In this paper, we study two different insulating three-dimensional (3D) quantum magnets. In the first part of this paper, we propose a strain-induced topological phase transition in 3D topological insulating antiferromagnets. We show that by applying (100) uniaxial strain, 3D antiferromagnetic Weyl magnons (WMs) in insulating antiferromagnets are an intermediate phase between a strain-induced 3D magnon Chern insulator (MCI) with integer Chern numbers and a 3D trivial magnon insulator with zero Chern number. In addition, we show that strain suppresses the topological thermal Hall conductivity of magnons. Our results provide a powerful mechanism for investigations of topological phase transitions in 3D chiral topological antiferromagnets. In the second part of this paper, we study the thermal Hall effect of magnons in the 3D insulating honeycomb ferromagnet CrI$_3$. Using the experimentally deduced parameters, we compute the 3D thermal Hall conductivity of magnons in CrI$_3$ and show that it is not negligible and it is positively enhanced by the interlayer coupling and the magnetic field. Our result provides an essential guide for future experimental measurements of magnon thermal Hall conductivity in CrI$_3$.

I. INTRODUCTION

Three-dimensional (3D) topological semimetals are exotic phases of matter with gapless electronic excitations, which are protected by topology and symmetry. Their theoretical predictions and experimental discoveries have attracted considerable attention in condensed-matter physics [1–8]. They currently remain an active field of study. Nevertheless, the condensed matter realization of topological semimetals is essentially independent of the statistical nature of the quasiparticle excitations. In fact the notion of Weyl points was first observed experimentally in bosonic quasiparticle excitations [9].

There has been an intensive search for bosonic analogs of 3D topological semimetals in insulating quantum magnets with broken time-reversal symmetry [10–22]. Recently, topological Dirac magnons protected by a coexistence of inversion and time-reversal symmetry have been experimentally observed in a 3D collinear antiferromagnet Cu$_3$TeO$_6$ [14, 15]. This has opened a great avenue for observing topological Weyl magnon (WM) points in 3D insulating quantum magnets. In magnetic bosonic systems, however, it is essentially important that the WM nodes occur at the lowest excitation if they were to make any significant contributions to observable thermal Hall transports. This is due to the population effect of bosonic quasiparticles at low temperatures. In this respect, WM nodes at the lowest excitation can be considered as the analog of electronic Weyl points close to the Fermi energy. The WM in the 3D kagome chiral antiferromagnet exhibit a topological thermal Hall effect [12]. Currently, they are the only known antiferromagnetic system in which the WM nodes occur at the lowest acoustic magnon branch and contribute significantly to the thermal Hall transports.

It is well-known that electronic ferromagnetic Weyl semimetal occurs as an intermediate phase between an ordinary insulator and a 3D quantum anomalous Hall insulator [2] [23]. To our knowledge, this interesting topological phase boundary has not been established in 3D topological antiferromagnets. Thus far, the topological Dirac and Weyl nodes that appear in 3D insulating antiferromagnets [10][17] cannot transit to another topological magnon phase. In this respect, strain provides...
an effective way to tune the band structure of crystal in quantum materials. For instance, uniaxial strain can induce chiral anomaly and topological phase transitions in 3D topological Dirac and Weyl semimetals \[24,25\]. Moreover, strain can also induce a 3D topological Dirac semimetal in epitaxially-grown α-Sn films on InSb(111) \[32\]. We envision that such strain effects could be possible in 3D topological antiferromagnets.

In addition, recent experiment has observed topological magnons in the bulk honeycomb ferromagnet CrI\(_3\) at zero magnetic field \[33\], which follows from earlier theoretical proposals in Ref. \[34\] followed by Ref. \[35\]. However, the observed topological magnons show a non-vanishing dispersion along the out-of-plane c axis and there is a non-negligible interlayer coupling. The fitted parameters also contain exchange interactions up to third nearest neighbours. Therefore, a complete 3D analysis of this system is desirable. In fact, the experimentally observed topological ferromagnetic magnons in CrI\(_3\) should also exhibit the magnon thermal Hall effect, which has been studied in other ferromagnetic insulators \[36–40\,42,43\].

In this paper, we study two different 3D insulating quantum magnets. In the first part of this paper, we propose a strain-induced topological magnon phase transition in 3D topological insulating antiferromagnets. Due to the nature of the topological magnon band distributions in the 3D kagome chiral antiferromagnet, we have chosen this system for our study. However, our results can be extended to other 3D topological insulating antiferromagnets such as Cu\(_3\)TeO\(_6\) \[14,15\]. We show that under (100) uniaxial strain, a topological magnon phase transition exist in the 3D topological insulating kagome chiral antiferromagnet.

We have identified four different magnon phases in this system as shown in Fig. 1. The 3D nodal-line magnon (NLM) and the triple point magnon (TPM) appear at zero magnetic field or at zero in-plane Dzyaloshinskii-Moriya interaction (DM) interaction \[14,15\] with a conventional 3D in-plane 120° non-collinear spin structure. They can be tuned by strain. The 3D WM phase appears in the unstrained limit at nonzero magnetic field or non-zero in-plane DM interaction with a noncoplanar chiral spin structure. The two new magnon phases that appear due to strained noncoplanar chiral spin structure are the fully gapped 3D MCI and the fully gapped 3D trivial insulator. We show that the former has integer Chern numbers, whereas the latter has zero Chern number. The study of the topological thermal Hall effect of magnons shows that the thermal Hall conductivity is suppressed in the fully gapped insulator phases. This implies that strain suppresses the thermal Hall conductivity of magnons.

