Real space Berry curvature of itinerant electron systems with spin-orbit interaction

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By considering an extended double-exchange model with spin-orbit coupling (SOC), we derive a general form of the Berry phase \( \gamma \) that electrons pick up when moving around a closed loop. This form generalizes the well-known result valid for SU(2) invariant systems, \( \gamma = \Omega/2 \), where \( \Omega \) is the solid angle subtended by the local magnetic moments enclosed by the loop. The general form of \( \gamma \) demonstrates that collinear and coplanar magnetic textures can also induce a Berry phase different from 0 or \( \pi \), smoothly connecting the result for SU(2) invariant systems with the well-known result of Karplus and Luttinger for collinear ferromagnets with finite SOC. By taking the continuum limit of the theory, we also derive the corresponding generalized form of the real space Berry curvature. The new expression is a generalization of the scalar spin chirality, which is presented in an explicitly covariant form. We finally show how these simple concepts can be used to understand the origin of the spontaneous topological Hall effect that has been recently reported in collinear and coplanar antiferromagnetic phases of correlated materials.

I. INTRODUCTION

The phenomenon of colossal magnetoresistance (CMR) provides a clear example of the dramatic effects of magnetism on electronic transport.\textsuperscript{1,2} The ability of changing the longitudinal electric resistivity by several orders of magnitude with an external magnetic field generated a wide interest,\textsuperscript{3,4} not only due to its multiple technological applications, including magnetic recording, but also because of the rich fundamental physics arising from the interplay between charge and spin degrees of freedom. Indeed, colossal magnetoresistance is an example of the profound influence of quantum mechanics on the macroscopic behavior of correlated materials.

The phenomenon of CMR only refers to the diagonal components of the conductivity tensor. It is natural to ask if a similar dramatic change of the off-diagonal components of the conductivity tensor can also be achieved by exploiting the interplay between localized magnetic moments and conduction electrons.\textsuperscript{5} Like in the case of CMR materials, the first affirmative answer to this question arose from the study of ferromagnets, whose transverse resistivity contains a term that remains non-zero even after switching off the applied magnetic field.\textsuperscript{6–8} Given that the magnetization, \( \mathbf{M} \), is apparently the only axial vector that characterizes the system in absence of the external field, it is not surprising that the observed “anomalous Hall effect” (AHE) turned out to be proportional to \( \mathbf{M} \). However, subsequent experiments showed that \( \rho_{xy} \) can be a non-monotonic function of \( \mathbf{M} \). This key observation led to the discovery of a much more interesting phenomenon of quantum mechanical origin.\textsuperscript{9}

Karplus and Luttinger made a seminal contribution to the problem of anomalous Hall effect by considering the band structure of ferromagnets in the presence of spin-orbit interaction.\textsuperscript{10} They pointed out that the anomalous velocity arises from inter-band matrix elements of the current operator. Smit provided an alternative explanation of the phenomenon by attributing the AHE to skew scattering with impurities.\textsuperscript{11} Later, another extrinsic mechanism, side jump, was proposed by Berger, which is related to the shift of the electron during its collision with an impurity.\textsuperscript{12} The skew scattering mechanism leads to a contribution to \( \rho_{xy} \) that is proportional to the longitudinal resistivity \( \rho \). In contrast, the intrinsic and side-jump mechanisms give \( \rho_{xy} \propto \rho^2 \). This behavior of \( \rho_{xy} \) was confirmed by a transport measurement in the spinel \( \text{CuCe}_2\text{Se}_4-x\text{Br}_x \).\textsuperscript{13} In general, the dominant mechanism depends on the material consideration. Our current understanding indicates that skew scattering is dominant in relatively clean materials, while the intrinsic mechanism is dominant in relatively dirty materials.\textsuperscript{14,15}

The vast implications of the explanation of the AHE offered by Karplus and Luttinger became clear after the derivation of the Hall conductance by Thouless \textit{et al.} and their analysis of the quantum Hall effect.\textsuperscript{16} In particular, it was understood that the AHE can be attributed to a Berry phase associated with the Bloch wave functions in solids.\textsuperscript{18,19} This Berry phase can arise through different mechanisms. Ye \textit{et al.}\textsuperscript{20} proposed a mechanism based on the observation that a carrier moving in a non-coplanar spin background acquires a real space Berry phase, which affects the motion of electrons in the same way as the Aharonov-Bohm phase arising from a physical magnetic field. Refs. 22 and 23 also discussed the relevance of non-coplanar spin configurations to the AHE in the context of perovskite-type manganites at high temperatures. A similar mechanism was proposed for pyrochlore ferromagnets and for noncoplanar antiferromagnets.\textsuperscript{25–31} However, Jungwirth \textit{et al.}\textsuperscript{19} showed that non-coplanar spin ordering is not actually necessary to produce an AHE. They related the AHE of collinear ferromagnets directly to a Berry phase in momentum space, which arises from the way in which the spin-orbit cou-
orderings are slightly higher than 100T. If we consider that the strongest pulsed field that can be achieved in a closed loop, which cannot be distinguished from the Aharonov-Bohm phase $2\pi$ acquired by the electronic wave function when the electron moves in a closed loop, which cannot be distinguished from the Aharonov-Bohm phase $2\pi$ acquired by the electronic wave function when the electron moves in a closed loop, which cannot be distinguished from the Aharonov-Bohm phase $2\pi$ produced by a magnetic flux equal to $\gamma\Phi_0/2\pi$ ($\Phi_0$ is the flux quantum). Given that spins of an elementary plaquette can subdue a solid angle comparable to $2\pi$, the effective magnetic flux produced by a non-coplanar spin ordering can be of the order of one flux quantum per elementary plaquette. For real materials, the area of an elementary plaquette can be as small as a few Å², implying that the effective magnetic field produced by a non-coplanar spin ordering can reach values of order $10^6$T. This is an enormous magnetic field if we consider that the strongest pulsed field that can be currently generated in the high magnetic field facilities are slightly higher than 100T.

The effective gauge field induced by non-coplanar spin-orderings can be illustrated with the so-called s-d exchange model. This idea originates from the seminal papers by Zener, and Anderson and Hasegawa, which discuss the double exchange interaction generated in the limit of large exchange coupling between the local moments and the conduction electrons. In this limit, the spin of the electron is forced to be aligned with the underlying spin field. As a consequence, the effective hopping matrix element between two sites $j$ and $k$ with local classical magnetic moments $\mathbf{S}_j = S\mathbf{n}_j$ and $\mathbf{S}_k = S\mathbf{n}_k$, becomes

$$\tilde{t}_{kj} = t_{kj} \langle n_j | n_k \rangle = t_{kj} \cos(\chi_{kj}/2)e^{i\Omega_{njk}/2},$$

(1)

where $| n_k \rangle$ is the coherent spin state polarized along the $n_k$ direction, $\mathbf{S}_k \cdot \mathbf{n}_k | n_k \rangle = S | n_k \rangle$, $\chi_{kj}$ is the angle between the $j$ and $k$ local moments, $\chi_{kj} = \arccos(\mathbf{n}_j \cdot \mathbf{n}_k)$, and $\Omega_{njk}$ is the solid angle subtended by $\mathbf{n}_j$, $\mathbf{n}_k$, and a reference unit vector $\mathbf{n}$. When the electron moves in a closed loop, such as a triangular plaquette, it picks up a Berry phase equal to the sum of the phases $\Omega_{njk}$ of each hopping amplitude. This sum is independent of the reference vector $\mathbf{n}$ (gauge invariance) and equal to half of the solid angle enclosed by the loop of spins on the unit sphere. In the continuum limit (infinitesimal small loops), this solid angle is proportional to the scalar spin chirality, $\mathbf{n}_j \cdot \mathbf{n}_k \times \mathbf{n}_i$, which then acts as an effective magnetic field on the orbital degree of freedom of the conduction electrons.

In general, the spin-orbit interaction, which is always present in solids, modifies the above argument based on the scalar spin chirality. For example, a theoretical study of Mo oxides has proposed that the spin-orbit interaction significantly modifies the Hall conductivity of the non-coplanar phase, producing a much larger Hall effect in multi-band systems. However, to date, a systematic understanding of how the spin-orbit interaction modifies the geometric picture associated with the scalar spin chirality mechanism is lacking. The purpose of this article is to derive the effective gauge field that emerges from a given magnetic texture in the presence of finite SOC. The SOC enters in the single-electron tight-binding Hamiltonian as a fixed SU(2) gauge field (defined on the lattice bonds), whose value is determined by the interplay between the relativistic spin-orbit interaction and the crystal structure. We note that this field can fluctuate in theories where the ionic positions are allowed to fluctuate (e.g., theories that include electron-phonon coupling). In this work, we only include the electronic degrees of freedom, implying that the SU(2) gauge field remains frozen. The inclusion of finite SOC coupling in the hopping term of the s-d model leads to a more general form of the real space Berry curvature (or effective magnetic field) in the double-exchange limit. In particular, it will become evident that non-coplanarity of the magnetic structure is no longer a requirement for producing a non-trivial real space Berry curvature, i.e., collinear and coplanar structures can also produce an effective magnetic field in the presence of SOC. We will also see that the case of collinear ferromagnets that was originally considered by Karpplus and Luttinger is simply a limiting case of the general formula that we will derive here. Moreover, by taking the continuum limit of the model Hamiltonian under consideration, we derive an explicitly gauge invariant form of the Berry curvature that generalizes the notion of scalar spin chirality. Finally, we consider a few simple examples to illustrate the applicability of these simple concepts to models and materials that exhibit topological Hall effect induced by coplanar and collinear magnetic orderings.

