Spontaneous Antisymmetric Spin Splitting in Noncollinear Antiferromagnets without Relying on Atomic Spin-Orbit Coupling

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We propose a realization of an antisymmetric spin-split band structure through magnetic phase transitions without relying on the atomic spin-orbit coupling. It enables us to utilize for a variety of magnetic-order-driven cross-correlated and nonreciprocal transport phenomena as similar to those in the atomic spin-orbit-coupling oriented systems. We unveil its general condition as an emergence of a bond-type magnetic toroidal multipole (polar tensor) in the triangular unit with the noncollinear 120°-AFM structures. By using the concept of augmented multipoles, we systematically analyze the phenomena in terms of an effective multipole coupling. Our multipole description is ubiquitously applied to any trigonal and hexagonal structures including the triangular, kagome, and breathing kagome structures, which provides how to design and engineer materials with a giant antisymmetric spin splitting and its physical responses even without the atomic spin-orbit coupling.

Presence of antisymmetric spin splitting in electronic band structure has drawn considerable interest in noncentrosymmetric materials, since it is a fundamental origin of rich spintronic functionalities, nonreciprocal transports, and magneto-electric effects [1–3]. It is typically realized in polar materials with the relatively large atomic spin-orbit coupling (SOC), for instance, the nonmagnetic Rashba compound, BiTeI, [4–6] and monolayer transition-metal dichalcogenides, MX₂ (M = Mo, W and X = S, Se) [7–10].

Even though a crystal structure is centrosymmetric, magnetic transition actualizes the antisymmetric spin splitting by an interplay between the kinetic motion of electrons and the magnetic structure via the SOC [11,12]. A spiral magnetic order is a typical example, which induces a linear magneto-electric effect in the presence of the nonzero vector spin chirality [13–15]. Another example is found in CoNb₃S₆ and Co₂Nb₂O₆ showing giant anomalous Hall and angle-dependent magneto-electric effects [16–21], respectively. It is emphasized that the emergent antisymmetric spin splitting through the magnetic phase transition is more flexibly controllable, i.e., the spin splitting driven by magnetic orders can be varied or even switched on and off by external fields, pressure and temperature. The complex interplay can be understood in a transparent manner by introducing the concept of the augmented multipole [22,24].

Since the above fascinating phenomena usually rely on the presence of the atomic SOC, candidate materials are limited to those constituted by moderately heavier elements in a crystal structure under low space-group symmetry. Such a limitation motivates a search for alternative mechanism to extend the occurrence of the spin-current generation. However, in the absence of the SOC it is proven that the collinear magnetic order leads only to the symmetric spin splitting in momentum space even with the broken spatial inversion symmetry due to SU(2) symmetry in spin space [26,27].

In the present study, we propose a realization of antisymmetric spin splitting by focusing on the triangular unit with the noncollinear 120°-AFM structures, and clarify microscopic conditions for the emergent spin splitting from a general point of view by introducing the multipole description [23,30]. The condition we found is that the magnetic toroidal (MT) multipoles present in the hopping Hamiltonian and they couple with the noncollinear AFM order parameters within the same irreducible representation in the high-temperature series expansion. We also predict possible cross-correlated and non-reciprocal transport phenomena in terms of an effective coupling among the multipole degrees of freedom, which can be modified by an external magnetic field for instance.

Our multipole description is ubiquitously applied to any trigonal and hexagonal structures including the triangular, kagome, and breathing kagome structures. Our proposal is demonstrated for the trigonal noncollinear AFM B₃MnNb₂O₇ based on the density-functional-theory (DFT) calculation. The present mechanism provides potentially gigantic antisymmetric spin splitting due to its kinetic-motion origin without relying on the atomic SOC, which can be directly detected in spin- and angle-resolved photoemission spectroscopy.

We start by considering a breathing kagome system with the noncollinear 120°-AFM structure in Fig. 1(a), which is an intuitive example showing an antisymmetric spin splitting. The positions of the three sublattice sites are defined by \( r_A = (0, 0, 0) \), \( r_B = a(1, 0, 0) \), and \( r_C = a(1/2, \sqrt{3}/2, 0) \) with \( a + b = 1 \). The tight-binding Hamiltonian is given by

\[
H = \left( t_A \sum_{\sigma, \langle ij \rangle} \epsilon_{\sigma} + t_B \sum_{\sigma, \langle ij \rangle} \epsilon_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma\sigma'} m_i \cdot c_{i\sigma}^\dagger c_{i\sigma'} \right),
\]

where \( c_{i\sigma}^\dagger (c_{i\sigma}) \) is the creation (annihilation) operator for site \( i \) and spin \( \sigma = \uparrow, \downarrow \). The first term represents the hop-
The origin of the antisymmetric spin splitting can be intuitively captured by applying the multipole description to the model in Eq. (1) [23, 26], as the type of an additional crystallographic symmetry breaking to the time-reversal symmetry is essential. To demonstrate this, first we introduce the triangular unit with three sublattices A-C, and define the 9 multipole degrees of freedom as shown in Fig. 1(c). Then, the spinless hopping matrix in the three-sublattice basis can be spanned by these multipoles. Moreover, the mean-field magnetic structure is also described by the multipoles, which are known as the cluster multipoles [35, 56].