In the second part of this paper, we provide a complete computation of the magnon thermal Hall conductivity in the bulk honeycomb ferromagnet CrI\(_3\) using a 3D Heisenberg spin model and the experimentally determined parameters \[33\]. We show that the magnitude of the magnon thermal Hall conductivity in CrI\(_3\) is not negligible and it is positively enhanced by the interlayer coupling and the magnetic field. We believe that our result provides a promising guide for future thermal Hall transport experiments in CrI\(_3\).

II. STRAINED 3D KAGOME CHIRAL ANTIFERROMAGNET

We study 3D kagome chiral antiferromagnets in the presence of (100) uniaxial strain and an external magnetic field along the (001) direction. The Heisenberg spin model is given by

\[
\mathcal{H} = \sum_{(ij),\ell} J_{ij} \vec{S}_i^\ell \cdot \vec{S}_j^\ell + \sum_{(ij),\ell} \vec{D}_{ij} \cdot \vec{S}_i^\ell \times \vec{S}_j^\ell + J_c \sum_{(\ell'\ell),i} \vec{S}_i^{\ell'} \cdot \vec{S}_i^\ell - \vec{H} \cdot \sum_{i,\ell} \vec{S}_i^\ell, \tag{1}
\]

where \(\vec{S}_i^\ell\) is the spin vector at site \(i\) in layer \(\ell\). The first term is the intralayer nearest-neighbour Heisenberg coupling. We model the effect of uniaxial strain along the (100) direction using the approximation that only the Heisenberg spin interaction along the in-plane \(x\) direction changes. In this case \(J_{ij} = J_1\) along the diagonal bonds and \(J_{ij} = J_1\delta\) along the horizontal bonds, where \(\delta\) is the strain as shown in Fig. 2(a). An alternative approximation is to consider isotropic Heisenberg interactions with lattice deformation in which only the primitive lattice vectors change. This will also modify the in-plane diagonal bonds, although to a lesser extent. We note that since the Weyl nodes in the isotropic limit is along the out-of-plane direction, it suffices to consider only the change along the in-plane horizontal bonds as the change along the in-plane diagonal bonds will not give any new topological phase transitions. In other words, the topological phase transition requires a modification of the in-plane coupling constants. The second term is the out-of-plane \((\vec{D}_{ij} = \pm D\hat{z})\) DM interaction due to inversion symmetry breaking between two sites on each kagome layer. The DM interaction alternates between the triangular plaquettes of the kagome lattice and it stabilizes the conventional in-plane 120° non-collinear spin structure. Its sign determines the vector chirality of the non-collinear spin order \[46\]. The third term is the nearest-neighbour interlayer antiferromagnetic coupling between the kagome layers, which is inherently present in real kagome materials \[47,51\]. Finally, the last term is an external magnetic field along the stacking direction \(\vec{H} = g\mu_B H\hat{z}\), where \(g\) is the Landé g-factor and \(\mu_B\) is the Bohr magneton.

In the absence of strain, \(i.e.,\ \delta = 1\), the 3D noncoplanar chiral kagome chiral antiferromagnets are intrinsic WM semimetals. The noncoplanar chiral spin texture with macroscopically broken time-reversal symmetry can be induced by an in-plane intrinsic DM interaction or an external magnetic field \[12\]. The WM phase in this system cannot transit to any other magnon phase by chang-
The bulk Brillouin zone of the hexagonal lattice. A uniaxial strain is applied along the (001) direction. The distribution of the scalar spin chirality on the kagome lattice. (d) Neighbours denoted by the blue and red lines. (c) Configuration of the spin structure at zero magnetic field. A uniaxial strain is applied along the midpoint of the second-nearest neighbours denoted by the blue and red lines. (b) Top view of stacked honeycomb-lattice ferromagnets along the (001) direction. The distribution of mirror reflection symmetry \( M_{z,y} \) of the kagome plane about the z axis and \( T \), \( i.e \, T M_{z,y} T \text{ or } M_{y} T \), is also a symmetry of the conventional in-plane 120° non-collinear spin structure [52–61]. These symmetries are known as the “effective time-reversal symmetry” and they lead to nodal-line magnons and triply-degenerate nodal magnon points in the conventional 3D in-plane 120° spin structure of the stacked kagome antiferromagnets.

B. Field-induced noncoplanar chiral spin texture

Next, we induce noncoplanar chiral spin texture in the non-collinear regime by applying a magnetic field along the (001) stacking direction. We note that a noncoplanar chiral spin texture can also be induced if the intrinsic in-plane DM interaction is present [47–51]. Due to the presence of an out-of-plane DM interaction, a magnetically-ordered phase is present at low temperatures. In the ordered phase the magnetic excitations are magnons (quantized spin waves). They can be captured clearly in the linear spin wave theory approximation. First, let us express the spins in terms of local axes, such that the z axis coincides with the spin direction. This can be done by performing a local rotation \( R_z(\theta, \ell) \) about the \( z \)-axis by the spin orientated angles \( \theta_{A,B,C} = 0, \varphi, -\varphi \), where \( \varphi \neq 120^\circ \) for \( \delta \neq 1 \). As the external magnetic field induces canting of spins in the out-of-plane direction, we perform another rotation \( R_y(\chi) \) about \( y \)-axis by the angle \( \chi \). Now, the spins transform as

\[
\vec{S}_{i,\ell} \rightarrow R_z(\theta_{i,\ell}) \cdot R_y(\chi) \cdot \vec{S}_{i,\ell},
\]

