Topological magnons: concepts and phenomenology

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Topological band structures are not restricted to fermionic systems and can also arise in bosonic systems such as linear spin waves or magnons. In this term paper I discuss the physics of topological magnons in the partially polarized phase of models in 2D honeycomb lattice, relevant for the physics in the high-field limit of Kitaev type quantum spin liquids and spin-orbit coupled magnetic insulators such as CrI_3. To study the phenomenology of topological aspects of magnons, I review the concepts of Berry phase (curvature), the Holstein-Primakoff transformation, and the semiclassical theory of thermal conductivity, followed by the linear response theory of thermal Hall coefficient κ_{xy} that relates to the Berry curvature of magnon bands. As a concrete example, I present the derivation of the magnon Hamiltonian from Kitaev model under high magnetic field; and from a more generic model with Kitaev, Γ, and Dzyaloshinskii–Moriya (DM) interactions relevant for CrI_3. In the latter example I show the Berry curvature of magnons which can be used to readily get thermal Hall conductivity at low temperature.

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CONTENTS

BERRY CURVATURE AND CHERN NUMBER

Consider a Hamiltonian that depends on time only via a set of time-dependent parameters $\mathbf{R}$. A system initially in an eigenstate $|n(\mathbf{R}(0))\rangle$ will stay as an instantaneous eigen state of the time-dependent Hamiltonian $H(\mathbf{R}(t))$ throughout the adiabatic evolution. If the parameter changes slowly in time such that adiabaticity is retained in the whole process, the only degree of freedom we have is the phase of the quantum state, which is responsible for a lot of topological effects such as Berry curvature and Chern invariant [1]. The state at time t is

$$|\psi(t)\rangle = \exp\left\{-\frac{i}{\hbar}\int_0^t dt' E_n(\vec{R}(t'))\right\}\exp\{i\gamma_n(t)\}\,|n(\vec{R}(t))\rangle \tag{1}$$

The reason for introducting this $\exp\{i\gamma\}$ term is clear from the Schrodinger equation The generic form of such evolution is:

$$|\psi(t)\rangle = c_n(t)\,|n(\mathbf{R}(t))\rangle \tag{2}$$

Plug into the Schrodinger equation we have:

$$\dot{c}_n(t)\,|n(\mathbf{R}(t))\rangle + c_n(t)\frac{d}{dt}\,|n(\mathbf{R}(t))\rangle = -\frac{i}{\hbar}c_n(t)E_n(t)\,|n(\mathbf{R}(t))\rangle \tag{3}$$

now project onto $|n(\mathbf{R}(t))\rangle$, it's readily to get:

$$\dot{c}_n(t) = \Big[-\langle n(\mathbf{R}(t))|\frac{d}{dt}|n(\mathbf{R}(t))\rangle - \frac{i}{\hbar}E_n(t)\Big]c_n(t) \tag{4}$$

therefore

$$\begin{aligned} c_n(t) = &\exp\left\{-\frac{i}{\hbar}\int_0^t dt' E_n(\mathbf{R}(t'))\right\} \\ &\times \exp\left\{-\int_0^t dt'\,\langle n(\mathbf{R}(t'))|\frac{d}{dt'}|n(\mathbf{R}(t'))\rangle\right\} \end{aligned} \tag{5}$$

compare with Eq.(2), the berry phase γ is:

$$\gamma(t) = i\int_0^t dt'\,\langle n(\mathbf{R}(t'))|\frac{d}{dt'}|n(\mathbf{R}(t'))\rangle \tag{6}$$

Since the wavefunction is time-dependent through $\mathbf{R}(t)$, we can rewrite the time derivative as:

$$\frac{d}{dt} = \dot{\mathbf{R}}\cdot\frac{d}{d\mathbf{R}} \equiv \dot{\mathbf{R}}\cdot\nabla_{\mathbf{R}}.$$

Plug into Eq.(6), the berry phase is then expressed in term of the trajactory in parameter space:

$$\gamma(\mathbf{R}) = i\int_0^{\mathbf{R}} d\mathbf{R}' \left\langle n(\mathbf{R}')\middle|\nabla_{\mathbf{R}'}\middle|n(\mathbf{R}')\right\rangle \tag{7}$$

which is necessarily a real number. On a closed loop in parameter space, we can define a *geometric phase change*:

$$\gamma_n(C) = i\oint_c \langle n(\mathbf{R})|\nabla_{\mathbf{R}}|n(\mathbf{R})\rangle \cdot d\mathbf{R} \tag{8}$$

such that

$$|\psi(T)\rangle = \exp\{i\gamma_n(C)\}\exp\left\{-\frac{i}{\hbar}\int_0^T dt' E_n(\mathbf{R}(t'))\right\}|\psi(0)\rangle\,.$$

From Eq.(7) we see that to calculate the Berry phase γ_n, we need to specify two index: the eigen state space index and the parameter space index. We define berry connection $\mathcal{A}$ - a rank 2 tensor, to meet this need:

$$\mathcal{A}^n_\mu \equiv i\,\langle n(\mathbf{R})|\frac{\partial}{\partial R_\mu}|n(\mathbf{R})\rangle \tag{9}$$

which is also a real number. In this way the Berry phase $\gamma_n(C)$ is expressed as:

$$\gamma_n(C) = \oint_C \vec{\mathcal{A}}^n(\mathbf{R})\cdot d\mathbf{R}.$$

Note that although $\mathcal{A}$ is not a gauge invariant, the geometric phase factor is gauge invariant. To show this, we start with the gauge transformation of ket $|n\rangle$:

$$|n\rangle \to e^{i\phi(\mathbf{R})}\,|n\rangle\,.$$

$$\nabla_{\mathbf{R}}\,|n\rangle \to \nabla_{\mathbf{R}} e^{i\phi(\mathbf{R})}\,|n\rangle = i\nabla_{\mathbf{R}}\phi(\mathbf{R})\,|n\rangle + e^{i\phi(\mathbf{R})}\nabla_{\mathbf{R}}\,|n\rangle\,.$$

therefore the Berry connection becomes $\vec{\mathcal{A}}^n \to \vec{\mathcal{A}}^n - \nabla_{\mathbf{R}}\phi(\mathbf{R})$, which is not gauge invariant, but γ(C) remains the same:

$$\gamma_n(C) \to \gamma_n(C) = \oint_c \Big(\vec{\mathcal{A}}^n - \nabla_{\mathbf{R}}\phi(\mathbf{R})\Big)\cdot d\mathbf{R} = \gamma_n(C).$$

The last step used the gradient theorem for line integrals. Particularly, for a 3D parameter space, e.g. the real space coordinate, we can define the Berry curvature:

$$\vec{\Omega}_n(\mathbf{R}) \equiv \nabla\times\vec{\mathcal{A}}^n \quad\Rightarrow\quad \gamma_n(C) = \iint_{\partial C}\vec{\Omega}_n(\mathbf{R})\cdot d\mathbf{S} \tag{10}$$

by Stokes' theorem. We write $\Omega = \nabla\times\mathcal{A}$ in Enstein notation:

$$\begin{aligned}\Omega^\alpha_n &= i\epsilon_{\alpha\beta\gamma}\nabla_\beta\,\langle n|\nabla_\gamma|n\rangle \\ &= i\epsilon_{\alpha\beta\gamma}\,\langle\nabla_\beta n|\nabla_\gamma n\rangle + i\epsilon_{\alpha\beta\gamma}\,\langle n|\nabla_\beta\nabla_\gamma n\rangle\end{aligned} \tag{11}$$

the second term goes to zero since ϵ is anti-symmetric while $\nabla_\alpha\nabla_\beta$ is symmetric. Therefore, inserting an resolution of idensity gives us

$$\vec{\Omega}_n = i\epsilon_{\alpha\beta\gamma}\sum_m\langle\nabla_\beta n|m\rangle\,\langle m|\nabla_\gamma n\rangle \tag{12}$$