The presentation of our results is organized as follows. In Sec. II we formulate the general problem and we introduce the model Hamiltonian that will be used in the rest of the manuscript. Sec. III introduces a geometric approach for the computation of the electronic Berry phase in the presence of SOC. Mathematically oriented readers may find this approach more appealing than the algebraic treatment that is introduced in Sec. IV. However, the algebraic approach is probably more amenable for the general reader, who can skip Sec. III in a first reading of the manuscript. A similar consideration can be applied to the continuum limit of the theory that is described in Sec. V. While it is important to understand how the notion of scalar spin chirality (i.e., the source of the Berry curvature in the SU(2) invariant case) must be generalized in the presence of SOC, this is not a requirement for...
understanding the subsequent section, which is devoted to applying the generalized form of the real space Berry curvature to simple lattice models. These simple models in Sec. VI capture the essence of the topological Hall effect that has been recently observed in materials with coplanar and collinear antiferromagnetic orderings, such as Mn₃Sn⁴² and CoNb₃S₆.⁴³

II. GENERAL FORMULATION

We will consider itinerant electrons that interact with localized magnetic moments via an exchange coupling \( J \). For simplicity, we will assume that quantum fluctuations are small, implying the localized spins can be approximated by classical moments, \( S_j = S n_j \), where \( n_j \) is a normalized vector field,

\[
  n_j = (\sin \theta_j \cos \phi_j, \sin \theta_j \sin \phi_j, \cos \theta_j),
\]

representing the direction of the classical moment \( S_j \). In this classical limit, the sign of the exchange interaction \( J \) can be changed by the unitary transformation: \( S_j \to -S_j \). Consequently, without loss of generality, we will adopt a ferromagnetic sign \( J > 0 \). The simplest Hamiltonian that describes this physics is:

\[
  H = H_t + H_J,
  H_t = \sum_{jk} (t_{kj} c_k \text{e}^{-i\alpha_{kj}} c_{j}^\dagger + t_{kj}^\ast c_{j}^\dagger \text{e}^{i\alpha_{kj}} c_k),
  H_J = -\frac{JS}{2} \sum_j c_j^\dagger \sigma c_j \cdot n_j.
\]

where \( \sigma = (\sigma_1, \sigma_2, \sigma_3) \) is a vector of the Pauli matrices. Here we are using the spinor notation:

\[
  c_k = \begin{bmatrix} c_k^\dagger \\ c_{k\perp} \end{bmatrix}, \quad c_k^\dagger = \begin{bmatrix} c_k^\dagger \\ c_{k\perp}^\dagger \end{bmatrix}.
\]

The unitary operator \( U_{kj} \) is an SU(2) rotation matrix taking the general form

\[
  U_{kj} = \exp \left[ -\frac{i\alpha_{kj}}{2} (a_{kj} \cdot \sigma) \right],
\]

where \( \alpha_{kj} \) is the rotation angle induced by the finite spin-orbit interaction, \( a_{kj} \) is the unit vector in the direction of the rotation axis. The complex hopping amplitudes \( t_{kj} \) can be expressed as \( t_{kj} = |t_{kj}| \text{e}^{i\beta_{kj}} \). We note that \( H \) becomes SU(2) invariant in absence of SOC: \( \alpha_{kj} = 0 \) (\( \forall k \)).

We will also assume that the exchange interaction \( J \) is comparable or larger than the bandwidth of the itinerant electrons. In this so-called double-exchange limit, the electronic spin orientation must remain parallel to the underlying localized spin. The resulting low-energy Hamiltonian is simply a spinless fermion tight-binding model with effective complex hopping amplitudes,

\[
  \tilde{t}_{kj} = \tau_{kj} \text{e}^{i\gamma_{kj}},
\]

determined by the configuration of the underlying magnetic moments:

\[
  \tau_{kj} = t_{kj} \sqrt{\frac{1 + n_k \cdot R_{kj} \cdot n_j}{2}}.
\]

The SO(3) rotation matrix

\[
  R_{kj} = \exp \left[ \alpha_{kj} (a_{kj} \cdot L) \right],
\]

corresponds to the SU(2) rotation defined by the matrix \( U_{kj} \) in Eq. (5), where \( L = (L^x, L^y, L^z) \) is a vector of the standard SO(3) generators \( [L^a]_{bc} = -\delta^{ab} \). This is just a generalization of the Anderson-Hasegawa or Double Exchange model to the case with finite SOC.⁴⁶,³⁷

We are interested in the net phase \( \Phi_{jkl} \) that the electronic wave function picks up as the electron moves around the triangle \( jkl \). This phase is equal to the sum of two contributions:

\[
  \Phi_{jkl} = \beta_{jkl} + \gamma_{jkl},
\]

where \( \beta_{jkl} = \beta_{jl} + \beta_{lk} + \beta_{kj} \), is the phase that arises from the complex nature of the hopping amplitudes \( t_{kj} \), which must be equal to 0 or \( \pi \) because \( H_t \) is time reversal invariant. The Berry phase,

\[
  \gamma_{jkl} = \gamma_{jl} + \gamma_{lk} + \gamma_{kj},
\]

arises from the strong exchange interaction between the electronic spin and the local moments, i.e., from the projection of the electronic spin state of each site \( j \) into the low-energy state:

\[
  |n_j\rangle = \cos \frac{\theta_j}{2} |\uparrow\rangle + \sin \frac{\theta_j}{2} \text{e}^{i\phi_j} |\downarrow\rangle.
\]

While our requirement of adiabaticity is not necessary for generating a real space Berry curvature, it greatly simplifies the analysis. In particular, it helps to identify the Berry curvature with a fictitious magnetic field that couples to the orbital motion of the itinerant electrons. In the absence of SOC, the flux of this effective magnetic field (in units of the flux quantum) through a closed loop is equal to half of the solid angle subtended by the local moments when moving around that loop. Correspondingly, in the long wavelength limit, the fictitious magnetic field on a triangular plaquette \( jkl \) is proportional to the scalar product of the three local moments: \( n_j \cdot n_k \times n_l \).

In the presence of finite SOC, the Berry connection \( \gamma_{kj} \) becomes

\[
  \gamma_{kj} = \text{arg} \left[ (n_k | U_{kj} | n_j) \right],
\]

where \( U_{kj} \) is the unitary operator in Eq. (5) describing the spin rotation as the electron hops from \( j \) to \( k \). The
goal of the next sections is to understand how this extra spin rotation induced by finite SOC modifies the effective magnetic field generated by the underlying vector field \( \mathbf{n} \). Along this process, we will find an explicitly covariant expression for this effective magnetic field and we will learn that such a field can be non-zero for collinear and coplanar magnetic orderings, in addition to the non-coplanar antiferromagnetism, that were previously identified as distinct potential sources of topological Hall effect.

III. GEOMETRIC APPROACH

A. Geodesic spin rotations

For any two spin states \( |p\rangle \) and \(|q\rangle \) corresponding to non-collinear unit vectors \( p \) and \( q \), we can define a “geodesic” SU(2) rotation \( \tilde{U}_{q,p} \) that rotates the spin direction from \( p \) to \( q \) along a geodesic (i.e., a great circle) of the Bloch sphere. If we choose the geodesic spin rotation to be along the shorter arc of the great circle containing both \( p \) and \( q \), it is unique and is given by

\[
\tilde{U}_{q,p} = \exp \left[ -\frac{i}{2} \chi_{q,p} (u_{q,p} \cdot \sigma) \right],
\]

where the rotation angle \( \chi_{q,p} = \arccos(p \cdot q) < \pi \) is the angle between the two unit vectors \( p \) and \( q \), and the unit vector specifying the rotation axis is

\[
u_{q,p} = \frac{p \times q}{|p \times q|} = \frac{p \times q}{\sin \chi_{q,p}}.
\]

It is instructive to consider the matrix element of this geodesic spin rotation \( \tilde{U}_{q,p} \) between the two spin states \( |p\rangle \) and \(|q\rangle \). By construction, \( \tilde{U}_{q,p}|p\rangle \propto |q\rangle \), and the geodesic matrix element \( \langle q|\tilde{U}_{q,p}|p\rangle \) is thus a complex number of unit modulus. To determine its complex argument, we first expand \( \tilde{U}_{q,p} \) in the standard way:

\[
\langle q|\tilde{U}_{q,p}|p\rangle = \langle q| \cos \frac{\chi_{q,p}}{2} - i \langle u_{q,p} \cdot \sigma \rangle \sin \frac{\chi_{q,p}}{2} \rangle|p\rangle.
\]