where the rotation matrices \( R_z(\theta_{i,\ell}), R_y(\chi) \) are given in the Appendix [A]. Using the Holstein Primakoff transformation [53], the non-interacting spin-wave Hamiltonian in momentum space can be written as

\[
\hat{H} = S \sum_{\vec{k},\alpha,\beta} 2 \left( \gamma^{(0)}_{\alpha\beta} \delta_{\alpha\beta} + \gamma^{(1)}_{\beta} \right) a^\dagger_{\vec{k}\alpha} a_{\vec{k}\beta} + \gamma^{(2)}_{\alpha\beta} \left( a^\dagger_{\vec{k}\alpha} a^\dagger_{-\vec{k}\beta} + a_{\vec{k}\alpha} a_{-\vec{k}\beta} \right),
\]

where \( \gamma^{(i)}_{\alpha\beta} \) are 3 x 3 matrices (see Appendix [A]), and \( S \) is the value for the spin. The three sublattices on the kagome lattice are \( \alpha, \beta = A, B, C \). Here, \( a^\dagger_{\vec{k}\alpha} (a_{\vec{k}\alpha}) \) are the bosonic creation (annihilation) operators.

As shown in Appendix [A], a finite magnetic field \( H \neq 0 \) induces a noncoplanar chiral spin texture with finite scalar spin chirality [see Fig. 2(c)] given by \( \chi_{ijk,\ell} = \cos \chi_{ijk,\ell} \cdot (\vec{S}_{i,\ell} \times \vec{S}_{j,\ell}) \), where \( \cos \chi = H/H_S(\delta) \) and the saturation field \( H_S(\delta) \) is given in the Appendix.

In contrast to other magnetic Weyl systems that rely on time-reversal symmetry breaking by magnetic order, it is important to note that the scalar spin chirality breaks time-reversal symmetry macroscopically, and induces Weyl nodes at \( \delta = 1 \). At \( H = 0 \) the scalar spin chirality vanishes. In this case, the unstrained 3D kagome

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**A. Symmetry protection of the conventional in-plane noncollinear spin structure**

As previously discussed in ref. [12], the conventional 3D in-plane 120° spin structure at zero magnetic field preserves all the symmetries of the kagomé lattice. In particular, the combination of time-reversal symmetry (denoted by \( T \)) and spin rotation denoted by \( R_z(\pi) \) is a good symmetry [52], where \( R_z(\pi) = \text{diag}(-1, -1, 1) \) denotes a \( \pi \) spin rotation of the in-plane coplanar spins about the \( z \)-axis, and ‘diag’ denotes diagonal elements. In addition, the system also has three-fold rotation symmetry along the \( z \) direction denoted by \( C_3 \). The combination of mirror reflection symmetry \( M_{x,y} \) of the kagome plane about the \( x \) or \( y \) axis and \( T \), \( i.e \, T M_{x,y} T \text{ or } M_{y} T \), is also a symmetry of the conventional in-plane 120° non-collinear spin structure [52–61]. These symmetries are known as the “effective time-reversal symmetry” and they lead to nodal-line magnons and triply-degenerate nodal magnon points in the conventional 3D in-plane 120° spin structure of the stacked kagome antiferromagnets.
FIG. 3: Color online. Strain-induced topological magnon phase transitions in 3D kagome chiral antiferromagnets. (a) 3D trivial magnon insulator for $\delta = 0.75$, (b) 3D acoustic WM for $\delta = 1$, (c) 3D MCI for $\delta = 1.05$. The other parameters are set as $J_c/J_1 = 0.6$, $D/J_1 = 0.2$, $H/J_1 = 0.5$.

FIG. 4: Color online. Heat map of the energy gap between the two acoustic magnon branches as a function of the momentum along the high symmetry line -$H$--$K$--$H$ and magnetic field. (a) 3D trivial magnon insulator for $\delta = 0.75$. (b) 3D WMs for $\delta = 1$. (c) 3D MCI for $\delta = 1.05$. The other parameters are set as $J_c/J_1 = 0.6$, $D/J_1 = 0.2$.

FIG. 5: Color online. Energy band gap between the two lowest acoustic magnon bands along $K$--$H$ high symmetry line as a function of strain. The parameters are $J_c/J_1 = 0.6$, $D/J_1 = 0.2$, and $H/J_1 = 0.5$.

C. Strain-induced topological phase transitions

Remarkably, the strained 3D kagome chiral antiferromagnet in the noncoplanar regime exhibits a topological...
magnon phase transition with interesting features. We will now investigate different aspects of these topological phase transitions. First, let us consider the 3D magnon band structures with varying \( \delta \). To establish a 3D spin structure, we fix a strong interlayer coupling \( J_c/J_1 = 0.6 \). In Fig. (3) we have shown the evolution of the 3D magnon bands along the Brillouin zone (BZ) paths in Fig. 2(d).

We can see that the uniaxial strain along the (100) direction gaps out the 3D WM phase at \( \delta = 1 \) along the high symmetry lines \( K-H \) and \( \Gamma-A \) of the BZ.