Note that only $m \neq n$ terms contribute to the above equation, i.e. $m = n$ term must vanish since Ω must be real. Hence

$$\Omega^\alpha_n = i\epsilon_{\alpha\beta\gamma}\sum_{m\neq n}\frac{\langle n|\nabla_\beta\mathcal{H}|m\rangle\;\langle m|\nabla_\gamma\mathcal{H}|n\rangle}{(E_n-E_m)^2} \tag{13}$$

from which it is clear that the Berry curvature is extremely large near degeneracy, where $E_n \to E_m$. In 2D translationally invariant systems, e.g. Bloch electrons or magnons, it is convenient to formulate this in the momentum space:

$$\Omega^\alpha_n = i\sum_{m\neq n}\frac{\langle n|\partial_{k_x}\mathcal{H}(\mathbf{k})|m\rangle\;\langle m|\partial_{k_y}\mathcal{H}(\mathbf{k})|n\rangle - (k_x\leftrightarrow k_y)}{(E_n-E_m)^2} \tag{14}$$

where $\mathcal{H}(\mathbf{k})$ is the Hamiltonian in the momentum space. The Berry curvature can lead to non-zero Chern number that is responsible for a lot of topological physics, including magnons to be disccused in the coming section. The Chern number is defined as:

$$\mathcal{C} = \frac{1}{2\pi}\int_{1^{st}B.L.} d^2\vec{k}\;\Omega_z(\vec{k}) \tag{15}$$

recall that the velocity with a generic Berry curvature is:

$$\vec{v} = \frac{1}{\hbar}\nabla_{\vec{k}}\epsilon_{\vec{k}} + \frac{e}{\hbar}\vec{E}\cdot\vec{\Omega}(\vec{k}) \tag{16}$$

under time-reversal transformation we have $\dot{\vec{r}} \to -\dot{\vec{r}}, \dot{\vec{k}} \to -\dot{\vec{k}}, \vec{E} \to \vec{E}, \vec{B} \to -\vec{B}$, so we must have $\vec{\Omega}(\vec{k}) \to -\vec{\Omega}(-\vec{k})$. Therefore the Chern number changes by:

$$\begin{aligned}\mathcal{C} \to \mathcal{C} &= -\frac{1}{2\pi}\int_{1^{st}B.L.} d^2\vec{k}\;\Omega_z(-\vec{k}) \\ &= -\frac{1}{2\pi}\int_{1^{st}B.L.} d^2\vec{k}'\;\Omega_z(\vec{k}')\end{aligned} \tag{17}$$

where in the last step we relabelled the dummy variable $\vec{k} \to \vec{k}'$. Comparing with with Eq.(15) we conclude:

$$\mathcal{C} \xrightarrow{\mathcal{T}} -\mathcal{C} \tag{18}$$

If the system respects $\mathcal{T}$ then we must have $\mathcal{C} = -\mathcal{C} \;\Rightarrow\; \mathcal{C} = 0$. Therefore in order to have a non-zero Chern number, the time-reversal symmetry must be broken. This condition is automatically satisfied in (partially) polarized magnets that support magnons.

THE HOLSTEIN-PRIMAKOFF TRANSFORMATION

To arrive at an approximate solution that does not use unwieldy spin operators, we would like to a representation that uses creation and annihilation operators in the second quantization. The transformation read:

$$S_i^+ = \sqrt{2S}\,\phi(n_i)\,a_i,\;\; S_i^- = \sqrt{2S}\,a_i^\dagger\,\phi(n_i),\;\; S_i^z = S - n_i \tag{19}$$

where we have defined:

$$n_i = a_i^\dagger a_i, \quad \phi(n_i) = \sqrt{1 - \frac{n_i}{2S}} \tag{20}$$

where $a, a^\dagger$ are bosonic operators. Before going to the implemetation, let us first have a review of its historical derivation. The building blocks of a spin Hamiltonian are:

$$S_j^+ = S_j^x + iS_j^y, \quad S_j^- = S_j^x - iS_j^y, \quad \hat{n}_j = S - S_j^z \tag{21}$$

with n_j the eigenvalue of $\hat{n}_j$, which is called the spin deviation of j-th site. For simplicity, let us consider the case in which S_j^z, thus n_l, is a good quantum number, such that the wavefunction can be labelled by local spin deviations:

$$|\psi\rangle = |n_1 \ldots n_l \ldots n_N\rangle \tag{22}$$

Now let us apply these operators to the state. The operator S_l^+ will raise S_l^z, thus lower n_l by 1. So we have:

$$S_l^+\,|n_1 \ldots n_l \ldots n_N\rangle = c\,|n_1 \ldots n_l - 1 \ldots n_N\rangle \tag{23}$$

it has to satisfy normalization condition:

$$|c|^2 = \langle n_1 \ldots n_l \ldots n_N | S_l^- S_l^+ | n_1 \ldots n_l \ldots n_N\rangle \tag{24}$$

in order to work under n_l basis, we rewrite the $S_l^- S_l^+$ as:

$$\begin{aligned} S_l^- S_l^+ &= (S_l^x - iS_l^y)(S_l^x + iS_l^y) \\ &= S_l^x S_l^x + S_l^y S_l^y + iS_l^x S_l^y - iS_l^y S_l^x \\ &= \mathbf{S}^2 - S_l^z S_l^z + i[S_l^x, S_l^y] \\ &= S(S+1) - (S - n_l)^2 - (S - n_l) \\ &= 2Sn_l - n_l(n_l - 1) = (2S)\left(1 - \frac{n_l - 1}{2S}\right) n_l \end{aligned} \tag{25}$$

so that

$$c = \sqrt{2S}\sqrt{1 - \frac{n_l - 1}{2S}}\sqrt{n_l} \tag{26}$$

$$S_l^+\,|\cdots n_l \cdots\rangle = \sqrt{2S}\sqrt{1 - \frac{n_l - 1}{2S}}\sqrt{n_l}\,|\cdots n_l - 1 \cdots\rangle \tag{27}$$

introducing the creation and annihilation operator $a^\dagger, a$, the above can be rewritten as:

$$\begin{aligned} S_l^+\,|n_1 \ldots n_l \ldots n_N\rangle &= \sqrt{2S}\sqrt{1 - \frac{\hat{n}_l}{2S}}\,\hat{a}_l\,|\cdots n_l \cdots\rangle \\ &\equiv \sqrt{2S}\,\phi(\hat{n}_l)\,\hat{a}_l \end{aligned} \tag{28}$$

where I have used $\hat{\bullet}$ to emphasize an operator. Hence we have the first Holstein-Primakoff transformation:

$$S_l^+ = \sqrt{2S}\,\phi(\hat{n}_l)\,\hat{a}_l \tag{29}$$

The mapping of S_l^- can be derived in the same way.