Employing Eq. (17) to turn the overlap in Eq. (18) into a geodesic matrix element, this Berry connection can be written as

\[
\gamma_{kj} = \arg \left[ \langle n_{kj} | U_{n_{kj},n_{j}} | n_{j} \rangle \right] = \arg \left[ \langle n_{kj} | U_{n_{kj},n_{j}}^{N-1} U_{n_{kj},n_{j}}^{(N-2)} ... U_{n_{kj},n_{j}}^{(1)} U_{n_{kj},n_{j}}^{(0)} | n_{j} \rangle \right],
\]

where \( N \rightarrow \infty \) is a large number, and \( n_{kj}^{(n)} \) in terms of \( n_{kj} \) are unit vectors equally spaced along the great circle connecting \( n_{j} \) and \( n_{k} \) [see Fig. 1 (a)]. At the intermediate step between the infinitesimal spin rotations \( U_{n_{kj},n_{j}}^{(0)}, U_{n_{kj},n_{j}}^{(1)}, ..., U_{n_{kj},n_{j}}^{(N-1)} \), the spin state is proportional to \( |n_{kj}^{(n)}\rangle \) by construction. If we then use the orthogonality relation \( \langle -p|p\rangle = 0 \) and the resolution of identity

\[
|p\rangle\langle p| + |-p\rangle\langle -p| = 1
\]

for \( |p\rangle = |n_{kj}^{(n)}\rangle \) at each intermediate step, and also Eq. (17) to turn each geodesic matrix element back into an overlap, the Berry connection in Eq. (19) becomes

\[
\gamma_{kj} = \arg \left[ \langle n_{kj} | U_{n_{kj},n_{j}}^{(N-1)} | n_{j} \rangle \right] + ... + \arg \left[ \langle n_{kj}^{(2)} | U_{n_{kj},n_{j}}^{(1)} | n_{j} \rangle \right] + \arg \left[ \langle n_{kj}^{(1)} | n_{j} \rangle \right].
\]
Consequently, the Berry phase in Eq. (10) is a sum of infinitely many infinitesimal Berry connections along a closed loop in the Hilbert space and can thus be converted into an appropriate integral of the Berry curvature along a surface bounded by this closed loop. For spin states, it is well known that the Berry curvature is 1/2 everywhere on the Bloch sphere, and the Berry phase $\gamma_{jkl}$ in Eq. (10) is therefore half the solid angle of the spherical nonagon spanned by $n_j$, $v_{kj}$, $w_{kj}$, $n_k$, $w_{lk}$, $w_{lk}$, $n_l$, $v_{lj}$, and $w_{lj}$. While this result is only valid modulo $\pi$, it can be used to deduce if the effective flux produced by the combination of magnetic ordering and SOC breaks the time-reversal symmetry or not.

The most important consequence of this result is that the axis $a_{kj}$ is not along a great circle of the Bloch sphere. However, there is a “mixed” representation between these two “pure” representations in which the spin direction is rotated along great circles all the way from $n_j$ to $n_k$: first along the one containing $n_j$ and $R_{kj}^{-1} \cdot n_k$, then along the one perpendicular to $a_{kj}$, and finally along the one containing $R_{kj} \cdot n_j$ and $n_k$.

To find the corresponding formula for the Berry connection, we start from Eq. (25) and notice that there is a general identity

$$U_{kj}^{*} \tilde{U}_{R_{kj}^{-1} \cdot n_k, n_j} = \pm U_{kj} \tilde{U}_{R_{kj}^{-1} \cdot n_k, w_{kj}} \tilde{U}_{v_{kj}, n_j}$$

for any unit vector $v_{kj}$ along the great circle containing $n_j$ and $R_{kj}^{-1} \cdot n_k$. The sign ambiguity in Eq. (26) reflects that the left-hand side and the right-hand side may differ in a $2\pi \times $ spin rotation $e^{i\pi} = -1$. We ignore this sign ambiguity as it does not matter for our purposes. Next, if the unit vector $v_{kj}$ is also along the great circle perpendicular to $a_{kj}$ [see Fig. 1 (d)], the spin rotation $U_{kj}$ becomes a geodesic spin rotation $U_{w_{kj}, v_{kj}}$, where $w_{kj} = R_{kj} \cdot v_{kj}$, and thus Eq. (26) takes the form

$$U_{kj}^{*} \tilde{U}_{R_{kj}^{-1} \cdot n_k, n_j} = \pm U_{nk, w_{kj}, R_{kj} \cdot v_{kj}} U_{v_{kj}, n_j}.$$  

The unit vector $v_{kj}$ is then along the intersection of the great circle perpendicular to $a_{kj}$ and the great circle containing $n_j$ and $R_{kj}^{-1} \cdot n_k$:

$$v_{kj} = a_{kj} \times \left[n_j \times \left(R_{kj}^{-1} \cdot n_k\right)\right],$$

while the unit vector $w_{kj}$ is along the intersection of the great circle perpendicular to $a_{kj}$ and the great circle containing $R_{kj} \cdot n_j$ and $n_k$:

$$w_{kj} = R_{kj} \cdot v_{kj} = \frac{a_{kj} \times ([R_{kj} \cdot n_j] \times n_k)}{|a_{kj} \times ([R_{kj} \cdot n_j] \times n_k)|}.$$  

Note that $-v_{kj}$ and $-w_{kj}$ are also along the intersections of the same great circles and could thus be used instead of $v_{kj}$ and $w_{kj}$ in Eq. (27). Substituting Eq. (27) into Eq. (25), and using Eqs. (17) and (20), the Berry connection finally becomes

$$\gamma_{kj} = \arg \left[\pm \langle \hat{n}_k | U_{nk, w_{kj}} U_{w_{kj}, v_{kj}} U_{v_{kj}, n_j} | n_j \rangle\right] = \arg \left[\pm \langle \hat{n}_k | U_{nk, w_{kj}} | w_{kj} \rangle \langle w_{kj} | U_{w_{kj}, v_{kj}} | v_{kj} \rangle \langle v_{kj} | U_{v_{kj}, n_j} | n_j \rangle\right]$$

$$= \arg \left[\langle \hat{n}_k | w_{kj} \rangle + \langle w_{kj} | v_{kj} \rangle + \langle v_{kj} | n_j \rangle \right] \mod \pi.$$
the Berry curvature (i.e., the effective magnetic field) can be non-zero even for **collinear** or **coplanar** spin configurations if the spin-orbit interaction is finite. This feature will become clearer in the next section, where we solve the same problem by using a convenient rotation of the local reference frame at each individual spin.

### IV. ALGEBRAIC APPROACH

#### A. SU(2) invariant case

We have seen in the previous section that, in absence of spin-orbit coupling, the Berry phase $\gamma_{jkl}$ picked up by an electron as it moves around a triangle of spins $jkl$ is half the solid angle subtended by the three spins:

$$\gamma_{jkl} = \frac{\Omega_{jkl}}{2}. \quad (30)$$

This simple equation can be rederived in the following way. We first introduce an arbitrary unit vector $\mathbf{n}$ that we choose as our quantization axis, i.e., $\mathbf{n} = \hat{z}$. In this frame, the states of the spins $j$ and $k$ are:

$$\left| n_j \right> = \cos \frac{\theta_j}{2} \left| \uparrow \right> + e^{i \phi_j} \sin \frac{\theta_j}{2} \left| \downarrow \right>,$$

$$\left| n_k \right> = \cos \frac{\theta_k}{2} \left| \uparrow \right> + e^{i \phi_k} \sin \frac{\theta_k}{2} \left| \downarrow \right>. \quad (31)$$

Given that $\phi_j - \phi_k$ is defined modulo $2\pi$, we will use this freedom to require that $|\phi_j - \phi_k| \leq \pi$. In absence of SOC, the Berry connection becomes

$$\gamma_{kj} = \arg \left[n_k | n_j \right] \quad (32)$$

implying that

$$\tan \gamma_{kj} = \frac{\sin (\phi_j - \phi_k)}{\cot \frac{\theta_j}{2} \cot \frac{\theta_k}{2} + \cos (\phi_j - \phi_k)} = \tan \frac{\Omega (\phi_j - \phi_k, \theta_j, \theta_k)}{2}, \quad (33)$$

where $\Omega (\phi_j - \phi_k, \theta_j, \theta_k)$ is the solid angle subtended by the vectors $(\mathbf{n}, \mathbf{n}_j, \mathbf{n}_k)$. Since the quantization axis $\mathbf{n}$ is the same for the three bonds of the triangle, the Berry phase is indeed given by Eq. (30):

$$\gamma_{jkl} = \gamma_{jk} + \gamma_{kl} + \frac{\Omega_{jkl}}{2}, \quad (34)$$

where $\Omega_{jkl}$ is the solid angle subtended by the vectors $(\mathbf{n}_j, \mathbf{n}_k, \mathbf{n}_l)$ corresponding to the spin directions.

#### B. General case with spin-orbit interaction

Our next goal is to generalize Eq. (34) for the case of finite SOC, where:

$$\gamma_{jkl} = \arg \left[ \left< n_k | U_{kj} | n_j \right> \left< n_l | U_{lk} | n_k \right> \left< n_j | U_{jl} | n_l \right> \right], \quad (35)$$

We first notice that the Berry phase $\gamma_{jkl}$ is invariant under local rotations of the spin reference frame,

$$\left| n'_j \right> = U_j | n_j \rangle, \quad \left| n'_k \right> = U_k | n_k \rangle, \quad \left| n'_l \right> = U_l | n_l \rangle, \quad (36)$$

$$\mathbf{n}'_j = \mathbf{R}_j \cdot \mathbf{n}_j, \quad \mathbf{n}'_k = \mathbf{R}_k \cdot \mathbf{n}_k, \quad \mathbf{n}'_l = \mathbf{R}_l \cdot \mathbf{n}_l, \quad (37)$$

where $\mathbf{R}_j$ is the SO(3) rotation matrix associated with the SU(2) matrix $U_j$, if we simultaneously transform the unitary operator on each bond in the following way:

$$U'_{kj} = U_k U_{kj} U'_l, \quad U'_{lk} = U_l U_{lk} U'_k, \quad U'_{jl} = U_j U_{jl} U'_l. \quad (38)$$

This observation simply reflects the gauge invariance of the Berry phase under rotations of the local spin spin reference frame and it motivates the introduction of the
Wilson loop operator

\[ A_{jkl} = U_{j}U_{lk}U_{kj} = \exp \left[ -\frac{i\alpha_{jkl}}{2} (a_{jkl} \cdot \sigma) \right], \quad (39) \]

which is also a gauge invariant quantity. We note that the exchange Hamiltonian \( \mathcal{H}_j \) between the spins of the itinerant electrons and the local magnetic moments remains invariant under the local spin rotations described by Eqs. (36) and (37).