Let us define the gap between the two acoustic magnon branches as

\[
E_{\text{gap}} = 2|E_2(\vec{k}) - E_1(\vec{k})|.
\]

At the WM points \( E_{\text{gap}} \) vanishes, and the fully gapped magnon insulators are characterized by a non-zero \( E_{\text{gap}} \) along the high symmetry lines of the BZ. Next, let us check if the regime \( \delta \neq 1 \) is truly a fully gapped magnon insulator with \( E_{\text{gap}} \neq 0 \) for varying magnetic field in the noncoplanar regime. For this purpose, we have fixed the antiferromagnetic interlayer coupling to \( J_c/J_1 = 0.6 \) and the DM interaction to \( D/J_1 = 0.2 \). We then plot the heat map of \( E_{\text{gap}} \) as a function of the momentum along the high symmetry lines and the magnetic field in the noncoplanar regime. The heat map of \( E_{\text{gap}} \) is shown in Figs. 4(a)–(c) for different regimes of \( \delta \). At the critical point \( \delta = 1 \) we can see that gapless points (black lines) appear between the two acoustic magnon branches, which signify the presence of WM points along \(-H-K-H\) lines. In the regimes \( \delta < 1 \) and \( \delta > 1 \) there are no discernible gapless points along the \(-H-K-H\) line of the BZ. Therefore these two regimes define fully gapped magnon insulators, however with different properties as we will see later. Furthermore, in Fig. 5 we have shown the evolution of the magnon energy band gap \( E_{\text{gap}} \) along the \( K-H \) high symmetry line as a function of the strain parameter \( \delta \). We can see that the three distinct regions are clearly identified. We have checked that similar trends are manifested along the \(-A-\Gamma-A\) line.

Now, we will consider the Chern number topological phase transition of the system. This will justify the topological and non-topological regimes of \( \delta \). We will focus on the lowest acoustic magnon branch in which the strain-induced topological phase transition occurs. In this case, we can formally define the 3D trivial magnon insulator as the state where the Chern number of the lowest acoustic magnon branch vanishes, and a 3D MCI as the state with non-zero integer Chern numbers. The 3D antiferromagnetic system can be considered as slices of 2D antiferromagnetic MCIs [55, 56] interpolating between the magnetic system can be considered as slices of 2D antiferromagnetic insulators, however with different properties as we will see later. Furthermore, in Fig. (5) we have shown the evolution of the magnon energy band gap \( E_{\text{gap}} \) along the \( K-H \) high symmetry line as a function of the strain parameter \( \delta \). We can see that the three distinct regions are clearly identified. We have checked that similar trends are manifested along the \(-A-\Gamma-A\) line.

Having identified the different magnon phases in the strained 3D kagome chiral antiferromagnet, we will now consider the Chern number evolution of the magnon energy band gap as a function of the magnetic field in the regime \( \delta < 1 \). For small magnetic field in the regime \( \delta < 1 \), however, the Chern number of lowest acoustic magnon band is \( C = -1 \) and changes it changes sign as the sign of the magnetic field is flipped. At the 3D WM phase \( \delta = 1 \), the Chern number is \( C = -2 \) for small magnetic field.

D. Topological thermal Hall effect

Having identified the different magnon phases in the strained 3D kagome chiral antiferromagnet, we will now consider the Chern number evolution of the magnon energy band gap as a function of the magnetic field in the regime \( \delta < 1 \). For small magnetic field in the regime \( \delta < 1 \), however, the Chern number of lowest acoustic magnon band is \( C = -1 \) and changes it changes sign as the sign of the magnetic field is flipped. At the 3D WM phase \( \delta = 1 \), the Chern number is \( C = -2 \) for small magnetic field.
study an experimentally feasible measurement that can be performed on this system. The topological thermal Hall effect of magnons refers to the generation of a transverse thermal Hall voltage in the presence of a longitudinal temperature gradient due to the presence of noncoplanar chiral spin textures. In principle, it does not necessarily require the DM interaction provided a noncoplanar chiral spin configuration can be established, for example by adding further nearest-neighbour interactions. Therefore, the topological thermal Hall effect of magnons is different from the conventional magnon thermal Hall effect in insulating ferromagnets which strictly requires the DM interaction [36][43].

In the 3D model, the topological thermal Hall conductivity has three contributions \(\kappa_3^{xy}, \kappa_3^{zx}, \text{ and } \kappa_3^{xy}\), where the components are given by

\[
\kappa_{\alpha\beta}^{3D} = -k_B T \int_{BZ} \frac{d\vec{k}}{(2\pi)^3} \sum_{n=1}^{N} c_2 \left( f_n^{B} \right) \Omega_{\alpha\beta}^{n}(\vec{k}),
\]

where \( f_n^{B} = \left( e^{E_n(\vec{k})/k_B T} - 1 \right)^{-1} \) is the Bose occupation function, \( k_B \) the Boltzmann constant which we will set to unity, \( T \) is the temperature and \( c_2(x) = (1 + x) \left( \ln \frac{1+x}{1-x} \right)^2 - (\ln x)^2 - 2 Li_2(-x) \), with \( Li_2(x) \) being the dilogarithm. In Eq. (7), we have dropped the term \(-2\pi^2 \sum_{n=1}^{N} \Omega_{\alpha\beta}^{n}(\vec{k})\), since the sum of the Berry curvature of the three magnon bands is zero.