BOSON HAMILTONIAN

The physics of linear spin waves or magnons can be considered in terms of bosonic Hamiltonian. Consider the generic magnon field $\Psi(\mathbf{r})$ in quadratic order [2]:

$$\mathcal{H} \equiv \frac{1}{2}\int d\mathbf{r}\;\Psi^\dagger(\mathbf{r})\mathcal{H}_0(\mathbf{r})\Psi(\mathbf{r}) \tag{30}$$

where $\Psi(\mathbf{r}) = [a_1(\mathbf{r}), \cdots, a_n(\mathbf{r}), a_1^\dagger(\mathbf{r}, \cdots, a_n^\dagger(\mathbf{r}))]^{\mathrm{T}}$, and $a_i^\dagger(\mathbf{r}),\; a_i(\mathbf{r})$ are bosonic creation and annihilation operators of i-th degrees of freedom (i-th boson within a unit cell, or a band index of spin waves) satisfying commutation $[a_i(\mathbf{r}), a_j^\dagger(\mathbf{r'})] = \delta_{ij}\delta_{rr'}$. Note that the total number of bosons may not be conserved due to the presence of spin-orbital coupling or many bond-dependent exchange interactions that are responsible for $a_i^\dagger a_j^\dagger$ or $a_i a_j$. In such cases, as I will show later in this note, we need to transform $a_i, a_i^\dagger$ into its eigen basis and study the quasiparticle thereof. Under the Fourier transform:

$$a_i(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} a_{i,\mathbf{k}}, \quad a_i^\dagger(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} a_{i,\mathbf{k}}^\dagger \tag{31}$$

where N is the number of unit cells. The Hamiltonian in momentum space representation reads

$$\mathcal{H} = \frac{1}{2}\sum_{\mathbf{k}}(\mathbf{a}_{\mathbf{k}}^\dagger,\; \mathbf{a}_{-\mathbf{k}})\mathcal{H}_{\mathbf{k}}\begin{pmatrix}\mathbf{a}_{\mathbf{k}} \\ \mathbf{a}_{-\mathbf{k}}^\dagger\end{pmatrix} \tag{32}$$

where $\mathbf{a}_{\mathbf{k}} = (a_{1,\mathbf{k}}^\dagger, \cdots a_{n,\mathbf{k}})^{\mathrm{T}}$. The Hamiltonian is diagonalized by a paraunitary matrix $T_{\mathbf{k}}$ such that

$$\begin{aligned} \mathcal{H} &= \frac{1}{2}\sum_{\mathbf{k}}(\boldsymbol{\gamma}_{\mathbf{k}}^\dagger,\; \boldsymbol{\gamma}_{-\mathbf{k}})\mathcal{E}_{\mathbf{k}}\begin{pmatrix}\boldsymbol{\gamma}_{\mathbf{k}} \\ \boldsymbol{\gamma}_{-\mathbf{k}}^\dagger\end{pmatrix} \\ &= \sum_{\mathbf{k}}\sum_{m=1}^{N}\varepsilon_{m\mathbf{k}}\left(\gamma_{m\mathbf{k}}^\dagger\gamma_{m\mathbf{k}} + \frac{1}{2}\right) \end{aligned} \tag{33}$$

where $\boldsymbol{\gamma}_{\mathbf{k}} = (\gamma_{1,\mathbf{k}}, \cdots \gamma_{n,\mathbf{k}})$ and $\varepsilon_{m\mathbf{k}}$ the magnon excitation energy of mth band. Let $T_{\mathbf{k}}$ be the matrix that diagonalize the $\mathbf{k}$th block of the bosonic Hamiltonian, that is

$$\begin{pmatrix}\boldsymbol{\gamma}_{\mathbf{k}} \\ \boldsymbol{\gamma}_{-\mathbf{k}}^\dagger\end{pmatrix} = T_{\mathbf{k}}^{-1}\begin{pmatrix}\mathbf{a}_{\mathbf{k}} \\ \mathbf{a}_{-\mathbf{k}}^\dagger\end{pmatrix} \tag{34}$$

and $\mathcal{E}_{\mathbf{k}}$ is given by

$$\mathcal{E}_{\mathbf{k}} = T_{\mathbf{k}}^{\dagger}\mathcal{H}_{\mathbf{k}}T_{\mathbf{k}} = \begin{pmatrix} \mathbf{E}_{\mathbf{k}} & \\ & \mathbf{E}_{-\mathbf{k}} \end{pmatrix},\ \mathbf{E}_{\mathbf{k}} = \begin{pmatrix} \varepsilon_{1\mathbf{k}} & & \\ & \ddots & \\ & & \varepsilon_{N\mathbf{k}} \end{pmatrix} \tag{35}$$

Note that the matrix $T_{\mathbf{k}}$ can also be regarded as an alignment of the eigenstates, i.e. $T_{\mathbf{k}}^{\dagger} \equiv (\boldsymbol{\gamma}_{1,\mathbf{k}}^{\dagger}, \cdots \boldsymbol{\gamma}_{1,\mathbf{k}}^{\dagger})\,|0\rangle$, then according to the boson commutation relation the following paraunitary conditions must be satisfied:

$$T_{\mathbf{k}}^{\dagger}\sigma_3 T_{\mathbf{k}} = T_{\mathbf{k}}\sigma_3 T_{\mathbf{k}}^{\dagger} = \sigma_3,\ \sigma_3 \equiv \begin{pmatrix} 1_{N\times N} & \\ & -1_{N\times N} \end{pmatrix} \tag{36}$$

To intuitively understand Eq.36 we can test is in 2 band boson states $b_{1,\mathbf{k}}$ and $b_{2,\mathbf{k}}$, where the paraunitary conditions gives

$$b_{1,\mathbf{k}}^{\dagger}b_{1,\mathbf{k}} - b_{2,\mathbf{k}}^{\dagger}b_{2,\mathbf{k}} = b_{1,\mathbf{k}}b_{1,\mathbf{k}}^{\dagger} - b_{2,\mathbf{k}}b_{2,\mathbf{k}}^{\dagger} \equiv \sigma_3 \tag{37}$$

which is true iff b and $b^{\dagger}$ satisfy the boson commutation relation $[b, b^{\dagger}] = 1$. For fermions, in contrast, we would have $\sigma_3 \equiv b_{1,\mathbf{k}}^{\dagger}b_{1,\mathbf{k}} - b_{2,\mathbf{k}}^{\dagger}b_{2,\mathbf{k}} \neq -(b_{1,\mathbf{k}}b_{1,\mathbf{k}}^{\dagger} - b_{2,\mathbf{k}}b_{2,\mathbf{k}}^{\dagger}) \equiv -\sigma_3$.

THERMAL HALL CONDUCTIVITY

The thermal hall effects is one of the most salient feature of topological magnons [3]. I first review the semiclassical picture of thermal conductivity using relaxation time approximation, follwed by the linear response theory of heat conduction under a temperature gradient and the derivation of the thermal current operator from the continuity equation. The section is converged by the discussion of the thermal Hall coefficient and its relation to Berry curvature of magnon band structure.

Semi-classical phenomenology

In this section I review the semi-classical theory of thermal transport based on Chapter 13 of Ashcroft and Mermin [4]. This picture is based on the relaxation-time approximation as fellows: (i) The distribution of electron emerging from collisions at any time does not depend on the non-equilibrium distribution function $g(\mathbf{r}, \mathbf{k}, t)$ prior to the collision – as is required by the Marchovian nature of collision; and (ii) the equilibrium distribution appropriate to a local temperature $T(\mathbf{r})$, $g_n^0(\mathbf{r}, \mathbf{k})$ of nth band, is a fixed point w.r.t. the collision, that is, effectively unaltered by any possible collisions. Therefore, if in the time interval dt a fraction of $dt/\tau_n(\mathbf{r}, \mathbf{k})$ of the electrons in band n with momentum $\mathbf{k}$ near position $\mathbf{r}$ suffers a collision that *alters* the band index and/or momentum, the distribution of electrons that emerge from collisions *into* the same band $\mathbf{n}$ and momentum $\mathbf{k}$ during the same time interval must precisely compenstate for this loss. This translates to the fellowing simple relation:

$$dg_n(\mathbf{r}, \mathbf{k}, t) = \frac{dt}{\tau_n(\mathbf{r}, \mathbf{k})}g_n^0(\mathbf{r}, \mathbf{k}) \tag{38}$$