The next step is to perform a convenient rotation of the local reference frame of two spins (say \( k \) and \( l \)) such that the unitary operator becomes the identity on two out of three bonds (say \( kj \) and \( jl \)). To this end, one can use the local unitary transformations

\[ U_j = I, \quad U_k = U_{kj}^T, \quad U_l = U_{lj}, \]

\[ R_j = I, \quad R_k = R_{lk}^T, \quad R_l = R_{lj}. \quad (40) \]

Given that the Wilson loop remains invariant under such a transformation, the unitary operator on the third bond \( lk \) must then be equal to the Wilson loop \( A_{jkl} \).

The final step is to align the global quantization axis \( n \) with the rotation axis of the Wilson loop operator: \( n = a_{jkl} \). The Berry connections can then be easily computed in the new reference frame:

\[ \gamma_{jkl} = \Omega_{jkl} + \tilde{\gamma}_{jkl}, \quad (42) \]

where \( \Omega_{jkl} \) is the solid angle subtended by the three vectors \( n'_j, n'_k, n'_l \) corresponding to the rotated spin directions in the new reference frame, and

\[ \tilde{\gamma}_{jkl} = -\frac{\alpha_{jkl}}{2} \]

in terms of

\[ \delta \Omega_{jkl} = \Omega(\phi'_k - \phi'_l + \alpha_{jkl}, \theta'_k, \theta'_l) - \Omega(\phi'_k - \phi'_l, \theta'_k, \theta'_l). \quad (44) \]

is an additional contribution due to the Wilson loop \( A_{jkl} \).

Eq. (42) generalizes Eq. (30), which is only valid for SU(2) invariant systems. In particular, it is easy to demonstrate that collinear or coplanar configurations can induce a Berry phase different from 0 or \( \pi \), which acts as an effective magnetic flux. As an example, we can consider the case of a collinear ferromagnet, \( n_j \parallel n_k \parallel n_l \) with the three vectors \( a_{kj}, a_{lk}, \) and \( a_{jl} \) being parallel (or antiparallel) to the magnetization. In this case, Eq. (42) tells us that \( \gamma_{jkl} = -\alpha_{jkl}/2 \), implying that the combination of ferromagnetism and SOC generates a real space Berry phase that is proportional to the rotation angle of the Wilson loop. In this way, we recover the essential result of Karplus and Luttinger\(^{10}\) in the minimal model that we are considering here. The potential emergence of real space Berry curvature in coplanar antiferromagnets will become clearer in the next section, where we discuss the limit of small SOC. However, one can immediately verify that Eq. (42) also gives a finite Berry curvature for the coplanar spin configuration illustrated in Figure 2.

### FIG. 2. Coplanar configuration with Berry phase different from 0 or \( \pi \). The clockwise circulation indicates the bond orientations required to define the directions of the spin-orbit vectors \( a_{kj}, a_{lk}, \) and \( a_{jl} \), indicated with blue arrows.

### C. Limit of small spin-orbit interaction

We will now consider the quite general case of small spin-orbit coupling: \( \alpha_{kj} \ll 1 \) for all bond bonds \( kj \) con-
nected by finite hopping amplitudes $t_{kj}$ (the hopping amplitudes are assumed to be zero beyond a characteristic distance of a few lattice spaces because of the exponential decay of the atomic orbitals). Expanding Eqs. (5) and (39) up to first order in $\alpha_{kl}$ and $\alpha_{jl}$, respectively, the parameters of the Wilson loop operator then easily follow from those of the individual unitary operators:

$$\alpha_{jkl} = |v_{jkl}|, \quad a_{jkl} = \frac{v_{jkl}}{|v_{jkl}|},$$

$$v_{jkl} = \alpha_{kj}a_{kj} + \alpha_{lk}a_{lk} + \alpha_{jl}a_{jl}.$$  \hspace{1cm} (45)

Moreover, the contribution to the Berry phase in Eq. (43) can be expanded up to first order in $\alpha_{jkl}$ as

$$\hat{\gamma}_{jkl} = \frac{\alpha_{jkl}}{2}\left[-1 + \frac{\partial \Omega_j(k) - \partial \Omega_i(k) + \alpha_{kl}a_{kl}}{\partial \alpha} \right],$$ \hspace{1cm} (46)

and can be brought to a simple form via Eq. (33):

$$\hat{\gamma}_{jkl} = -\frac{\alpha_{jkl}(\cos \theta^l_k + \cos \theta^l_i)}{2[1 + \cos \theta^l_k \cos \theta^l_i + \sin \theta^l_k \sin \theta^l_i \cos(\phi^l_k - \phi^l_i)].}$$ \hspace{1cm} (47)

In particular, when the spin directions are close to a ferromagnetic configuration, such that $\theta^l_k \approx \theta^l_i \approx \theta'$ and $\theta^l_k \approx \theta^l_i \approx \theta''$, this contribution becomes

$$\hat{\gamma}_{jkl} = -\frac{\alpha_{jkl} \cos \theta'}{2},$$ \hspace{1cm} (48)

which is simply the projection of the net spin-orbit rotation to the common direction of the spins.

In the special case when the Wilson loop is equal to the identity ($\alpha_{jkl} = 0$), the Berry phase $\hat{\gamma}_{jkl}$ in Eq. (43) vanishes. The total Berry phase $\gamma_{jkl}$ in Eq. (42) is then half the solid angle $\Omega_{jkl}$ subtended by the three magnetic moments in the local reference frame that is required to “gauge away” the SOC. Clearly, even in this case, an antiferromagnetic ordering that is coplanar in the original reference frame can become non-coplanar in the rotated reference frame and thus produce a finite real-space Berry curvature.

For example, in the $C_3$ invariant system depicted in Figure 2, the three angles, $\alpha_{k} = \alpha_{l} = \alpha_{j} = \alpha \ll 1$, are identical, and the three vectors, $a_{k}$, $a_{l}$, and $a_{j}$, are related by $2\pi/3$ rotations around the $\hat{z}$ axis. Consequently,

$$v_{jkl} = \alpha(a_{k} + a_{l} + a_{j}) = 0$$ \hspace{1cm} (49)

if the $z$-component of $a_{k}$ vanishes. In other words, to first order in the SOC, the Wilson loop is equal to the identity: $A_{jkl} = 1$. To the same order, the three spin directions in the new reference frame are

$$n_j^\prime = n_j, \quad n_k^\prime = n_k - \alpha a_{kj} \times n_k, \quad n_l^\prime = n_l + \alpha a_{jl} \times n_l,$$ \hspace{1cm} (50)

and the Berry phase is thus given by

$$\gamma_{jkl} = \frac{\partial \Omega_{jkl}}{2} = \pi - 6\alpha + O(\alpha^2).$$ \hspace{1cm} (51)

The simple message of this example is that, whenever the SOC can be gauged away in a particular local reference frame (i.e., the Wilson loop is equal to the identity), the magnetic ordering must be non-coplanar in that reference frame to produce a finite real-space Berry curvature. It is easy to imagine that antiferromagnetic orderings that are collinear or coplanar in the original reference frame can become non-coplanar in the rotated reference frame leading to a finite Berry curvature.

V. CONTINUUM LIMIT

The simple ideas that we discussed in the previous section can be presented in a more formal and elegant way by taking the continuum limit. This limit is appropriate for describing situations where the SU(2) Wilson loop bond defined by $A_{jkl}$, associated with the SOC, and the magnetic texture vary over a length scale which is much longer than the lattice parameter. The first condition can be realized by long wavelength lattice deformations induced by strain. The second condition arises naturally in materials with a very small magnetic ordering wave vector.

By taking the continuum limit, we will find an explicitly covariant form of the effective magnetic field or real space Berry curvature produced by the underlying vector field $n_j$ in presence of SOC. We have seen that the unitary “hopping” matrices $U_{jkl}$ correspond to a non-Abelian SU(2) gauge field which is fixed by the interplay between the lattice structure and the SOC. After taking the continuum limit, the bond matrices $U_{jkl}$ become infinitesimal SU(2) rotations connecting the points $x$ and $x + dx$ which are parametrized by the field $A^a_{\mu}$:

$$U_{x+d\vec{x}} = \exp \left(\frac{1}{2} \int_{x}^{x+d\vec{x}} \sigma^a A^a_{\mu} dx_{\mu}\right).$$ \hspace{1cm} (52)

where repeated indices are implicitly summed over.