Due to the Bose occupation function, the dominant contribution to \(\kappa_3^{xy}\) comes from the lowest magnon branch, where the topological phase transitions occur in the current system. As the noncoplanar chiral spin configuration is induced along the \(z\) direction, the first two components \(\kappa_3^{xy}\) and \(\kappa_3^{zx}\) vanish. The nonzero component \(\kappa_3^{xy}\) can be written as

\[
\kappa_3^{xy} = -k_B T \int_{BZ} \frac{d\vec{k}}{(2\pi)^3} \sum_{n=1}^{N} c_2(f_n^{B}) \Omega_{3D}^{xy}(\vec{k}),
\]

III. THREE-DIMENSIONAL HONEYCOMB FERROMAGNET

Motivated by recent experiment [33], we study the bulk 3D honeycomb ferromagnet CrI\(_3\). The Heisenberg spin model is given by

\[
\mathcal{H} = -\sum_{ij,\ell} J_{ij} \vec{S}_i^\ell \cdot \vec{S}_j^\ell + \sum_{(ij),\ell} \vec{D}_{ij} \cdot \vec{S}_i^\ell \times \vec{S}_j^\ell
\]

\[
- K \sum_{i,\ell} \left( S_{i}^{\ell,\ell'} \right)^2 - J_c \sum_{(\ell'),i} \vec{S}_i^{\ell'} \cdot \vec{S}_i - \vec{H} \cdot \sum_{i,\ell} \vec{S}_i^\ell.
\]

The first term is the intralayer Heisenberg coupling up to third-nearest-neighbours \(J_{ij} = J_1, J_2, J_3\). The second term is the DM interaction due to inversion symmetry breaking on the second-nearest-neighbour bonds \(\vec{D}_{ij} = \nu_{ij} \vec{D}_z\), where \(\nu_{ij} = \pm1\) for clockwise and counterclockwise hopping magnons on each honeycomb layer sublattices as depicted in Fig. 2(b). The third term is the easy-axis anisotropy. The fourth term is the nearest-neighbour ferromagnetic interlayer coupling. Finally, the last term is an external Zeeman magnetic field along the stacking \(c(z)\) direction \(\vec{H} = g\mu_B H\hat{z}\), where \(g\) is the Landé factor and \(\mu_B\) is the Bohr magneton. We consider congruently-stacked honeycomb ferromagnetic layers. Due to a nonzero easy-axis anisotropy in CrI\(_3\), recent experiment shows that the magnetic spin moments are already polarized along the \(c\) axis at zero magnetic field, which enables the observation of topological magnon dispersions without an external applied magnetic field [33]. This is in stark contrast to the in-plane kagome ferromagnet Cu(1,3-bdc) [37], where the magnetic field is required to polarize the spins along the \(z\) axis.

By fitting the observed topological magnon dispersions, the following parameters were deduced [33]: \(J_1 = 2.01\text{ meV}, J_2 = 0.16\text{ meV}, J_3 = 0.18\text{ meV}, D = 0.31\text{ meV}, K = 0.22\text{ meV}, J_c = 0.59\text{ meV}.\)
Magnon Hamiltonian in momentum space can be written using the bosonic creation \( a^\dagger_i \) and annihilation \( a_i \) operators, and \( S_i^{x,y} \) denote the spin raising and lowering operators. The resulting noninteracting magnon Hamiltonian in momentum space can be written as

\[
\mathcal{H} = E_0 + S \sum_k \psi^\dagger(\vec{k}) \cdot \mathcal{H}(\vec{k}) \cdot \psi(\vec{k}),
\]

where \( E_0 \) is the mean-field energy, \( \psi^\dagger(\vec{k}) = (a^\dagger_{k,A}, a^\dagger_{k,B}) \) is the basis vector. The momentum space Hamiltonian is given by

\[
\mathcal{H}(\vec{k}) = \begin{pmatrix}
    m(\vec{k}) + f_1(\vec{k}) & f_2(\vec{k}) + f_3(\vec{k}) \\
    f_2^*(\vec{k}) & f_3^*(\vec{k}) + m(-\vec{k}) + f(\vec{k})
\end{pmatrix}.
\]
B. Topological spin excitations and Chern numbers

The topological magnon dispersions are depicted in Fig. 8 with the experimentally deduced parameters at zero magnetic field. We can see that the acoustic (lower) and the optical (upper) magnon modes are well-separated. As observed in the experiment [33], the optical magnon mode extends up to $\hbar\omega = 20$ meV in the $k_z = 0$ plane and the acoustic magnon mode extends up to $\hbar\omega = 2$ meV along the line $k_x = k_y = 0$. The small gap at the $\Gamma$ point is due to nonzero easy-axis anisotropy $K = 0.22$ meV. The gaps at the Dirac points at $K$ and $H$ can be attributed to a nonzero DM interaction $D = 0.31$ meV. This leads to nonzero Chern numbers. Using the experimentally deduced parameters [33], we find $C_\pm = \mp 1$ for the lower and upper spin wave modes of the 3D system. The inset of Fig. 8 shows the variation of the Chern numbers as a function of $J_3$.

C. Thermal Hall effect of magnons in CrI$_3$

The thermal Hall effect of magnons in insulating ferromagnets has been extensively studied both theoretically and experimentally in different insulating ferromagnets [39–40, 42, 43]. However, the thermal Hall effect in CrI$_3$ has not been studied using the 3D model in Eq. (10). The thermal Hall effect provides a way to access the magnetic excitations in quantum magnets, and it is believed to be due to topological magnons in ordered insulating ferromagnets. Therefore, a nonzero thermal Hall conductivity will solidify the belief that the observed magnon modes in CrI$_3$ are indeed topological. Similar to the 3D chiral kagome antiferromagnets, the total intrinsic anomalous thermal Hall conductivity in the present case also has the three contributions $\kappa_{y^y}$, $\kappa_{z^z}$, and $\kappa_{z^y}$, but only the intrinsic contributions of $\kappa_{y^y}$ are nonzero as the spins are fully polarized along the $z$ axis. Therefore, Eqs. (8) and (9) are also valid in the present case.