Given this relation, now we can calculate the nonequilibrium distribution function under temperature gradient and/or external fields. Consider a phase space volumn $d\mathbf{r}d\mathbf{k}$ abour $\mathbf{r}, \mathbf{k}$. The number of particles therein is given by

$$dN = g_n(\mathbf{r}, \mathbf{k}, t)\frac{d\mathbf{r}d\mathbf{k}}{4\pi^3} \tag{39}$$

This can be expressed in an alternative form whereby dN is grouped into different patches emerging from collisions at earlier times. The dN electrons that locate at the aforementioned phase space volumn must have emerged due to the last collision at t' prior to t within a phase space volumn $d\mathbf{r}'d\mathbf{k}'$ about $\mathbf{r}_n(t'),\ \mathbf{k}_n(t')$. After the collision at t' the motion of part of these electrons (those that remain unscattered until t) is completely determined by the semi-classical equation of motion whose solution gives $\mathbf{r}_n(t) = \mathbf{r},\ \mathbf{k}_n(t) = \mathbf{k}$. Eq.38 tells us that the number of particles that are scattered out of the equilibrium distribution around the phase space volumn $d\mathbf{r}'d\mathbf{k}'$ is the same as the number of those emerging from collisions at $\mathbf{r}_n(t'),\ \mathbf{k}_n(t')$ into the volumn element $d\mathbf{r}'d\mathbf{k}'$ in the interval dt'. Therefore, the number of particles that are scattered out of the phase space volumn $d\mathbf{r}'d\mathbf{k}'$ during dt' around t' is given by

$$dn(t') = \frac{dt'}{\tau_n(\mathbf{r}_n(t'), \mathbf{k}_n(t'))}g_n^0(\mathbf{r}_n(t'), \mathbf{k}_n(t'))\frac{d\mathbf{r}d\mathbf{k}}{4\pi^3} \tag{40}$$

where we used Liouville's theorem to make the replacement $d\mathbf{r}'d\mathbf{k}' = d\mathbf{r}d\mathbf{k}$. Among these particles, only a fraction $P_n(\mathbf{k}, \mathbf{k}, t; t')$ survive from t' to t without suffering any further collisions and arrive at the phase volumn $d\mathbf{r}d\mathbf{k}$ around $\mathbf{r}, \mathbf{k}$ driven by the equations of motion. Considering the probability P and all possible t' where collisions happen, the total number of electrons in $d\mathbf{r}d\mathbf{k}$ around $\mathbf{r}, \mathbf{k}$ and time t can be written as

$$dN = \int_{-\infty}^{t} dn(t')P(t, t') = \frac{d\mathbf{r}d\mathbf{k}}{4\pi^3}\int_{-\infty}^{t}\frac{dt' g_n^0(t')P_n(t, t')}{\tau_n(t')} \tag{41}$$

where we have suppressed the notation $\mathbf{r}(t')$ and $\mathbf{k}(t')$, etc. Comparing this equation to Eq.39 we have

$$g_n(t) = \int_{-\infty}^{t}\frac{dt'}{\tau_n(t')}g_n^0(t')P(t, t') \tag{42}$$

It still remains to compute the specific form of $P(t, t')$. Noting that the fraction that survive from t' to t is less than the fration that survive from $t' + dt'$ to t by the factor $(1 - dt'/\tau(t'))$, i.e. the fraction of electrons that *do* *not* suffer from collision at a time interval dt'. Hence we readily have

$$P(t,t') = P(t,t'+dt')\left(1-\frac{dt'}{\tau(t')}\right) \tag{43}$$

by having $dt' \to 0$ we immediatel have the following differential equation

$$\frac{\partial}{\partial t'}P(t,t') = \frac{P(t,t')}{\tau(t')}, \quad s.t.\ P(t,t)=1 \tag{44}$$

such that Eq.42 becomes $g_n(t) = \int_{-\infty}^{t} dt' g_n^0(t')\frac{\partial}{\partial t'}P(t,t')$. Integral by parts gives us

$$g_n(t) = g_n^0(t) - \int_{-\infty}^{t} dt' P(t,t')\frac{d}{dt'}g_n^0(t') \tag{45}$$

Note that the time evolution of the position and momentum are determined by the equations of motion:

$$\dot{\mathbf{r}} = \mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\mathbf{k})}{\partial \mathbf{k}} + \mathbf{v}_{\text{ano}}(\mathbf{k}) \tag{46}$$

$$\hbar\dot{\mathbf{k}} = -e\left[\mathbf{E}(\mathbf{r},t) + \frac{1}{c}\mathbf{v}_n(\mathbf{k})\times\mathbf{H}(\mathbf{r},t)\right] \tag{47}$$

with $\mathbf{v}_{\text{ano}}(\mathbf{k})$ the anormalous velocity potentially induced by Berry curvature and external field $\mathbf{H}$. The second equation due to the Lorentzian force and $\mathbf{E}$ the electric field. This allows us to relate the distribution function to the Berry curvature and external field. At equilibrium, g_n^0 becomes the Fermi distribution function $f(\varepsilon(\mathbf{k}))$, and is time dependent only through $\varepsilon(\mathbf{k}_n(t'))$, $T(\mathbf{r}_n(t'))$, $\mu(\mathbf{r}_n(t'))$. Therefore the time derivative of g_n^0 above becomes

$$\begin{aligned}\frac{dg_n^0(t')}{dt'} =& \frac{\partial g_n^0}{\partial \varepsilon_n}\frac{\partial \varepsilon_n}{\partial \mathbf{k}}\cdot\frac{d\mathbf{k}_n}{dt'} + \frac{\partial g_n^0}{\partial T}\frac{\partial T}{\partial \mathbf{r}}\cdot\frac{d\mathbf{r}_n}{dt'} \\ &+ \frac{\partial g_n^0}{\partial \mu}\frac{\partial \mu}{\partial \mathbf{k}}\cdot\frac{d\mathbf{k}_n}{dt'}\end{aligned} \tag{48}$$

which can be expanded according to Eq.46 and Eq.47. Therefore, Eq.45 becomes

$$g_n(t) = g_n^0(t) + \int_{-\infty}^{t} dt' P(t,t')\left[\left(-\frac{\partial f}{\partial \varepsilon}\right)\mathbf{v}\cdot\left(-e\mathbf{E} - \nabla\mu - \left(\frac{\varepsilon-\mu}{T}\right)\nabla T\right)\right] \tag{49}$$

where we have set $\mathbf{H}=0$, $c=\hbar=1$; and used the following equivalence:

$$\frac{\partial f}{\partial T} = -\frac{\partial f}{\partial \varepsilon}\left(\frac{\varepsilon-\mu}{T}\right), \quad \frac{\partial f}{\partial \mu} = -\frac{\partial f}{\partial \varepsilon} \tag{50}$$

as can be readily checked in the Fermi-Dirac distribution. Eq.49 is of central importance in all kinds of semiclassical theories of conductivity. For the interest of this paper, I will focus on the thermal transport relevant for the thermal Hall effects of topological magnons.