The Hamiltonian in Eq. (1) is Fourier transformed with respect to the unit cell as

\[ \mathcal{H} = \sum_{k, \sigma \sigma', l' l} c_{k l \sigma}^\dagger \left[ \delta_{\sigma \sigma'} (H^Q_t + H^T_t)_{ll'} + \delta_{ll'} H^\sigma_{ml} \right] c_{k l' \sigma'}, \]

where \( c_{k l \sigma} \) is the Fourier transform of \( \hat{c}_{k n \sigma} \) at wave vector \( \mathbf{k} \) and sublattice \( l \). \( H^Q_t \) and \( H^T_t \) stand for the real and imaginary hopping matrices, respectively, which comes from the first term in Eq. (1), and \( H_m \) are the mean-field matrix from the second term in Eq. (1). The matrices \( H^Q_t \), \( H^T_t \), and \( H_m \) are decomposed in terms of the triangular-unit multipoles defined in Table I as

\[ H^Q_t = Q_0(k) \hat{Q}_0^{(1)} + Q_v(k) \hat{Q}_v^{(1)} + Q_{xy}(k) \hat{Q}_{xy}^{(1)}, \]
\[ H^T_t = T_{3a}(k) \hat{T}_{3a}^{(1)} + T_{3b}(k) \hat{T}_{3b}^{(1)} + T_{3g}(k) \hat{T}_{3g}^{(1)}, \]
\[ H_m = -m (\hat{Q}_{xy}^{(0)} \delta_x + \hat{Q}_v^{(0)} \delta_y). \]

Here, three onsite potentials and three bonds with real hoppings are described by the linear combination of the electric monopole \( \hat{Q}_0^{(n)} \) and two electric quadrupoles \( \hat{Q}_v^{(n)}, \hat{Q}_{xy}^{(n)} \), whereas three bonds with imaginary hoppings by two MT dipoles \( \hat{T}_{3a}^{(1)}, \hat{T}_{3b}^{(1)} \) and a MT octupole \( \hat{T}_{3g}^{(1)} \), where the superscripts \( n = 0 \) and 1 stand for onsite and bond indices, respectively [23, 26]. We use the standard Gell-Mann matrices to express each multipole in Table I and their schematic pictures are shown in Fig. 1(c). Each multipole is normalized as \( \text{Tr}[X^2] = 1 \). By using the molecular-orbital basis in the triangular unit [26, 37], we identify the symmetry of each multipoles as indicated by the subscript. The linear coefficients, the electric and MT multipoles \( \hat{Q}(k) \) and \( \hat{T}(k) \), represent the form factors, which are even and odd functions of \( k \), respectively. Note that their \( k \) dependences are consistent with the general definition of multipoles in momentum representation [23].

In the multipole description, the active odd-rank MT bond multipoles (imaginary hoppings) can become the origin of the antisymmetric spin splitting, once the effective coupling between them and the mean-field multipoles is activated under spontaneous magnetic orders [38]. Such an effective coupling is systematically obtained from the high-temperature expan-

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FIG. 1. (a) Noncollinear 120°-AFM pattern in the breathing kagome structure. (b) (left panel) The band structure of the model in Eq. (1) at \( t_a = 1, t_b = 0.5, \) and \( m = 0.3 \) and (right panel) the isoenergy surfaces at \( \mu = -1 \). The dashed lines show the band dispersions and the colormap shows the spin polarization of the \( z \) components at each wave vector. (c) Schematic pictures of the triangular-unit multipoles. The red (blue) circles represent the positive (negative) onsite potential, and the red (blue) lines and arrows on each bond represent the positive (negative) real and imaginary hoppings, respectively.