In Fig. (10) we have shown the temperature dependence of the 3D magnon thermal Hall conductivity of CrI$_3$ up to $T = J_1 \sim 23$ K, which is below $T_c = 61$ K. We can see that the magnon thermal Hall conductivity is negative and drops with increasing temperature (note that $T_c/J_1 \sim 2.6$). The magnon thermal Hall conductivity also increases positively with increasing $J_3$. The inset of Fig. (10) shows that the fully 3D model has a positively enhanced magnon thermal Hall conductivity than the 2D system at $J_3 = 0$. Indeed, experiment shows that the magnon dispersion along the $c$ axis does not vanish and $J_c \neq 0$ [33]. In Fig. (10) we have shown the heat map of $\kappa_{z^y}$ in CrI$_3$ in the plane of the magnetic field and temperature (a), the trend of $\kappa_{z^y}$ vs. $D$ (b), and the trend of $\kappa_{z^y}$ vs. $J_3$ (c) for some values of $T/J_1$. In (a) and (c) we can see that $\kappa_{z^y}$ is also positively enhanced by increasing magnetic field and $J_3$, whereas it decreases negatively with increasing $D$ as shown in (b).

IV. CONCLUSION

We have proposed a strain-induced topological phase transition in 3D topological insulating antiferromagnets and studied the 3D magnon thermal Hall effect in CrI$_3$.

In the first part of our results, we have shown that in the presence of (100) uniaxial strain, the antiferromagnetic WM in 3D topological insulating antiferromagnets is an intermediate phase between a 3D antiferromagnetic MCI with integer Chern numbers and a 3D antiferromagnetic trivial insulator with zero Chern number. We further showed that the thermal Hall conductivity of magnons is suppressed in the 3D insulator phases. Besides, we found that the 3D trivial magnon insulator with zero Chern number possess a non-zero thermal Hall conductivity due to the bosonic nature of magnons. We believe that our results can be investigated experimentally in various 3D insulating antiferromagnets by...
applying uniaxial strain or pressure. For the 3D kagome chiral antiferromagnets, there are various promising materials that have been synthesized lately [47, 51]. Furthermore, it will be interesting to experimentally investigate the effects of strain on the recently observed 3D topological Dirac magnons in the insulating antiferromagnet Cu$_3$TeO$_6$ [14, 15]. Due to the similarity between 3D insulating and metallic kagome chiral antiferromagnets, we envision that the current results could also manifest in the 3D antiferromagnetic topological Weyl semimetals Mn$_3$Sn/Ge [57, 62].

In the second part of our results, we computed the magnon thermal Hall conductivity of CrI$_3$ using the experimentally determined values of the parameters [33]. We found that the magnon thermal Hall conductivity of CrI$_3$ can be observed in experiment and it can be also be enhanced by the interlayer coupling and the magnetic field. The temperature dependence of the magnon thermal Hall conductivity is also negative, which suggests electron-like. Therefore, if the observed magnon dispersions in CrI$_3$ are topological, we believe that our results will pave the way for future experimental measurements of magnon thermal Hall conductivity in CrI$_3$.

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Appendix A: Spin wave theory

The rotation matrices that transform the spins are given by

\[ \mathcal{R}_z(\theta_{i,\ell}) = \begin{pmatrix} \cos \theta_{i,\ell} & -\sin \theta_{i,\ell} & 0 \\ \sin \theta_{i,\ell} & \cos \theta_{i,\ell} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{A1} \]

\[ \mathcal{R}_y(\chi) = \begin{pmatrix} \cos \chi & 0 & \sin \chi \\ 0 & 1 & 0 \\ -\sin \chi & 0 & \cos \chi \end{pmatrix}, \tag{A2} \]

\[ \mathcal{R}_z(\theta_{i,\ell}) \cdot \mathcal{R}_y(\chi) = \begin{pmatrix} \cos \theta_{i,\ell} \cos \chi - \sin \theta_{i,\ell} \sin \chi & \sin \theta_{i,\ell} \cos \chi & \cos \theta_{i,\ell} \sin \chi \\ \sin \theta_{i,\ell} \cos \chi + \cos \theta_{i,\ell} \sin \chi & \cos \theta_{i,\ell} \cos \chi - \sin \theta_{i,\ell} \sin \chi & 0 \\ -\sin \chi & 0 & \cos \chi \end{pmatrix}. \tag{A3} \]

Next, we apply the transformation in Eq. (2). The terms that contribute to linear spin wave theory are given by

\[ \mathcal{H}_J = \sum_{\langle ij,\ell \rangle} J_{ij} \left[ \cos \theta_{ij,\ell} \vec{S}_{i,\ell} \cdot \vec{S}_{j,\ell} + 2 \sin^2 \left( \frac{\theta_{ij,\ell}}{2} \right) \sin^2 \chi \vec{S}_{i,\ell}^x \vec{S}_{j,\ell}^x + \cos^2 \chi \vec{S}_{i,\ell}^y \vec{S}_{j,\ell}^y \right] \]

\[ + \sin \theta_{ij,\ell} \cos \chi \vec{z} \cdot \vec{S}_{i,\ell} \times \vec{S}_{j,\ell} \], \tag{A4} \]