The thermal current is intimately related to entropy current by $dQ = TdS$. In a fixed volumn element, changes in entropy reduces to the change of internal energy and particle number:

$$TdS = dU - \mu dN \tag{51}$$

that is, the total thermal transport can be decomposed into the energy current and the particle current density i.e. $\mathbf{j}^q = T\mathbf{j}^s = \mathbf{j}^\varepsilon - \mu\mathbf{j}^n$, respectively given by

$$\mathbf{j}^n = \sum_n \int \frac{d\mathbf{k}}{4\pi}\mathbf{v}_n(\mathbf{k})g_n(\mathbf{k}) \tag{52}$$

$$\mathbf{j}^\varepsilon = \sum_n \int \frac{d\mathbf{k}}{4\pi}\varepsilon_n(\mathbf{k})\mathbf{v}_n(\mathbf{k})g_n(\mathbf{k}) \tag{53}$$

therefore the total thermal current density is

$$\mathbf{j}^q = \sum_n \int \frac{d\mathbf{k}}{4\pi}(\varepsilon_n(\mathbf{k})-\mu)\mathbf{v}_n(\mathbf{k})g_n(\mathbf{k}) \tag{54}$$

Under static field and temperature gradient, the only time-dependent piece is $P(t,t')$. Here we assume the energy-dependent relaxation time, that is, τ depends on momentum only through $\varepsilon(\mathbf{k})$, thus τ is no longer dependent on t' and $P = e^{-(t-t')/\tau_n(\mathbf{k})}$; and the integral in dt' acts only on $P(t,t')$. This gives us the distribution function:

$$g_n(\mathbf{k}) = g_n^0(\mathbf{k}) + \tau(\mathbf{k})\left(\frac{\partial f}{\partial \varepsilon}\right)\mathbf{v}(\mathbf{k})\cdot\left[\left(\frac{\partial \mu}{\partial T} + \frac{\varepsilon(\mathbf{k})-\mu}{T}\right)\nabla T\right] \tag{55}$$

where we used $\int_{-\infty}^{t} P(t,t')dt' = \int_{-\infty}^{t} e^{-(t-t')/\tau}dt' = \tau$, $\nabla\mu = \frac{\partial\mu}{\partial T}\nabla T$, and assumed $\mathbf{E},\mathbf{H}=0$ for convenience. Therefore Eq.54 can be written as

$$\mathbf{j}^q = \mathbf{L}_1\cdot\nabla T + \mathbf{L}_2\cdot\frac{\nabla T}{T} = \mathbf{L}_1\cdot\nabla T - \mathbf{L}_2\cdot\left(\nabla\frac{1}{T}\right)T \tag{56}$$

where $\mathbf{L}_1$ and $\mathbf{L}_2$ are tensors (dyadics). This expression describes the thermal current along different directions w.r.t the temperature gradient. The thermal hall measurement is intersted in the thermal current in transverse directions. Hence it is convenient to write the total phenomenological thermal current in the form

$$J^q_\mu = L_{\mu\nu}\left(T\nabla_\nu \frac{1}{T} - \nabla_\nu T\right) \tag{57}$$

where the semiclassical coefficient can be read from Eq.54 and Eq.55.

Thermal current operator and pseudo-gravitational potential

In the standard linear response theory where particles are coupled to external fields, the field should enter the Hamiltonian as a perturbation and can be treated by usual time-dependent perturbation theory. However, the temperature gradient affects transport in a different way: temperature does not affect the Hamiltonian, but affects the Boltzmann factor $\exp(-\beta\mathcal{H})$. This problem was first overcame by Luttinger who introduced a fictitious gravitational field.

The temperature gradiate can be written in terms of the deviation from one end to the other:

$$T(\mathbf{r}) = T_0(1-\chi(\mathbf{r})) \tag{58}$$

where T_0 is a constant and $\chi(\mathbf{r})$ is a weak spacial perturation to the uniform temperature. The key insight is that this $\chi(\mathbf{r})$ can be regarded as a space-dependent prefactor to the original Hamiltonian. To the leading order, this is

$$e^{-\mathcal{H}/k_BT} = e^{-\mathcal{H}/[k_BT_0(1-\chi(\mathbf{r}))]} \approx e^{-(1+\chi(\mathbf{r}))\mathcal{H}/k_BT_0} \tag{59}$$

where we used $(1-\chi)^{-1} = 1+\chi+O(\chi^2)$ with the assumption $\chi \ll 1$. Thereofre $\chi(\mathbf{r})\mathcal{H}$ can be regarded as a perturbation to the Hamiltonian due to the temperature gradient. In the dimensionless measure this gradient is

$$\nabla\left(\frac{T}{T_0}\right) = -\nabla\chi(\mathbf{r}) \tag{60}$$

such grandient causes a change in effective Hamiltonian that is propotional to the energy $\delta\mathcal{H}(\mathbf{r}) = \mathcal{H}_{\text{eff}}(\mathbf{r}) - \mathcal{H} \approx \chi(\mathbf{r})\mathcal{H}$, where $\mathcal{H}$ is considered uniform in a translationally invariant system. Hence

$$\delta\mathcal{H} = \int d\mathbf{r}[\nabla\chi(\mathbf{r})]\mathcal{H} = -\int d\mathbf{r}\left[\nabla\left(\frac{T}{T_0}\right)\right]\mathcal{H} \tag{61}$$

compare with the usual setup of perturbation theory

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}',\ \mathcal{H}' = \int f(\mathbf{r})\mathbf{B}(\mathbf{r})d\mathbf{r} \tag{62}$$

where in magnets B usually takes the form $\mathbf{B} = (\mathbf{H}\cdot\mathbf{S})\hat{n}$. We can then interpret $\nabla\chi(\mathbf{r})$, thus $\nabla\left(\frac{T}{T_0}\right)$, as a fictitious force due to the pseudogravitational potential $\chi(\mathbf{r})$ or $T(\mathbf{r}))/T_0$; and that such a force is proportional to the particle energy encoded in $\mathcal{H}$ in analogy to that spins density are coupled to local magnetic field.

The total Hamltonian that incorporates such field is

$$\mathcal{H}_T = \mathcal{H} + \mathcal{F} \tag{63}$$

where $\mathcal{F}$ is the contribution from temperature gradient (in a symmetrized form):

$$\mathcal{F} = \frac{1}{4}\int d\mathbf{r}\Psi^\dagger(\mathbf{r})(\mathcal{H}_0\chi + \chi\mathcal{H}_0)\Psi(\mathbf{r}) \tag{64}$$

According to the semiclassical picture, we are interested in the thermal transport coefficient as a linear response to the gradient of the pseudo-gravitational potential,

$$\langle J^q_\mu\rangle = L_{\mu\nu}\left(T\nabla_\nu\frac{1}{T} - \nabla_\nu\chi\right) \tag{65}$$

The thermal hall conductivity $\kappa_{\mu\nu}$ is then defined as

$$\kappa_{\mu\nu} = L_{\mu\nu}/T \tag{66}$$

Let us now calculate the thermal current density operator in the presence of χ. The total Hamiltonian defined previously can be rewritten as

$$\mathcal{H}_T = \frac{1}{2}\int d\mathbf{r}\left(1+\frac{\chi}{2}\right)\Psi^\dagger(\mathbf{r})\mathcal{H}_0\left(1+\frac{\chi}{2}\right)\Psi(\mathbf{r}) \tag{67}$$

the form of current density operator can be derived from the continuity equation

$$\dot{h}_T + \nabla\cdot\mathbf{j}^q(\mathbf{r}) = 0 \tag{68}$$

where $h_T = \frac{1}{2}(1+\frac{\chi}{2})\Psi^\dagger(\mathbf{r})(1+\frac{\chi}{2})\Psi(\mathbf{r})$ is the local energy density. Here without delving into details, which can be found in Ref.[2], the thermal hall conductivity reads

$$\kappa_{xy} = -\frac{k_B^2T}{\hbar V}\sum_{\mathbf{k}}\sum_{n=1}^{N}\left\{c_2[g(\varepsilon_n(\mathbf{k}))] - \frac{\pi^2}{3}\right\}\Omega_n(\mathbf{k}) \tag{69}$$

where g is the Bose distribution $1/[\exp(\varepsilon/k_BT)-1]$, $\Omega_n(\mathbf{k})$ the Berry curvature of nth band, and c_2 is defined as