This threefold out-of-plane antisymmetric spin splitting has close resemblance to that observed in the monolayer dichalcogenides with the atomic SOC, which is so-called the Ising-type spin splitting [31, 33]. However, the microscopic origin is totally different, i.e., the present case is the non-SOC origin, although the resultant antisymmetric spin splitting becomes a source of various cross-correlated and transport phenomena, such as the magneto-electric effect and nonreciprocal transport, as discussed below. The out-of-plane antisymmetric spin splitting can be detected by using spin- and angle-resolved photoemission spectroscopy [34].
TABLE I. Multipole degrees of freedom in the triangular unit. The onsite potentials and nearest-neighbor hoppings are described by these multipoles. \( \lambda_a (\alpha = 0\text{-}8) \) are the Gell-Mann matrices. We use the abbreviated notations, \( k_x = k_\parallel/2, k_y = \sqrt{3}k_\parallel/2, p_a = t_a \), and \( p_b = -t_b \).

| electric | \( Q_0 \) | \( Q_0 \) | \( Q_{xy} \) |
|---|---|---|---|
| onsite | \( \frac{1}{\sqrt{3}} \lambda_0 \) | \( \frac{1}{\sqrt{3}} \lambda_0 \) | \( \frac{1}{\sqrt{3}} \lambda_3 \) |
| real bond | \( \frac{1}{\sqrt{3}} (\lambda_1 + \lambda_4 + \lambda_6) \) | \( \frac{1}{2} (\lambda_4 + \lambda_6 - 2\lambda_1) \) | \( \frac{1}{2} (-\lambda_4 + \lambda_6) \) |
| form factor | \( \sum k \theta (\cos k_x \eta + 2 \cos k_y \eta \cos \tilde{k}_y \eta) \) \( \frac{1}{\sqrt{3}} \sum k \theta (\cos k_x \eta \cos \tilde{k}_y \eta - \cos k_x \eta \) \( \frac{1}{2} \sum \eta \) \eta \cos \tilde{k}_y \eta \) | \( \frac{1}{\sqrt{3}} \sum \eta \) \eta \sin \tilde{k}_y \eta \) \( \frac{1}{2} \sum \eta \) \eta \sin \tilde{k}_y \eta \) |
| magnetic | \( T_{3a} \) | \( T_x \) | \( T_y \) |
| imaginary bond | \( \frac{1}{\sqrt{3}} (\lambda_7 - \lambda_5 - \lambda_7) \) | \( \frac{1}{2} (\lambda_7 - \lambda_5 - 2\lambda_2) \) | \( -\frac{1}{2} (\lambda_5 + \lambda_7) \) |
| form factor | \( -\sum p_0 \) \( \sin k_x \eta \) \( -2 \sin k_x \eta \cos \tilde{k}_y \eta \) \( \frac{1}{\sqrt{3}} \sum \eta \) \eta \sin \tilde{k}_y \eta \) \( \frac{1}{2} \sum \eta \) \eta \sin \tilde{k}_y \eta \) |

TABLE II. Effective multipole couplings under an external magnetic field \([39]\). The lowest-order band deformations \( q_x (k) \cdot \sigma \) of the wave-vector \( k \) dependences around \( k = 0 \), and relevant physical responses are shown, where \( Q \) and \( T \) are the electric polarization and magnetic toroidalization. ME and NR indicate magneto-electric and nonreciprocal responses, respectively.

| \( H \) | \( q_x (k) \cdot \sigma \) | \( k \to 0 \) limit | response |
|---|---|---|---|
| 100 | \( m^2 H_x Q_{xy}(k) T_{3a}(k) | \sigma_x \) | \( k_0^3 \) \( \sim H_x \) ME |
| 010 | \( m^2 H_y Q_{xy}(k) T_{3a}(k) | \sigma_y \) | \( k_0^3 \) \( \sim H_y \) ME |
| 001 | \( m^2 H_z Q_{xy}(k) T_{3a}(k) | \sigma_z \) + \( Q_x(k) T_{3a}(k) | \sigma_y \) | \( k_0^3 \) \( \sim H_z \) NR |
| 101 | \( m^3 H_x Q_{xy}(k) T_{3a}(k) | \sigma_0 \) + \( Q_x(k) T_{3a}(k) | \sigma_y \) | \( k_0^3 \) \( \sim H_x \) ME |
| 110 | \( m^3 H_y Q_{xy}(k) T_{3a}(k) | \sigma_0 \) + \( Q_x(k) T_{3a}(k) | \sigma_y \) | \( k_0^3 \) \( \sim H_y \) NR |