Once again, we want to compute the Berry phase that the electronic wave function acquires when the electron moves along a one dimensional closed path $C = \{x_{\mu}(\tau) \mid \tau \in [0; T], x_{\mu}(0) = x_{\mu}(T)\}$. As we did for the lattice case, we will first derive the well-known expression of the Berry phase in the SU(2) invariant case and we will use this result as an introduction for obtaining a gauge invariant form of the Berry curvature or effective magnetic field in the presence of SOC.

A. SU(2) invariant case

For the SU(2) invariant case on the lattice, we have seen that the Berry phase for a closed loop $C : j \rightarrow k \rightarrow l \rightarrow \ldots \rightarrow m \rightarrow j$ is:

$$\gamma_C = \arg \langle n_j|n_m\rangle \ldots \langle n_l|n_k\rangle \langle n_k|n_j\rangle.$$ \hspace{1cm} (53)
Note that an arbitrary closed loop can be obtained from a superposition of multiple “elementary” triangular loops. To find the counterpart of Eq. (53) in the continuum, we will divide the interval \( T \) into \( N \) equal subintervals \( \Delta \tau = T/N \) to finally take the \( N \to \infty \) limit. In this way we obtain:

\[
\gamma_C = \lim_{N \to \infty} \frac{1}{T} \sum_{j=0}^{N-1} \left\langle n_{x(\tau_j + \Delta \tau)} | n_{x(\tau_j)} \right\rangle
\]

where \( \tau_j = j \Delta \tau \). The geometric character of the Berry phase becomes evident after reexpressing Eq. (54) in terms of a closed integral over the loop \( C \):

\[
\gamma_C = i \oint_C \langle n | \partial_\tau | n \rangle dx_\mu = \frac{1}{2} \oint_{S_C} n \cdot \partial_\tau n \times \partial_\tau n \ d^2 \sigma^{\mu \nu} = \frac{\Omega_C}{2},
\]

(55)

and following the same steps that appear in the derivation of Eq. (54), we obtain

\[
\gamma_C = -i \int_C \langle n | D_\mu | n \rangle dx_\mu = \int_C A_\mu dx^\mu.
\]

(59)

Here we have introduced the covariant derivative,

\[
D_\mu \equiv \partial_\mu - \frac{i}{2} \sigma^a A_\mu^a,
\]

(60)

and the covariant Berry connection,

\[
A_\mu = i \langle n | \partial_\mu | n \rangle + \frac{1}{2} n^a A_\mu^a,
\]

(61)

to make the gauge invariance of \( \gamma_C \) more explicit.

We can now use Stokes theorem to convert the closed integral of Eq. (59) into an integral over the area \( S_C \):

\[
\oint_C A_\mu dx^\mu = \int_{S_C} \left[ \partial_\mu A_\nu - \partial_\nu A_\mu \right] d^2 \sigma^{\mu \nu} = \frac{1}{2} \int_{S_C} \left[ \partial_\mu (n^a A_\nu^a) + \partial_\nu (n^a A_\mu^a) \right] d^2 \sigma^{\mu \nu}
\]

\[
= \int_{S_C} n \cdot [\partial_\mu n \times \partial_\nu n] d^2 \sigma^{\mu \nu}.
\]

(62)

The second term is the contribution (55) that we derived for the SU(2) invariant case. While this term is zero for collinear or coplanar magnetic orderings, the first term can still be finite, implying that collinear and magnetic textures can generate an effective magnetic field if the SOC is finite. In these cases, the effective magnetic field is \( B_\mu = \epsilon_{\mu
u\lambda} \partial_\mu (n^a A_\nu^a) / 2 \). In other words, the effective U(1) vector potential is obtained by projecting the SU(2) vector potential into the direction of the \( n \) field.

Our next goal is to find a covariant form for the two contributions that appear in Eq. (62). The integral that...
appears in the first term can be reexpressed as

\[
\int_{S_c} [\partial_\mu (n^\alpha A^\alpha_\mu) - \partial_\nu (n^\alpha A^\alpha_\mu)]d^2\sigma^{\mu\nu}
\]

\[
= \int_{S_c} [n^\alpha \partial_\mu A^\alpha_\nu - n^\nu \partial_\mu A^\alpha_\mu + (\partial_\mu n^\alpha) A^\alpha_\nu - (\partial_\nu n^\alpha) A^\alpha_\mu]d^2\sigma^{\mu\nu}
\]

\[
= \int_{S_c} [n^\alpha F^\alpha_{\mu\nu} + n^\alpha \varepsilon^{abc} A^a_\mu A^b_\nu + A^\alpha_\mu \partial_\nu n^\alpha - A^\alpha_\nu \partial_\mu n^\alpha]d^2\sigma^{\mu\nu}
\]

\[
= \int_{S_c} \left[n^\alpha \varepsilon^{abc} A^a_\mu A^b_\nu + A^\alpha_\mu \partial_\nu n^\alpha - A^\alpha_\nu \partial_\mu n^\alpha\right]d^2\sigma^{\mu\nu},
\]

\[
(63)
\]

By combining this equation with Eqs. (62), (63), and (64), we find a concise covariant form of the Berry phase:

\[
\gamma_C = \frac{1}{2} \int_{S_c} [n^\alpha F^\alpha_{\mu\nu} + n \cdot (D_\mu n \times D_\nu n)]d^2\sigma^{\mu\nu}.
\]

\[
(67)
\]

This final equation is one of the key contributions of this work. This equation simply tells us that the strength of the effective U(1) gauge field that is generated by the localized magnetic moments is the sum of the covariant scalar spin chirality and the projection of the SU(2) field strength along the local direction \( n \) of the localized moments.\(^{41,46}\) This is essentially the same result that was obtained in Eq. (48) by working on the lattice and taking the long wavelength limit at the end of the process.

Another interesting aspect of this derivation is that it can be immediately generalized to the case of time-dependent magnetic configurations by allowing the Greek indices \( \mu \) and \( \nu \) to run from 0 to \( d \), where 0 is the time coordinate and the \( d \) is the spatial dimension of the system under consideration. The zeroth component of the SU(2) vector potential arises from a Zeeman coupling between the spin of the conduction electrons and an external magnetic field \( H \),

\[
A^a_0 = -\frac{g\mu_B}{2} H^a,
\]

\[
(68)
\]

where \( g \) is the \( g \)-factor of the electron and \( \mu_B \) is the Bohr magneton. The action that results from adding the Zeeman term to the effective Hamiltonian in Eq. (3),

\[
S[\Psi] = \int dt (\bar{\psi} i \partial_t \Psi - \mathcal{H}),
\]

\[
(69)
\]

preserves the invariance under time dependent transformations of the local spin reference frame,\(^{41}\)

\[
\Psi \rightarrow U \Psi, \quad A^a_\mu \sigma^a \rightarrow U A^a_\mu \sigma^a U^{-1} - 2i(\partial_\mu U)U^{-1},
\]

\[
(70)
\]

where \( \Psi \) is the electronic wave function in the continuum and \( U = e^{i\theta(x,t)\sigma^a/2} \). Eq. (70) generalizes the time-independent rotations of the local reference frame in Eqs. (36)-(38) that were introduced for the lattice Hamiltonian. The effective electromagnetic field tensor produced by a time-dependent configuration of the local magnetic moments is then given by

\[
\frac{1}{2} [n^\alpha F^\alpha_{\mu\nu} + n \cdot (D_\mu n \times D_\nu n)],
\]

\[
(71)
\]

where \( 0 \leq \mu, \nu \leq d \) and the strength of the SU(2) gauge field is still given by Eq. (64). This equation generalizes then well-known result for SU(2) invariant systems.\(^{38}\)

VI. MOMENTUM SPACE BERRY CURVATURE

In this section we will discuss a few examples to apply the notion of the generalized Berry curvature that was introduced in previous sections. In particular, we will consider an extended version of the model Hamiltonian (3) that includes potentially anisotropic exchange interactions between the local moments:

\[
\mathcal{H} = \mathcal{H}_t + \mathcal{H}_J + \mathcal{H}_H,
\]

\[
(72)
\]

where \( \mathcal{H}_t \) and \( \mathcal{H}_K \) have been introduced in Eq. (3) and

\[
\mathcal{H}_H = \sum_{\langle jk \rangle} S_j^a \mathcal{J}_{jk}^{\mu\nu} S_k^a.
\]

\[
(73)
\]

We will consider different 2D and 3D variants of this model comprising single or vertically stacked Kagome
layers. The first case corresponds to a very simple version of the model, which is useful for illustrating the connection between real space Berry curvature introduced in the previous sections and the resulting momentum space Berry curvature and AHE.

![Diagram of Berry curvature and AHE](image)

**FIG. 3.** Uniform 120° magnetic ordering (black arrows) on the Kagome lattice. This is a straightforward extension of the single triangle state shown in Figure 2. The clockwise circulation indicates the bond orientation. The in-plane components of the SOC vectors $a_{12}, a_{23}, a_{13}$ are indicated with blue arrows. $u_{1,2}$ are the primitive lattice vectors of the Bravais lattice.