$$c_2(x) \equiv \int_0^x dt\left(\ln\frac{1+t}{t}\right)^2 \tag{70}$$

POLARIZED KITAEV MAGNET

In this section I discuss the linear spin waves in the polarized phase of Kitaev model under a polarizing out-of-plane magnetic field along e_3, as shown in Fig.2. The [111] direction corresponds to the e_3 direction in the lab coordinate. The lab coordinate is related to the intrinsic coordinate defined by the ligands (See Fig.2(b)) according to the relation between the orthogonal (e_1, e_2, e_3) basis and the intrinsic basis shown in Fig. 2(a,b), where unit vectors are related through: $\hat{e}_1 = \frac{1}{\sqrt{6}}(-\hat{x} - \hat{y} + 2\hat{z})$, $\hat{e}_2 = \frac{1}{\sqrt{2}}(\hat{x} - \hat{y})$, $\hat{e}_3 = \frac{1}{\sqrt{3}}(\hat{x} + \hat{y} + \hat{z})$, hence the projection of spins:

$$S_i^{e_1} = \frac{1}{\sqrt{6}}(-S_i^x - S_i^y + 2S_i^z) = \frac{1}{2}(S_i^+ + S_i^-) \tag{71}$$

$$S_i^{e_2} = \frac{1}{\sqrt{2}}(S_i^x - S_i^y) = \frac{1}{2i}(S_i^+ - S_i^-) \tag{72}$$

$$S_i^{e_3} = \frac{1}{\sqrt{3}}(S_i^x + S_i^y + S_i^z) \tag{73}$$

where we defined $S^\pm \equiv S_i^{e_1} \pm iS_i^{e_2}$. We can write the intrinsic spin operator in terms of the lab frame operators

$$S_i^x = \frac{1}{\sqrt{6}}(\theta S_i^+ + \theta^* S_i^- + \sqrt{2}S_i^{e_3}) \tag{74}$$

$$S_i^y = \frac{1}{\sqrt{6}}(\theta^* S_i^+ + \theta S_i^- + \sqrt{2}S_i^{e_3}) \tag{75}$$

$$S_i^z = \frac{1}{\sqrt{6}}(S_i^+ + S_i^- + \sqrt{2}S_i^{e_3}) \tag{76}$$

where $\theta \equiv -\frac{1}{2}(1 + \sqrt{3}i) = e^{-i\frac{2\pi}{3}}$. Note $\theta\theta^* = 1$, $\theta^2 = \theta^*$, $\theta + \theta^* + 1 = 0$ and $(\theta^*)^2 = \theta$. For the partially polarized state along [111] we define the boson as fluctuation againt the e_3 direction:

$$S_i^{e_3} = S - a_i^\dagger a_i, \tag{77}$$

$$S_i^+ \approx \sqrt{2S}\left(1 - \frac{a_i^\dagger a_i}{4S}\right) a_i, \tag{78}$$

$$S_i^- \approx \sqrt{2S}a_i^\dagger\left(1 - \frac{a_i^\dagger a_i}{4S}\right) \tag{79}$$

Then the spin operators can be approximated by

$$S_i^x = \frac{1}{\sqrt{3}}[\sqrt{S}(\theta a_i + \theta^* a_i^\dagger) - a_i^\dagger a_i + S] \tag{80}$$

$$S_i^y = \frac{1}{\sqrt{3}}[\sqrt{S}(\theta^* a_i + \theta a_i^\dagger) - a_i^\dagger a_i + S] \tag{81}$$

$$S_i^z = \frac{1}{\sqrt{3}}[\sqrt{S}(a_i + a_i^\dagger) - a_i^\dagger a_i + S] \tag{82}$$

up to the quadratic order. So the Kitaev exchange can be written as quadratic boson operators shown in Appendix.; and the magnetic field per unit cell is

$$-h_i^{e_3}(S_{i,A}^{e_3} + S_{i,B}^{e_3}) \approx -h_i^{e_3}(2S - a_i^\dagger a_i - b_i^\dagger b_i) \tag{83}$$

Then the non-interacting part of Kitaev Hamiltonian under [111] field is

$$\begin{aligned}\mathcal{H}_K^0 =& \frac{1}{3}\sum_{i\in A}\Big[(3S^2 - 6Sh^{e_3}) - 3(S - h^{e_3})a_i^\dagger a_i \\ &- (S - 3h^{e_3})b_i^\dagger b_i - Sb_{i+\mathbf{n}_1}^\dagger b_{i+\mathbf{n}_1} - Sb_{i+\mathbf{n}_2}^\dagger b_{i+\mathbf{n}_2} \\ &+ S(\theta^* a_i b_{i+\mathbf{n}_1} + \theta a_i b_{i+\mathbf{n}_2} + a_i b_i \\ &+ a_i b_{i+\mathbf{n}_1}^\dagger + a_i b_{i+\mathbf{n}_2}^\dagger + a_i b_i^\dagger + h.c.)\Big]\end{aligned} \tag{84}$$

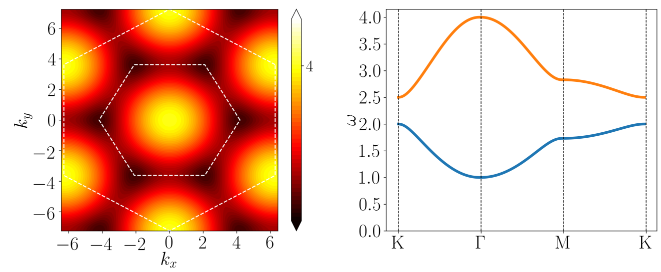

FIG. 1. Linear spin wave bands in the bulk of the polarized Kitaev magnet with $h^{e_3}/K = 4$. (a) The first Brillouin zone (b) cuts of linear spin wave bands along $K - \Gamma - M - K$.

where we have restricted the bond-dependent interactions to be identical in strength ($K_x = K_y = K_z \equiv 1$) such that linear bosonic operators cancel due to $\theta + \theta^* + 1 = 0$. In momentum space we have:

$$\begin{aligned}\mathcal{H}_K^0 =& \frac{N}{2}(S^2 - 2Sh^{e_3}) - (S - h^{e_3})\sum_{\mathbf{k}}(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}}) \\ &+ \frac{S}{3}\sum_{\mathbf{k}}\left[\Delta_{\mathbf{k}} a_{\mathbf{k}} b_{\mathbf{k}}^\dagger + \Delta_{\mathbf{k}}^\theta a_{\mathbf{k}} b_{-\mathbf{k}} + h.c.\right]\end{aligned} \tag{85}$$

where we defined

$$\Delta_{\mathbf{k}} \equiv \left(1 + e^{-i\mathbf{k}\cdot\mathbf{n}_1} + e^{-i\mathbf{k}\cdot\mathbf{n}_2}\right), \tag{86}$$

$$\Delta_{\mathbf{k}}^\theta \equiv \left(1 + \theta^* e^{-i\mathbf{k}\cdot\mathbf{n}_1} + \theta e^{-i\mathbf{k}\cdot\mathbf{n}_2}\right) \tag{87}$$

By diagonalizing this bosonic Hamiltonian we get the magnon band structure of the polarized Kitaev magnet along e_3 direction, as is shown in Fig.1.

TOPOLOGICAL MAGNONS IN J-K-Γ

In this section I discuss the topological magnons in the $J - K - \Gamma$ model relevant for the quasi-2D magnetic material CrI_3 [5], which includes energy contribution from (i) Kitaev exchange, (ii) Heisenberg exchange, (iii) DM interaction, (iv) off-diagonal or Γ exchange, (v) on-site single ion anisotropy and (iv) other next-to-nearest-neighbor interactions which are of minor importence in the context. I will present the linear spin wave theories on (i) - (v) and their resultant magnon band with non-trivial Berry curvature responsible for thermal Hall effects. The energy scale for these interactions are reported in Ref.[5] using density functional theory.