\( \sum_{i \sigma \sigma'} c_i^\dagger \sigma \sigma \sigma \sigma \sigma_i \sigma \sigma' \), yielding a rich variety of band deformations depending on the field direction. For \( H \parallel [100] \), the directional antisymmetric spin splitting with \( k_0^3 \) \( \sigma_z \) is induced by the coupling between \( T_{3a}, Q_{xy} \), and \( \sigma_z \). This band deformation describes the emergent magneto-electric (ME) effect where the electric polarization along the \( x \)-direction, \( Q_x \), is induced by \( H_z \), since \( k_0^3 \) \( \sigma_z \) is the same symmetry as \( Q_x \) \([23]\). In a similar way, different ME couplings are obtained for \( H \parallel [010] \) and \( H \parallel [001] \); the \( k_0^3 \) \( \sigma_z \)-type band deformation corresponding to \( Q_y \) for \( H \parallel [100] \) and the \( k_0^3 \) \( \sigma_y - k_0^3 \) \( \sigma_z \)-type band deformation corresponding to \( Q_z \) for \( H \parallel [001] \). Thus, the 120°-AFM order in the breathing kagome system exhibits the longitudinal ME effect \( (Q \parallel H) \). Note that the qualitatively similar results are also obtained by the symmetry analysis based on the cluster multipole theory \([35]\), although our approach is apparent for microscopic conditions to induce the antisymmetric spin splitting in a systematic way. We summarize the effective coupling and relevant responses under the magnetic fields in Table II \([39]\).

Interestingly, spin-independent antisymmetric band deformations are realized when the magnetic field is applied along the \( z \)-direction as shown in Fig. 2(a), where the effective multipole coupling is expressed as \( m^3 H_z T_{3a}(k) | \sigma_0 \) \( \sim m^3 H_z k_{xy}(k)^2 - 3k_0^2) \sigma_0 \). This type of antisymmetric band deformation becomes a microscopic source of the angle-dependent nonreciprocal transport. Moreover, when \( H \) is rotated from \([001] \) to \([011] \), the additional contribution,
responding isoenergy surfaces where the contour shows the kagome structures. Similar analyses can be directly applied to any model [40].

So far, we have considered the specific breathing kagome structure. Similar analyses can be directly applied to any other systems with the triangular unit, such as the triangular and kagome systems. For example, as the multipoles $Q_0^{(1)}$ and $T_{3a}^{(1)}$ are active in the three-sublattice 120°-AFM order on a triangular lattice, the antisymmetric spin splitting is expected [Fig. 3(a)]. Note that there are no additional antisymmetric band deformations induced by the magnetic field, since there are no active $Q_v^{(1)}$ and $\hat{T}_{zy}^{(1)}$ [see also Table 1]. The nearly 120°-AFM materials, such as CsFeCl₃ [41] and PdCrO₂ [42, 43], are candidates to exhibit the antisymmetric spin splitting. In a similar way, the antisymmetric spin splitting is expected for the $\sqrt{3} \times \sqrt{3}$ AFM order on the simple kagome structure, where only $\hat{Q}_{0}^{(1)}$ and $\hat{T}_{3a}^{(1)}$ are active multipoles as shown in Fig. 3(b). Moreover, the lower-symmetry trigonal material also shows spin-split physics, such as trimer and triangular tube magnets, LuFeO₃ [44] and CsCrF₃ [45, 46], which possesses the same active multipoles as the breathing kagome structure.

Finally, we demonstrate the emergent antisymmetric spin splitting in Ba₃MnNb₂O₉ [47]. This compound belongs to the trinodal space group $P3m1$ (No. 164), and the high-spin state ($S = 5/2$) of Mn²⁺ ions exhibits the 120°-AFM structure with out-of-plane cantings on the triangular lattice at low temperatures as shown in Figs. 4(a) and (b) [47]. We calculate the expected AFM band structure of Ba₃MnNb₂O₉ based on the DFT with the generalized gradient approximation by using the WIEN2k package [48]. We analyze a realistic tight-binding Hamiltonian obtained from the Wannier90 code [49, 50], and introduce the mean field to induce the 120°-AFM order by neglecting the out-of-plane component for simplicity. Figures 4(c) and (d) show the band structure and the isoenergy surfaces projected onto the $\sigma_z$-component in the AFM state at zero magnetic field, respectively. The results are consistent with the analysis in the simple triangular AFM in Fig. 4(a), i.e., the antisymmetric $z$-spin polarization in the form of $k_y(3k_x^2 - k_y^2)$. In addition, we also confirmed that the isoenergy surfaces are deformed antisymmetrically for $H \parallel [001]$. Therefore, this compound can be an archetypal example of the antisymmetric SOC physics induced by a noncollinear magnetic ordering.

In summary, we clarify general conditions for emergent antisymmetric spin-split band structures in noncollinear magnets. The following three conditions are enough to obtain the antisymmetric spin splitting in the band structure without the atomic SOC: (1) the triangular unit with the 120°-AFM structure, (2) inversion symmetry breaking and (3) active MT multipoles (imaginary hopping) in the one-body Hamiltonian. We also demonstrate the origin of the cross-correlated coupling and nonreciprocal transport is attributed to the effective
microscopic multipole couplings. As our analysis on the basis of the multipole description is ubiquitously applied to any systems with the triangular unit, the result will shed light on potential candidate materials with a giant spin splitting even without the atomic SOC.

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