\[ \mathcal{H}_D = D \sum_{\langle ij,\ell \rangle} \left[ -\cos \theta_{ij,\ell} \cos \chi \vec{z} \cdot \vec{S}_{i,\ell} \times \vec{S}_{j,\ell} + \sin \theta_{ij,\ell} \left( \sin^2 \chi \vec{S}_{i,\ell}^x \vec{S}_{j,\ell}^y + \cos^2 \chi \vec{S}_{i,\ell}^y \vec{S}_{j,\ell}^x \right) \right] \]

\[ + 2 \sin^2 \left( \frac{\theta_{ij,\ell}}{2} \right) \sin^2 \chi \vec{S}_{i,\ell}^y \vec{S}_{j,\ell}^y + \cos^2 \chi \vec{S}_{i,\ell}^x \vec{S}_{j,\ell}^x \], \tag{A5} \]

where \( \theta_{\alpha \beta} = \theta_{\alpha} - \theta_{\beta} \). The emergent field-induced scalar spin chirality due to non-coplanar spin structure is given by

\[ \chi_{ijk,\ell} \propto \cos \chi \vec{S}_{i,\ell}^z \cdot \left( \vec{S}_{j,\ell} \times \vec{S}_{k,\ell} \right). \tag{A7} \]

The magnetic field term is given by

\[ H_Z = -H \cos \chi \sum_{i,\ell} \vec{S}_{i,\ell}^z. \tag{A8} \]

The classical ground state energy is given by

\[ E_{cl}(\varphi)/NS^2 = 2J_1(2+\delta) \left[ (1-\cos \varphi) \cos^2 \chi + \cos \varphi \right] - 4D \sin^2 \chi \sin \varphi \cos \varphi \]

\[ - 2J_1(1 - 2 \cos^2 \chi) - 3H \cos \chi, \tag{A9} \]

where \( N \) is the number of sites per unit cell. The magnetic field has been rescaled in unit of \( S \). By minimizing the classical energy we get the canting angle \( \cos \chi = H/H_S(\delta) \), where \( H_S(\delta) = \frac{1 - \cos^2 \varphi}{3} \left[ 4J_1(2 + \delta) + 8D \sin \varphi \right] - 4J_1 \).

We can now perform the linearized Holstein Primakoff transformation [53]

\[ S_{i,\ell}^z = S - a_{i,\ell}^\dagger a_{i,\ell}, \quad S_{i,\ell}^+ = \sqrt{2S} a_{i,\ell} = (S_{i,\ell}^-)^\dagger, \tag{A10} \]

where \( a_{i,\ell}^\dagger(a_{i,\ell}) \) are the bosonic creation (annihilation) operators, and \( S_{i,\ell}^x = S_{i,\ell}^z \pm iS_{i,\ell}^y \) denote the spin raising and lowering operators.

The noninteracting spin wave Hamiltonian for the intralayer interactions is given by

\[ \mathcal{H}_{J_{ij,D}} = S \sum_{\langle ij \rangle} \left[ M_{ij}^{(0)}(a_{i,\ell}^\dagger a_{j,\ell} + a_{j,\ell}^\dagger a_{i,\ell}) \right] \]

\[ + M_{ij}^{(1)}(e^{-\phi_{ij,\ell}} a_{i,\ell}^\dagger a_{j,\ell} + \text{H.c.}) \]

\[ + M_{ij}^{(2)}(a_{i,\ell}^\dagger a_{j,\ell} + \text{H.c.}) \]  \[ + h_x \sum_{\ell} a_{i,\ell}^\dagger a_{i,\ell}, \tag{A11} \]
where \( h_\chi = h \cos \chi \),

\[
M^{(0)}_{ij} = -J_{ij}[\cos \theta_{ij} + 2\cos^2 \chi \sin^2(\theta_{ij}/2)] - D \sin^2 \chi \sin \theta_{ij},
\]

\[
M^{(1)}_{ij} = \sqrt{(M^{(0)}_{ij})^2 + (M^{(m)}_{ij})^2},
\]

\[
M^{(m)}_{ij} = J_{ij} \left( \cos \theta_{ij} + \frac{2\sin^2 \chi \sin^2(\theta_{ij}/2)}{2} \right) + D \sin \theta_{ij} \left( 1 - \frac{\sin^2 \chi}{2} \right),
\]

\[
M^{(2)}_{ij} = \frac{\sin^2 \chi}{2} (2J_{ij} \sin^2(\theta_{ij}/2) - D \sin \theta_{ij}).
\]

Recall that \( \theta_{ij} = \theta_i - \theta_j \), with \( \theta_A, \theta_B, \theta_C = 0, \varphi, -\varphi \), where \( \varphi \not\equiv 120^\circ \) for \( \delta \neq 1 \). The fictitious magnetic flux or solid angle subtended by three non-coplanar spins is given by

\[
tan \Phi_{ij} = \frac{M^{(m)}_{ij}}{M^{(2)}_{ij}}.
\]

The noninteracting spin wave Hamiltonian for the interlayer coupling is given by

\[
\mathcal{H}_{J_c} = S \sum_{i,\ell} t_c^{(0)} a_{i,\ell}^\dagger a_{i,\ell} + S \sum_{i,\ell,\ell'} [t_c^{(1)} (a_{i,\ell}^\dagger a_{i,\ell'} + \text{H.c.}) + t_c^{(2)} (a_{i,\ell}^\dagger a_{i,\ell'}^\dagger + \text{H.c.})],
\]

where

\[
t_c^{(0)} = -2J_c \cos 2\chi,
\]

\[
t_c^{(1)} = -J_c \cos 2\chi,
\]

\[
t_c^{(2)} = J_c \sin 2\chi.
\]