Heisenberg Exchange

By the same token used in the previous section, the Heisenberg exchange can be written in the boson language as

$$\sum_{i\in A}\vec{S}_{i,A}\cdot\vec{S}_{j,B}=\sum_{i\in A}S^{e_3}_{i,A}S^{e_3}_{j,B}+\frac{1}{2}\left(S^{+}_{i,A}S^{-}_{j,B}+S^{-}_{i,A}S^{+}_{j,B}\right)$$
$$\approx\sum_{i\in A}S(a_ib_j^\dagger+a_i^\dagger b_j-a_i^\dagger a_i-b_j^\dagger b_j)$$
$$+\frac{1}{4}(4a_i^\dagger a_i b_j^\dagger b_j-a_i^\dagger a_i^\dagger a_i b_j$$
$$-a_i^\dagger a_i a_i b_j^\dagger-a_ib_j^\dagger b_j^\dagger b_j-a_i^\dagger b_j^\dagger b_j b_j)+S^2 \tag{88}$$

where $j\in\{i,\ i+\mathbf{n}_1,\ i+\mathbf{n}_2\}$. The quadratic part of Heisenberg exchange is

$$\mathcal{H}^0_J=\frac{3N}{2}S^2-3S\sum_{\mathbf{k}}(a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+b^\dagger_{\mathbf{k}}b_{\mathbf{k}})+S\sum_{\mathbf{k}}(\Delta_{\mathbf{k}}a_{\mathbf{k}}b^\dagger_{\mathbf{k}}+h.c.) \tag{89}$$

Γ exchange

The Γ exchange, i.e. the off-diagonal exchange is allowed by symmetry of CrI_3. Its contribution to Hamiltonian is

$$\mathcal{H}_\Gamma=\Gamma\sum_{\langle ij\rangle\in\alpha\beta(\gamma)}(S_i^\alpha S_j^\beta+S_i^\beta S_j^\alpha) \tag{90}$$

where the notation $\langle ij\rangle\in\alpha\beta(\gamma)$ stands for bonds $(i,j=i+\delta_\gamma)$ with $\gamma\neq\alpha,\ \beta$. The Γ exchange in terms of linear spin waves is shown in Appendix.. The quadratic part reads

$$\mathcal{H}^0_\Gamma=NS^2-\frac{1}{3}\sum_{i\in A}2S(3a_i^\dagger a_i+b_i^\dagger b_i+b^\dagger_{i+\mathbf{n}_1}b_{i+\mathbf{n}_1}$$
$$+b^\dagger_{i+\mathbf{n}_2}b_{i+\mathbf{n}_2})+\frac{1}{3}\sum_{i\in A}S(2\theta^*a_ib_{i+\mathbf{n}_1}+2\theta a_ib_{i+\mathbf{n}_2}$$
$$+2a_ib_i-a_ib^\dagger_{i+\mathbf{n}_1}-a_ib^\dagger_{i+\mathbf{n}_2}-a_ib_i^\dagger+h.c.) \tag{91}$$

Now we move to the momentum space by a Fourier transform of boson operators. This gives:

$$\mathcal{H}^0_\Gamma=NS^2-2S\sum_{\mathbf{k}}(a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+b^\dagger_{\mathbf{k}}b_{\mathbf{k}})$$
$$+\frac{S}{3}\sum_{\mathbf{k}}(2\Delta^\theta_{\mathbf{k}}a_{\mathbf{k}}b_{-\mathbf{k}}-\Delta_{\mathbf{k}}a_{\mathbf{k}}b^\dagger_{\mathbf{k}}) \tag{92}$$

DM exchange

We now turn to D-M interaction. From previous texts it is readily to see that the real space Hamiltonian up to 2nd order reads

$$\mathcal{H}^0_D=S\sqrt{3}\sum_{\langle\langle ij\rangle\rangle}(ia_ia_j^\dagger+h.c.)$$
$$=S\sqrt{3}\sum_{i\in A}(ia_ia^\dagger_{i-\mathbf{n}_1}+ia_ia^\dagger_{i+\mathbf{n}_2}+ia_ia^\dagger_{i+\mathbf{n}_1-\mathbf{n}_2}+h.c.)$$
$$+S\sqrt{3}\sum_{i\in B}(ib_ib^\dagger_{i+\mathbf{n}_1}+ib_ib^\dagger_{i-\mathbf{n}_2}+ib_ib^\dagger_{i+\mathbf{n}_2-\mathbf{n}_1}+h.c.) \tag{93}$$

where $\sqrt{3}$ comes from $\theta^*-\theta$; and note that i,j belong to the same sublattice. In momentum space we have

$$\mathcal{H}^0_D=S\sqrt{3}\sum_{\mathbf{k}}\left[i\left(e^{i\mathbf{k}\cdot\mathbf{n}_1}+e^{-i\mathbf{k}\cdot\mathbf{n}_2}+e^{-i\mathbf{k}\cdot(\mathbf{n}_1-\mathbf{n}_2)}\right)a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+h.c.\right]$$
$$+S\sqrt{3}\sum_{\mathbf{k}}\left[i\left(e^{-i\mathbf{k}\cdot\mathbf{n}_1}+e^{i\mathbf{k}\cdot\mathbf{n}_2}+e^{i\mathbf{k}\cdot(\mathbf{n}_1-\mathbf{n}_2)}\right)b^\dagger_{\mathbf{k}}b_{\mathbf{k}}+h.c.\right]$$
$$=2\sqrt{3}S\sum_{\mathbf{k}}\left(\Xi_{\mathbf{k}}a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+\Xi_{-\mathbf{k}}b^\dagger_{\mathbf{k}}b_{\mathbf{k}}\right) \tag{94}$$

where we defined

$$\Xi_{\mathbf{k}}=-\sin(\mathbf{k}\cdot\mathbf{n}_1)+\sin(\mathbf{k}\cdot\mathbf{n}_2)+\sin[\mathbf{k}\cdot(\mathbf{n}_1-\mathbf{n}_2)] \tag{95}$$

Single-ion anisotropy

Finally, the single-ion anisotropy, to the leader order, is

$$\mathcal{H}^0_A=NS^2-2S\sum_{\mathbf{k}}(a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+b^\dagger_{\mathbf{k}}b_{\mathbf{k}}) \tag{96}$$

Therefore, the full LSW Hamiltonian is

$$\mathcal{H}^{\mathrm{LSW}}=\mathcal{H}^0_J+\mathcal{H}^0_K+\mathcal{H}^0_\Gamma+\mathcal{H}^0_D+\mathcal{H}^0_A-\mathcal{H}_{e_3}$$
$$=\sum_{\mathbf{k}}\Big[d_{\mathbf{k}}a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+d_{-\mathbf{k}}b^\dagger_{\mathbf{k}}b_{\mathbf{k}}$$
$$+\left(p_{\mathbf{k}}a_{\mathbf{k}}b^\dagger_{\mathbf{k}}+q_{\mathbf{k}}a_{\mathbf{k}}b_{-\mathbf{k}}+h.c.\right)+C \tag{97}$$

where

$$d_{\mathbf{k}}=-S(3J+K+2\Gamma+2A-2\sqrt{3}D\Xi_{\mathbf{k}})+h^{e_3} \tag{98}$$
$$p_{\mathbf{k}}=S\left(J+\frac{K}{3}-\frac{\Gamma}{3}\right)\Delta_{\mathbf{k}} \tag{99}$$
$$q_{\mathbf{k}}=S\left(\frac{K}{3}+\frac{2\Gamma}{3}\right)\Delta^\theta_{\mathbf{k}} \tag{100}$$