### A. Single Kagome Layer

We will first assume that $H_{t}$ is a tight-binding Hamiltonian on a single Kagome layer with nearest-neighbor hopping $t$ and that $H_{ij}$ stabilizes the ground state magnetic ordering shown in Fig. 3: $S_{j} = Sn_{j}$, with

$$n_{1} = \hat{y}, \quad n_{2} = \frac{\sqrt{3}}{2} \hat{x} - \frac{\hat{y}}{2}, \quad n_{3} = -\frac{\sqrt{3}}{2} \hat{x} - \hat{y}.$$

(74)

The SOC vectors introduced in Eq. (5) are

$$a_{23} = \cos \theta a_{23}^{1} + \sin \theta \hat{z},$$

$$a_{31} = \cos \theta a_{31}^{1} + \sin \theta \hat{z},$$

$$a_{12} = \cos \theta a_{12}^{1} + \sin \theta \hat{z},$$

(75)

where $a_{ij}^{1} = -\epsilon_{ijk} n_{k}$. Before proceeding with the actual calculation, it is instructive to analyze the distribution of the real-space Berry curvature in the double-exchange limit $J/t \rightarrow \infty$. For $\theta = \frac{\pi}{3}$, the SOC vectors $a_{ij}$ are collinear and parallel to the $\hat{z}$-axis. The Berry phase $2\gamma_{123}$ picked up by an electron that moves around the triangle 123 (see Fig. 3) is equal to $\pi$ (the same is true for the hexagonal plaquettes). Given that these $\pi$-phases remain invariant under time-reversal symmetry, there is no effective magnetic field in real space. The tight-binding spectrum of the double-exchange Hamiltonian exhibits two Dirac points at the K points of the Brillouin zone (BZ); $(\pm \frac{\pi}{3u}, 0)$ with $u \equiv |u_{1}|$. In the opposite limit of in-plane SOC vectors ($\theta = 0$), the Berry phase becomes $\gamma_{123} = \pi - 6\alpha$ to first order in the strength of the SOC ($\alpha_{ij} \equiv \alpha$). The resulting effective magnetic flux per triangle gaps out the two Dirac points, giving rise to a finite Chern number $C = -\text{sign}(\alpha)$ of the lower band of the massive Dirac fermions.

In the more general case (away from the double-exchange limit), we need to consider six bands. The matrix of $H_{t} + H_{ij}$ in momentum space is the 6 × 6 matrix:

$$[H_{k}] = \begin{pmatrix}
H_{k}^{11} & H_{k}^{12} & (H_{k}^{21})^{\dagger} & H_{k}^{22} & (H_{k}^{31})^{\dagger} & H_{k}^{33} \\
(H_{k}^{12})^{\dagger} & (H_{k}^{11})^{\dagger} & (H_{k}^{21})^{\dagger} & (H_{k}^{22})^{\dagger} & (H_{k}^{31})^{\dagger} & (H_{k}^{33})^{\dagger} \\
H_{k}^{23} & (H_{k}^{22})^{\dagger} & H_{k}^{21} & H_{k}^{33} & H_{k}^{32} & H_{k}^{31} \\
(H_{k}^{31})^{\dagger} & (H_{k}^{32})^{\dagger} & (H_{k}^{33})^{\dagger} & H_{k}^{11} & H_{k}^{12} & (H_{k}^{21})^{\dagger} \\
H_{k}^{31} & H_{k}^{32} & (H_{k}^{33})^{\dagger} & (H_{k}^{21})^{\dagger} & (H_{k}^{11})^{\dagger} & (H_{k}^{12})^{\dagger} \\
H_{k}^{33} & H_{k}^{32} & H_{k}^{31} & (H_{k}^{21})^{\dagger} & (H_{k}^{11})^{\dagger} & (H_{k}^{12})^{\dagger}
\end{pmatrix}$$

(76)

with

$$H_{k}^{12} = t e^{i \frac{2}{3} \sigma} a_{12} (1 + e^{-i k_{z} (u_{2} - u_{1})}),$$

$$H_{k}^{23} = t e^{i \frac{2}{3} \sigma} a_{23} (1 + e^{-i k_{z} u_{1}}),$$

$$H_{k}^{31} = t e^{i \frac{2}{3} \sigma} a_{31} (1 + e^{i k_{z} u_{2}}),$$

$$H_{k}^{11} = -\frac{JS}{2} n_{1} \cdot \sigma, \quad H_{k}^{22} = -\frac{JS}{2} n_{2} \cdot \sigma, \quad H_{k}^{33} = -\frac{JS}{2} n_{3} \cdot \sigma.$$

In the absence of SOC ($\alpha = 0$), the tight-binding model hosts multiple Dirac points. As explained above, these Dirac points are gapped out for finite SOC ($\alpha \neq 0$) as long as the in-plane component of $a_{ij}$ is non-zero. The resulting energy bands become topologically non-trivial, namely, they acquire a finite Chern number. We note that this result is consistent with our simple analysis of the double-exchange limit. As an example, for $J = 0.5t$, $\alpha = 0.2\pi$ and $\theta = 0$, the Chern numbers of each band are $C(n=1) = 1$, $C(n=2) = -3$, $C(n=3) = 2$, $C(n=4) = 2$, $C(n=5) = -3$ and $C(n=6) = 1$, where $n = 1$ ($n = 6$) refers to the lowest (highest) energy band. The resulting energy bands for this example are shown in Fig. 4. Note, however, that these bands are not adiabatically connected with the six bands that are obtained in the double-exchange limit (three low-energy bands separated by an energy $J$ from the three high-energy bands) because the Chern numbers in the double-exchange limit must satisfy the property $C(n) = -C(n+3)$ for $1 \leq n \leq 3$. This is just a consequence of the opposite sign of the real space Berry curvature for bands of opposite spin, i.e., aligned or anti-aligned with the local moments.

### B. Vertically stacked Kagome layers

We first consider a toy model of vertically stacked Kagome layers with an SU(2) invariant hopping between adjacent layers. The intra-layer magnetic ordering is assumed to be the same uniform 120° structure that we used in the previous 2D analysis, while the inter-layer ordering is assumed to be ferromagnetic. For concreteness, we will assume that the inter-layer hopping is finite only between nearest-neighbor ($l_{z}^{1}$) and next-nearest-neighbor ($l_{z}^{2}$) sites on adjacent Kagome layers. The resulting inter-
layer Hamiltonian in momentum space is:

\[
\tilde{H}^\text{inter} = \begin{bmatrix}
\tilde{H}^{11}_{k} & \tilde{H}^{12}_{k} & (\tilde{H}^{21}_{k})^\dagger \\
(\tilde{H}^{12}_{k})^\dagger & \tilde{H}^{22}_{k} & \tilde{H}^{23}_{k} \\
(\tilde{H}^{21}_{k})^\dagger & (\tilde{H}^{23}_{k})^\dagger & \tilde{H}^{33}_{k}
\end{bmatrix},
\tag{77}
\]

where

\[
\tilde{H}^{12}_{k} = 2t^2_x \cos(\mathbf{k} \cdot \mathbf{u}_3)(1 + e^{-i\mathbf{k} \cdot (\mathbf{u}_2 - \mathbf{u}_1)}),
\]

\[
\tilde{H}^{23}_{k} = 2t^2_x \cos(\mathbf{k} \cdot \mathbf{u}_3)(1 + e^{-i\mathbf{k} \cdot \mathbf{u}_1}),
\]

\[
\tilde{H}^{31}_{k} = 2t^2_x \cos(\mathbf{k} \cdot \mathbf{u}_3)(1 + e^{i\mathbf{k} \cdot \mathbf{u}_2}),
\]

\[
\tilde{H}^{11}_{k} = 2t^2_x \cos(\mathbf{k} \cdot \mathbf{u}_3), \quad \tilde{H}^{12}_{k} = \tilde{H}^{11}_{k}, \quad \tilde{H}^{23}_{k} = \tilde{H}^{11}_{k},
\]

and \( \mathbf{u}_3 \) is the primitive lattice basis vector along the \( c \)-axis.

We will start by considering the trivial 2D limit of zero inter-layer hopping. In this limit the spectrum does not depend on \( k_z \), i.e., it is the same for each two-dimensional layer \( (k_x, k_y) \) in momentum space. We have seen that, in the absence of SOC, each \( (k_x, k_y) \) layer hosts several Dirac points, which become nodal lines in the 3D BZ. These nodal lines are fully gapped out by a finite SOC, implying that we can introduce a \( k_z \)-independent Chern number on any \( (k_x, k_y) \) plane, \( C^{(n)}(k_z) \), for each of the six bands.

The band structure obtained in the 2D limit changes qualitatively for finite inter-layer hopping because the Dirac lines are gapped everywhere, except for isolated points that turn out to be Weyl points of the 3D band structure. The finite inter-layer hopping leads to a \( k_z \)-dependence of the single-particle dispersion and, consequently, of the Chern number \( C^{(n)}(k_z) \). The Chern number remains well-defined unless the \( (k_x, k_y) \) layer crosses the Weyl points and the spectrum is thus gapless. In terms of momentum space Berry curvature, the Weyl points are magnetic monopoles, i.e., sources and sinks of the momentum space Berry curvature. From Gauss’s law, we get that the difference between the \( n \)th band Chern numbers at the \( k_z \) and \( k'_z \) planes is equal to the sum of the charges of the Weyl points connected to that band which are enclosed by the two planes. Fig. 5 shows an example of \( C^{(n)}(k_z) \), where each Kagome layer is identical to that in Fig. 4, and a finite inter-layer hopping is included. Only the Chern numbers of the lower and the upper two bands \( (n = 1, 2, 5, 6) \) are changing because the \( n = 2 \) and \( n = 3 \) bands are not connected to any Weyl point.

\[
C^{(n)}(k_z) = \begin{cases} 
+1 & \text{for } n \neq 2, 3, 5, 6, \\
-3 & \text{for } n = 2, \\
+2 & \text{for } n = 4, \\
+2 & \text{for } n = 5, \\
-3 & \text{for } n = 6.
\end{cases}
\]

FIG. 4. Band structure of the tight-binding model of Eq. (77) for Hamiltonian parameters \( J = 0.5t, \alpha = 0.2\pi, \theta = 0 \).