Next, we Fourier transform Eqs. (A11) and (A18) into momentum space and assemble all the terms together. Let us define the basis vector \( \psi^{\dagger}(\vec{k}) = (a_{\vec{k},A}^\dagger, a_{\vec{k},B}^\dagger, a_{\vec{k},C}^\dagger, a_{-\vec{k},A}^\dagger, a_{-\vec{k},B}^\dagger, a_{-\vec{k},C}^\dagger) \), the resulting spin wave Hamiltonian in momentum space can be written as

\[
\mathcal{H} = \frac{1}{2} \sum_{\vec{k}} \psi^{\dagger}(\vec{k}) \cdot \mathcal{H}(\vec{k}) \cdot \psi(\vec{k}),
\]

where

\[
\mathcal{H}(\vec{k}) = S \begin{pmatrix}
\mathcal{A}(\vec{k}) & \mathcal{B}(\vec{k}) \\
\mathcal{B}^\dagger(-\vec{k}) & \mathcal{A}^\dagger(\vec{k})
\end{pmatrix}
\]

where \( \mathcal{A}(\vec{k}) = \gamma^{(0)}(\vec{k}) + \gamma^{(1)}(\vec{k}) \) and \( \mathcal{B}(\vec{k}) = \gamma^{(2)}(\vec{k}) \).

The matrices are given by

\[
\gamma^{(0)}(\vec{k}) = \begin{pmatrix}
\gamma_{AA} & 0 & 0 \\
0 & \gamma_{BB} & 0 \\
0 & 0 & \gamma_{CC}
\end{pmatrix},
\]

\[
\gamma^{(1)}(\vec{k}) = \begin{pmatrix}
\gamma_{AB} e^{-i \phi_{AB}} & 0 & \gamma_{AC} e^{-i \phi_{AC}} \\
0 & \gamma_{BC} e^{-i \phi_{BC}} & 0 \\
\gamma_{CA} e^{i \phi_{AC}} & 0 & \gamma_{CB} e^{i \phi_{BC}}
\end{pmatrix},
\]

\[
\gamma^{(2)}(\vec{k}) = \begin{pmatrix}
\gamma_{AB}^{(2)} & \gamma_{AC}^{(2)} & \gamma_{BC}^{(2)} \\
\gamma_{CA}^{(2)} & \gamma_{CB}^{(2)} & \gamma_{AC}^{(2)} \\
\gamma_{AB}^{(2)} & \gamma_{AC}^{(2)} & \gamma_{CB}^{(2)}
\end{pmatrix},
\]

where

\[
\gamma_{AA} = M^{(0)}_{AB} + M^{(0)}_{CA} + t_c^{(1)} \cos k_z + \frac{h_\chi}{2},
\]

\[
\gamma_{BB} = \gamma_{CC} = M^{(0)}_{AB} + M^{(0)}_{BC} + t_c^{(1)} \cos k_z + \frac{h_\chi}{2}.
\]

The momentum vectors are \( k_i = \vec{k}_i \cdot \vec{a}_i \), with \( \vec{a}_1 = -1/2, \sqrt{3}/2 \), \( \vec{a}_2 = (1, 0) \), \( \vec{a}_3 = (-1/2, \sqrt{3}/2) \).

**Appendix B: Generalized Bogoliubov transformation**

The Hamiltonian (13) can be diagonalized by paraunitary operators \( \mathcal{P}_k \). This is equivalent to diagonalizing the bosonic Bogoliubov Hamiltonian \( \mathcal{H}_B(\vec{k}) = \tau_3 \mathcal{H}(\vec{k}) \) with \( \tau_3 = \text{diag}(I_{N \times N}, -I_{N \times N}) \), where \( I_{N \times N} \) is an identity \( N \times N \) matrix. The magnon Hamiltonian \( \mathcal{H}(\vec{k}) \) can be diagonalized using the bosonic Bogoliubov transformation: \( \psi_\vec{k} = \mathcal{P}_k \psi_\vec{k} \), where \( \mathcal{Q}_k^\dagger = (b_{\vec{k}A}^\dagger, b_{\vec{k}B}^\dagger, b_{\vec{k}C}^\dagger, b_{-\vec{k}A}^\dagger, b_{-\vec{k}B}^\dagger, b_{-\vec{k}C}^\dagger) \) are the Bogoliubov quasiparticles, and \( \mathcal{P}_k \) is a \( 2N \times 2N \) paraunitary matrix defined as

\[
\mathcal{P}_k = \begin{pmatrix}
u^t_k & u^t_k \\
u_k & u_k
\end{pmatrix},
\]

where \( |u_k|^2 - |v_k|^2 = I_{N \times N} \).

The matrix \( \mathcal{P}_k \) satisfies the relations

\[
\mathcal{P}_k^\dagger \tau_3 \mathcal{P}_k = \tau_3, \quad \mathcal{P}_k^\dagger \mathcal{H}(\vec{k}) \mathcal{P}_k = \mathcal{E}_k,
\]
where
\[
\mathcal{E}(\vec{k}) = \begin{pmatrix} E_n(\vec{k}) & 0 \\ 0 & E_n(-\vec{k}) \end{pmatrix}, \quad \tau_3 = \begin{pmatrix} I_{N \times N} & 0 \\ 0 & -I_{N \times N} \end{pmatrix},
\]
with energy band $E_n(\vec{k})$ and band index $n$.\[\text{(B4)}\]

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