By symmetrizing the momentum we have

$$\mathcal{H}^{\mathrm{LSW}}=\frac{1}{2}\sum_{\mathbf{k}}\Big[d_{\mathbf{k}}a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+d_{-\mathbf{k}}a^\dagger_{-\mathbf{k}}a_{-\mathbf{k}}+d_{-\mathbf{k}}b^\dagger_{\mathbf{k}}b_{\mathbf{k}}$$
$$+d_{\mathbf{k}}b^\dagger_{-\mathbf{k}}b_{-\mathbf{k}}+\Big(p_{\mathbf{k}}a_{\mathbf{k}}b^\dagger_{\mathbf{k}}+p_{-\mathbf{k}}a_{-\mathbf{k}}b^\dagger_{-\mathbf{k}}$$
$$+q_{\mathbf{k}}a_{\mathbf{k}}b_{-\mathbf{k}}+q_{-\mathbf{k}}a_{-\mathbf{k}}b_{\mathbf{k}}+h.c.\Big)\Big] \tag{101}$$

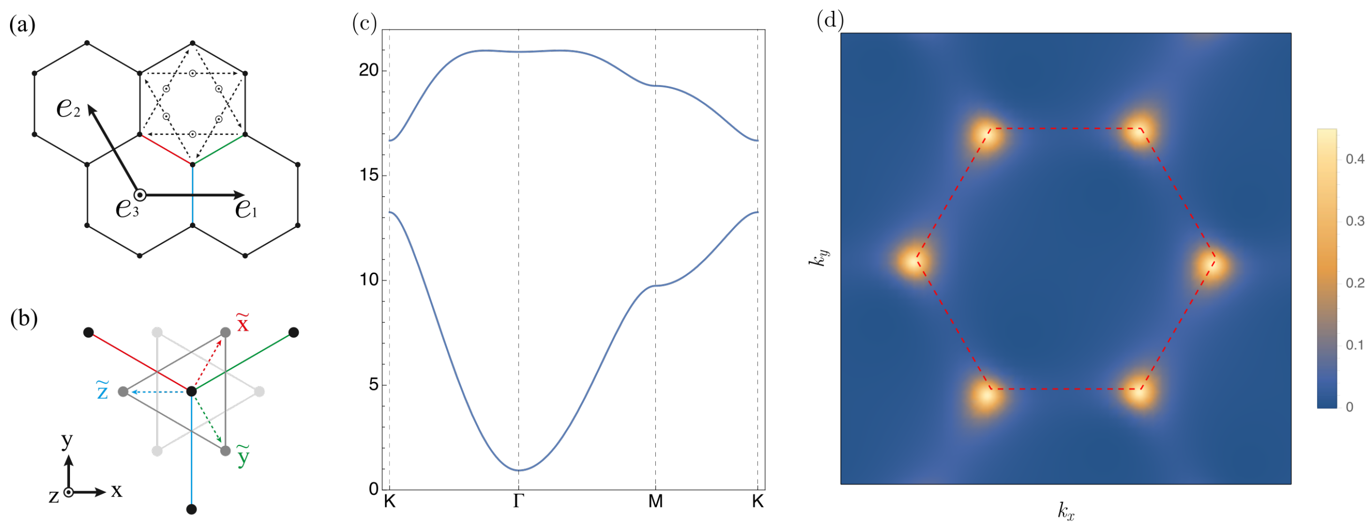

FIG. 2. (a) A 2D plane of CrI_3 on honeycomb lattice, with the crystal cooridnate defined by ligands shown in panel (b). (c) Magnon band structure with respect to the [111] i.e. the $\mathbf{e}_3$ direction, the data is obtained by including the in-plane next-to-nearest neighbor coupling according to Ref.[5]. (d) the Berry curvature of the aforementioned magnon band.

Now we diagonalize this Hamiltonian. In the matrix form we have

$$\Psi_{\mathbf{k}} \equiv (a_{\mathbf{k}}, b_{\mathbf{k}}, a^\dagger_{-\mathbf{k}}, b^\dagger_{-\mathbf{k}})^{\mathrm{T}}, \quad \mathcal{H}^{\mathrm{LSW}} = \frac{1}{2}\sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} \mathcal{H}_{\mathbf{k}} \Psi_{\mathbf{k}} \tag{102}$$

where

$$\mathcal{H}_{\mathbf{k}} = \begin{pmatrix} d_{\mathbf{k}} & p^*_{\mathbf{k}} & 0 & q^*_{\mathbf{k}} \\ p_{\mathbf{k}} & d_{-\mathbf{k}} & q^*_{-\mathbf{k}} & 0 \\ 0 & q_{-\mathbf{k}} & d_{-\mathbf{k}} & p_{-\mathbf{k}} \\ q_{\mathbf{k}} & 0 & p^*_{-\mathbf{k}} & d_{\mathbf{k}} \end{pmatrix} \tag{103}$$

Diagonalizing the Hamiltonian in $\mathbf{k}$ space gives the band structure of linear spin waves around e_3 axis, as is shown in Fig.2(c). Then by using Eq.14 we know the Berry curvature Ω. Then we can use it to derive the thermal hall coefficient in finite temperature (assuming anharmonic terms and higher order effects are negligible) by Eq.69, which will be discussed in future investigation that relates to experiments.

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APPENDIX

In this appendix I show the spin-spin exchange in terms of Holstein-Primakoff bosons. They are then kept upto the quardatic order to get the band structure. Note that the linear terms are cancelled with each other due to $\theta + \theta^* + 1 = 0$.

Spin exchanges relevant for Kitaev interaction:

$$S^x_{i,A} S^x_{i+\mathbf{n}_1,B} = \frac{1}{3}\left[S(\theta^* a_i b_{i+\mathbf{n}_1} + a_i b^\dagger_{i+\mathbf{n}_1} + h.c.) - S(a^\dagger_i a_i + b^\dagger_{i+\mathbf{n}_1} b_{i+\mathbf{n}_1}) + S^{\frac{3}{2}}(\theta a_i + \theta b_{i+\mathbf{n}_1} + h.c.) + S^2\right] \tag{104}$$

$$S^y_{i,A} S^y_{i+\mathbf{n}_2,B} = \frac{1}{3}\left[S(\theta a_i b_{i+\mathbf{n}_2} + a_i b^\dagger_{i+\mathbf{n}_2} + h.c.) - S(a^\dagger_i a_i + b^\dagger_{i+\mathbf{n}_2} b_{i+\mathbf{n}_2}) + S^{\frac{3}{2}}(\theta^* a_i + \theta^* b_{i+\mathbf{n}_2} + h.c.) + S^2\right] \tag{105}$$

$$S^z_{i,A} S^z_{i,B} = \frac{1}{3}\left[S(a_i b_i + a_i b^\dagger_i + h.c.) - S(a^\dagger_i a_i + b^\dagger_i b_i) + S^{\frac{3}{2}}(a_i + b_i + h.c.) + S^2\right] \tag{106}$$

The Γ exchange reads (will leave out A, B. Assume $i \in A$ and $j \in B$):

$$S^x_i S^y_i = \frac{1}{3}\left[S(a_i b_i + \theta^* a_i b^\dagger_i + h.c.) - S(a^\dagger_i a_i + b^\dagger_i b_i) + S^{3/2}(\theta a_i + \theta^* b_i + h.c.) + S^2\right] \tag{107}$$

$$S^y_i S^z_j = \frac{1}{3}\left[S(\theta^* a_i b_j + \theta^* a_i b^\dagger_j + h.c.) - S(a^\dagger_i a_i + b^\dagger_j b_j) + S^{3/2}(\theta^* a_i + b^\dagger_j + h.c.) + S^2\right] \tag{108}$$

$$S^z_i S^x_j = \frac{1}{3}\left[S(\theta a_i b_j + \theta^* a_i b^\dagger_j + h.c.) - S(a^\dagger_i a_i + b^\dagger_j b_j) + S^{3/2}(a_i + \theta b_j + h.c.) + S^2\right] \tag{109}$$

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