FIG. 5. Chern number \( C(k_z) \) for each \( (k_x, k_y) \) plane in momentum space. The in-plane parameters are the same as in Fig. 4, while the inter-layer hopping amplitudes are \( t_x = 0.1t \) and \( t_z = 0.3t \).

C. Minimal model for Mn\(_3\)Sn

We will consider now a modified version of the previous model that can be regarded as a minimal Hamiltonian for the lattice and magnetic ordering of Mn\(_3\)Sn.\(^{42,48}\) While this Hamiltonian is not a realistic model for Mn\(_3\)Sn, it includes the essential ingredients that are required for capturing the qualitative behavior of this material. More specifically, the model reveals the origin of the real space Berry curvature that leads to the Weyl points that are obtained by more realistic band structure calculations\(^{48–50}\) and that are the sources and drains of momentum space Berry curvature. The crystallographic unit cell of Mn\(_3\)Sn is shown in Fig. 6 (a): each unit cell includes six Mn atoms distributed in two Kagome layers. As shown in Fig. 6 (b), the \( P6_3/mmc \) space group of this material includes

- Mirror symmetries \( \mathcal{M}_i \), \( i = 1, 2, 3; \)
- Glide symmetries \( \mathcal{G}_i \equiv \mathcal{M}_i' \otimes T_{\mathbf{z}} \), \( i = 1, 2, 3 \), with \( T_{\mathbf{z}} \) the translation along the \( c \)-axis by \( \frac{1}{2} \mathbf{u}_3 \);
- Mirror symmetry \( \mathcal{M}_z \) about the Kagome layer;
- Inversion symmetry \( \mathcal{I} \).

The experimental data\(^{42}\) shows that Mn\(_3\)Sn displays the magnetic ordering depicted in Fig. 7, which is stable within the temperature range 50K < \( T < T_N \), with a
Néel temperature $T_N \approx 420$K. To a good approximation, this magnetic ordering consists of a 120° structure with fixed vector spin chirality: the spin rotates anticlockwise when circulating clockwise around each triangular plaquette. Several discrete symmetries are spontaneously broken by this magnetic ordering. The residual symmetry group includes $M_{1}, G_{2} \otimes \Theta, M_{3} \otimes \Theta,$ and $I$, where $\Theta$ is the time reversal operation. The $C_{3}$ symmetry is spontaneously broken because the spin and the lattice must be rotated in opposite directions to keep the system invariant.

Once again, we will use the minimal Hamiltonian (3) to capture the essential features of Mn$_3$Sn. The site index $j$ (or $k$) in Eq. (3) will be decomposed into two indices $(\alpha, r)$, where, as shown in Fig. 6 (a), $\alpha = 1, \ldots, 6$ is a sublattice index and $r$ is the coordinate of the crystallographic unit cell. We will also assume that the abovementioned magnetic ordering of the Mn moments is stabilized by the additional exchange interaction term that is included in Eq. (72). The corresponding orientations of the magnetic moments on each sublattice are:

$$n_{1} = n_{4} = \hat{x},$$

$$n_{2} = n_{5} = \frac{1}{2} \hat{x} + \frac{\sqrt{3}}{2} \hat{y},$$

$$n_{3} = n_{6} = \frac{1}{2} \hat{x} - \frac{\sqrt{3}}{2} \hat{y}. \quad (78)$$

The unit vectors $a_{jk}$ are constrained by symmetry considerations. For instance, the in-plane components of $a_{kj}$ vanish for bonds lying in each Kagome layer because of the mirror symmetry plane $M_{z}$, implying that $a_{kj} = a_{ij}$. In addition, as shown in Fig. 6 (a), the two Kagome layers in the unit cell are related by the inversion symmetry, $I$: $j \rightarrow j, k \rightarrow k$, implying that $a_{kj} = a_{ij}$. By combining these results with the $C_{3}$ symmetry of the lattice, we obtain that the six in-plane hopping matrices must be the same:

$$t_{12} = t_{23} = t_{31} = t_{45} = t_{56} = t_{64} = t e^{i \frac{2}{3} \pi} \sigma_{z}. \quad (79)$$

A similar symmetry analysis leads to the following parametrization of the inter-layer hopping matrices:

$$t'_{\alpha \beta} = t' e^{i \frac{\pi}{3} \alpha_{\alpha \beta} \sigma}, \quad (80)$$

$$t''_{\alpha \beta} = t' e^{i \frac{2}{3} \pi \alpha_{\alpha \beta} \sigma}, \quad (81)$$

where $\alpha, \beta$ are sublattice indices connected by inter-layer bonds (see Fig. 7) and $t'_{\alpha \beta}$ ($t''_{\alpha \beta}$) are the hopping amplitudes on the inter-layer bonds depicted in Fig. 7 (a) (Fig. 7 (b)). The corresponding spin-orbit vectors,

$$a'_{\alpha \beta} = \pm \cos \theta' a_{\alpha \beta} \hat{z}, \quad (82)$$

$$a''_{\alpha \beta} = \mp \cos \theta' a_{\alpha \beta} \hat{z}, \quad (83)$$

are constrained by the mirror symmetries $M_{1}, M_{2},$ and $M_{3}$. The upper (lower) sign corresponds to $\alpha = 1, 2, 3$ ($\alpha = 4, 5, 6$), and the vector $a_{\alpha \beta}$ refers to the (normalized) projection of the bond vector $a_{\alpha \beta}$ on the basal plane

$$a_{16} = (\frac{\sqrt{3}}{2}, 1, 0, a_{24} = (-\frac{\sqrt{3}}{2}, -1, 0, a_{13} = (0, 0, 1, 0),$$

$$a_{62} = a_{35}, \quad a_{43} = a_{16}, \quad a_{51} = a_{24}. \quad (84)$$

In momentum space, the electron kinetic term is $H_{k} = \sum_{k} \psi_{k}^\dagger H_{k} \psi_{k}$ with $\psi_{k} = (c_{1k}, c_{2k}, c_{3k}, c_{4k}, c_{5k}, c_{6k})^T$ and

$$H_{k} = \begin{bmatrix} H_{11} & H_{12}^{\dagger} & H_{13} & 0 & H_{15}^{\dagger} & H_{16}^{\dagger} \\ H_{21} & H_{22} & H_{23}^{\dagger} & H_{24}^{\dagger} & 0 & H_{26}^{\dagger} \\ H_{31} & H_{32} & H_{33}^{\dagger} & H_{34}^{\dagger} & H_{35}^{\dagger} & 0 \\ H_{41} & H_{42}^{\dagger} & H_{43} & H_{44}^{\dagger} & H_{45}^{\dagger} & H_{46}^{\dagger} \\ H_{51} & 0 & H_{53} & H_{54}^{\dagger} & H_{55}^{\dagger} & H_{56}^{\dagger} \\ H_{61} & H_{62}^{\dagger} & 0 & H_{63}^{\dagger} & H_{64}^{\dagger} & H_{65}^{\dagger} \end{bmatrix}, \quad (85)$$

where the diagonal elements are $H_{k}^{\alpha \alpha} = -\frac{1}{2} \hbar S e_{\alpha} \cdot \sigma$, the off-diagonal elements $H_{k}^{\alpha \beta}$ arise from the intra-layer
For concreteness, we will consider the following set of Hamiltonian parameters: \( t' = t, J = 2t, \alpha = 0.2\pi, \alpha' = 0.2\pi, \) and \( \theta' = \pi/4 \approx 0.785. \) While this set does not correspond to the particular case of MnSb, it is enough to illustrate the physical origin of the Weyl points that appear in the band structure of this material.\(^{31}\) As shown in Fig. 8 (a), there are two Weyl points located at each of the \( K \) points of the BZ, connecting the fifth and the sixth bands and the seventh and the eight bands at \( k_z = 2.04. \) In general, the Weyl points connecting the fifth and the sixth bands turn out to be distributed over the surface of the BZ, as shown in Figs. 8 (b) and (c). This is not true for the other bands. Except for equivalent points related by reciprocal lattice vectors, they are classified according to the symmetries \( M_1, G_2 \otimes \Theta, M_2 \otimes \Theta, \) and \( I. \)

Weyl points connecting bands \( n \) and \( n+1 \) are singularities of the vector field \( B_{\mu\nu}^{(n)} = \sum_{\mu\nu} \epsilon_{\mu\nu}\mathcal{B}_{\mu\nu}^{(n)} \), where \( \mathcal{B}_{\mu\nu}^{(n)} \) is the momentum space Berry curvature of the \( n \)-band given by the Kubo formula,\(^ {52}\)

\[
\mathcal{B}_{\mu\nu}^{(n)} = -2\hbar^2 \sum_{m \neq n} \left[ \frac{\langle \psi_{nk}\partial_{\mu}\mathcal{H}\psi_{mk}\rangle \langle \psi_{mk}\partial_{\nu}\mathcal{H}\psi_{nk}\rangle}{(E_{nk} - E_{mk})^2} \right].
\]  

\( E_{nk} \) is the dispersion relation of the \( n \)-th band and \( |\psi_{nk}\rangle \) is the associated Bloch wave function. The singularity at the Weyl point is characterized by the quantized topological charge of the monopole

\[
Q^{(n)} = \frac{1}{4\pi} \int_{\Sigma} d^2s \cdot B^{(n)},
\]

where \( \Sigma \) is a closed surface enclosing the Weyl point. Each Weyl point is then a source (sink) of the Berry curvature field \( B^{(n)} \) if \( Q^{(n)} > 0 \) or \( Q^{(n)} < 0 \). This charge \( Q^{(n)} \) changes sign under mirror and spatial inversion transformations, while it remains invariant under time-reversal. Fig. 8 shows the Weyl points with \( Q^{(n)} > 0 \) (red color) and \( Q^{(n)} < 0 \) (blue color). Pairs related by the residual symmetries \( M_1, G_2 \otimes \Theta, M_2 \otimes \Theta, \) and \( I \) have opposite monopole charges.

