2\pi)^3 h} \int dk_{\|} \left[ \hat{v}_{k_{\|} l, x} \hat{v}_{k_{\|} l, \beta} R_{L,k_\|} - \hat{v}_{k_{\|} l, x} \hat{v}_{k_{\|} l, \beta} T_{L,k_\|} \right]_{E=E_F},$$

(C4) by

$$j_x = \frac{e^2 \Delta V_x}{2(2\pi)^3 h} \int dk_{\|} \left[ 1 - R_{L,k_\|} + T_{L,k_\|} \right]_{E=E_F},$$

(C5) This is the familiar Landauer formula which relates conductance to transmission coefficients.

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