The vector field \( B^{(n=5)} \) on the \( k_z = 0 \) plane is shown in Fig. 8 (c). Symmetry restrictions imply that

- \( M_1 : (k_x, k_y, k_z) \rightarrow (-k_x, k_y, k_z) \)
- \( (B_x^{(n)}, B_y^{(n)}, B_z^{(n)}) \rightarrow (B_x^{(n)}, -B_y^{(n)}, -B_z^{(n)}) \); \( \quad \) (89)
- \( G_2 \otimes \Theta : (k_x, k_y, k_z) \rightarrow (-k_x, k_y, -k_z) \)
- \( (B_x^{(n)}, B_y^{(n)}, B_z^{(n)}) \rightarrow (B_x^{(n)}, -B_y^{(n)}, B_z^{(n)}) \); \( \quad \) (90)
- \( M_2 \otimes \Theta : (k_x, k_y, k_z) \rightarrow (-k_x, -k_y, k_z) \)
- \( (B_x^{(n)}, B_y^{(n)}, B_z^{(n)}) \rightarrow (B_x^{(n)}, B_y^{(n)}, -B_z^{(n)}) \); \( \quad \) (91)
Hall conductivities \( \sigma \) and curvature of Mn

deerly strategy for controlling momentum space Berry
der the listed residual symmetry transformations, while

tance that is still present in doped Weyl semimetals.
tial consequence is a finite anomaly-related magnetoresis-
ture induced by the momentum space Berry curvature. Another poten-
tions, such as the Hall response, that are strongly

The first two transformations imply that \( B_z^{(n)} \equiv 0 \) for

eq 0 (\( k_z \) is fixed at \( 10^{-4} \) in Fig. 8 (e) such that \( B_z^{(n)} \neq 0 \)
near the Weyl points). Note that \( B_x^{(n)} \) remains even un-
der the listed residual symmetry transformations, while

\( B_y^{(n)}, B_z^{(n)} \) are odd under some of them (e.g., the mirror

symmetry plane \( M_1 \)). This observation implies that the

Hall conductivities \( \sigma_{xx} \) and \( \sigma_{xy} \) must vanish.

At this point it is interesting to ask what is the distri-
bution of the \textit{real space} Berry curvature that leads to
the distribution of \textit{momentum space} Berry curvature de-
picted in Fig. 8. This result is shown in Fig. 9. The first
observation is that the effective flux is zero for intra-layer

triangles. The flux (Berry phase) is concentrated on the

triangular plaquettes that connect different layers. The

sign of the flux alternates between the two types of tri-
angles that connect consecutive layers. Identifying the

origin of the real space Berry curvature is potentially

useful for achieving a more efficient control of response
functions, such as the Hall response, that are strongly

influenced by the momentum space Berry curvature. For

instance, Fig. 9 indicates that changing the lattice pa-

ter parameter or the SOC of the \textit{interlayer} triangles is the

correct strategy for controlling momentum space Berry

curvature of Mn\(_3\)Sn via the modification of its real space

Berry curvature.

\section*{E. Hall conductivity}

Our final step is to compute the Hall conductivity pro-
duced by the momentum space Berry curvature. The

only purpose of this calculation is to quantify the order

of magnitude of the effect. We note, however, that a finite

Hall conductivity is not the only measurable consequence

of the momentum space Berry curvature. Another poten-
tial consequence is a finite anomaly-related magnetoresis-
tance that is still present in doped Weyl semimetals.\(^{53,54}\)

\[ \sigma_{\mu\nu} = -\frac{e^2}{h} \int_{BZ} d^3k \sum_n f(E_{nk}) B_{\mu\nu}^{(n)}(k), \]

(92)

where \( f(x) = 1/(e^{(x-\mu)/k_B T} + 1) \) the Fermi-Dirac dis-
tribution function. The residual mirror symmetry plane

\( M_2 \) times a spin rotation \( B_z^{(s)}(-\frac{2\pi}{3}) \) becomes an

element of the residual symmetry group for \( a_{ij} \parallel \hat{z} \) on
every bond.

As expected, the value of \( \sigma_{yz} \) depends strongly on the

position of the Fermi level \( \mu \). However, it is interesting
to note that the order of magnitude of the overall ampi-
itude of the \( \sigma_{yz}(\mu) \) curve coincides with the experimen-
tal value in Mn\(_3\)Sn\(^{42}\). In other words, our minimal model for

Mn\(_3\)Sn not only captures the key qualitative aspects of

the problem, but also the correct order of magnitude of
response functions enabled by the finite momentum space

Berry curvature. This attribute of the model can be ex-

loited for further understanding the interplay between

real and momentum space Berry curvature induced by the

combination of magnetic ordering and SOC.

Finally, we mention that the small uniform magneti-
zation that is observed in Mn\(_3\)Sn should have the same

origin as the spontaneous Hall conductivity. The same

symmetry analysis that enables a finite \( \sigma_{yz} \) for the anti-
ferromagnetic ordering depicted in Fig. 7 also enables a
finite uniform orbital magnetization along the \( x \)-axis that

should also produce a uniform spin magnetization along

the same direction via the SOC. This effect can be cap-
tured by our minimal model if we allow the antiferromag-
netic state of Fig. 7 to relax into the magnetically ordered

state that minimizes the total energy \( \langle \mathcal{H}_I + \mathcal{H}_J + \mathcal{H}_H \rangle \).\(^{55}\)

As for the case of Mn\(_3\)Sn\(^{42}\) this uniform magnetization,
which must be present in any antiferromagnet that pro-
roduces a spontaneous Hall effect, can be used to orient the antiferromagnetic domains and induce a net Hall conductivity.

VII. CONCLUSIONS

In summary, we have shown that the real space Berry phase that electrons pick up when they move in a closed loop while interacting with local magnetic moments is a geometric property that combines rotation matrices associated with the finite SOC and the underlying magnetic ordering. From a more physical point of view, the finite SOC rotates the electronic spin while the electron hops from one atomic orbital to another. This rotation enables a non-trivial Berry phase (different from 0 or $\pi$) induced by collinear and coplanar magnetic configurations. In view of the fact that collinear and coplanar magnetic orderings are more common than noncoplanar orderings, we can conclude that SOC should play a crucial role in the discovery of new materials with large topological Hall effect, or even finite temperature Chern insulators, induced by spontaneous antiferromagnetic ordering. While material candidates can be identified by applying a simple symmetry analysis, understanding the underlying microscopic mechanism for the generation of Berry curvature is of crucial importance for the optimization and control of the effect. Understanding the microscopic mechanism is also necessary to estimate the value of the topological contribution to different response functions of interest and to anticipate the change of these response functions under the application of external fields, such as pressure, strain or magnetic field.

Here we have reduced this microscopic mechanism to its simplest form by considering the minimal model introduced in Eq. (3). Like for the SU(2) invariant case of zero SOC, the mechanism becomes transparent in the double-exchange limit of this model because the low-energy theory maps into a theory of spinless fermions coupled to an effective U(1) gauge field. We have shown that the strength of this emergent U(1) field has two covariant contributions. The first contribution is the covariant SU(2) extension of the skyrmion density in the underlying configuration of localized magnetic moments. The second contribution is simply the projection of the strength of the SU(2) gauge field produced by the SOC along the direction of the localized magnetic moments. This simple result reveals the role of SOC in the generation of real space Berry curvature. The new scenario becomes particularly clear when the SOC can be gauged away by a local rotation of the spin reference frame. The real space Berry curvature is then equal to the skyrmion density of the localized magnetic moments in that particular reference frame. It is then clear that magnetic configurations that are collinear or coplanar in the laboratory reference frame can become noncoplanar in the new reference frame.

We have illustrated these concepts by applying them to a simple minimal model that captures the essential aspects of Mn$_3$Sn. A similar analysis can in principle be applied to other materials that exhibit topological Hall effect induced by coplanar or collinear magnetic orderings. Moreover, given that the SU(2) gauge field produced by the SOC is a bond variable (i.e., it depends on the relative position of the two ions connected by that bond), it is natural to expect that pressure and strain could play an important role in the external control of the topological Hall effect. This is a new control variable enabled by the SOC, in addition to the external magnetic field that controls the orientation of the localized magnetic moments via the Zeeman term. It is then clear that SOC is crucially important for expanding the spectrum of materials and external fields that can be used to produce and control potentially large topological contributions to response functions.

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