Supporting Information for

Resonant thermal Hall effect of phonons coupled to dynamical defects

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In this supplement material, we present detailed calculations of the thermal Hall effects discussed in the main text. We will discuss model C in Part I because some of the expressions are simpler in this model due to the simplicity of phonon-defect coupling. We later generalize the formalism to account for the more complicated couplings in models A and B in Part II. We also include a calculation that reproduces the Berry curvature formula of phonon Hall effect for quadratic phonon systems in Part III.

**Part I**

**Model C**

In this part, we evaluate the thermal Hall effect of model C by keeping all contributions to the modified Kubo formula.

1. **Quadratic Phonon Hamiltonian**

In this part, we discuss properties of the quadratic phonon Hamiltonian.

In the main text, the quadratic phonon Hamiltonian without dissipation is given by

$$H_{ph} = \sum_p \frac{\pi^i_p \pi^i_p}{2m} + \frac{1}{2} \sum_{pq} u^i_p C^{ij}_{pq} u^j_q , \quad [S1]$$

where $m$ is the ion mass and $C^{ij}_{pq}$ is the elastic matrix, and the variables $u^i_p$ and $\pi^i_p$ satisfy the commutation relation

$$[u^i_p, \pi^j_q] = i\delta^{ij}\delta_{pq} . \quad [S2]$$

It is convenient to treat $u$ and $\pi$ on equal footing, by introducing the variable $\zeta^I_p = (u^i_p, \pi^i_p)$. Then any quadratic phonon Hamiltonian can be written as

$$H = \frac{1}{2} \sum_{pq} \zeta^I_p h^{IJ}(p,q) \zeta^J_q , \quad [S3]$$

where $\zeta$'s satisfy the canonical commutation relation

$$[\zeta^I_p, \zeta^J_q] = iJ^{IJ}(p,q) . \quad [S4]$$

Here repeated $I, J, \ldots$ indices are Einstein summed. Assuming $\zeta$'s are Hermitian, then the matrix $h$ is Hermitian and $J$ is real antisymmetric. Furthermore, by adding a suitable constant to $H$ we can make $h$ real and symmetric.

For the Hamiltonian Eq. (S1), we have explicitly

$$h^{IJ}(p,q) = \begin{pmatrix} C^{ij}_{pq} & 0 \\ 0 & \frac{1}{m}\delta^{ij}\delta_{pq} \end{pmatrix} , \quad [S5]$$

and

$$J^{IJ}(p,q) = \begin{pmatrix} 0 & \delta^{ij}\delta_{pq} \\ -\delta^{ij}\delta_{pq} & 0 \end{pmatrix} \quad [S6]$$

respectively.
A. Diagonalization. First we diagonalize the Hamiltonian Eq. (S3). For notational simplicity, in this subsection we group the indices together, writing $\zeta^I_p = \zeta_a$. The starting point is

$$H = \frac{1}{2} \sum_{ab} \zeta_a h_{ab} \zeta_b, \quad [\zeta_a, \zeta_b] = i J_{ab}. \tag{S7}$$

The Heisenberg equation reads

$$\frac{d\zeta_a}{dt} = i[H, \zeta_a] = (Jh\zeta) a. \tag{S8}$$

The normal modes satisfy the eigenvalue equation

$$\omega_a \psi_a = iJh \psi_a. \tag{S9}$$

Suppose the matrix $iJh$ is diagonalized by matrix $M$:

$$iJhM = ME, \tag{S10}$$

where $E$ is a diagonal matrix. Multiply $(iJ)^{-1}$ on both sides of Eq. (S10), and contract with $M^\dagger$, we obtain

$$M^\dagger hM = M^\dagger (iJ)^{-1} ME. \tag{S11}$$

Taking the diagonal elements of the above equation, and using the fact that $h, iJ$ are Hermitian, we conclude that $E$ is real. Because $h$ is positive definite, $E$ is nonzero.

Taking the Hermitian conjugation of Eq. (S11), we obtain

$$M^\dagger (iJ)^{-1} M = M^\dagger h M = E M^\dagger (iJ)^{-1} M. \tag{S12}$$

Here we have used the fact that $E$ is real. Therefore $M^\dagger (iJ)^{-1} M$ can also be chosen to be diagonal. The positive definiteness of $h$ implies that $M^\dagger (iJ)^{-1} M$ has the same sign as $E$, therefore we normalize it as

$$M^\dagger (iJ)^{-1} M = \text{sgn} E. \tag{S13}$$

Because $J, h$ are real, the complex conjugate of Eq. (S10) yields

$$iJh M^* = -M^* E. \tag{S14}$$

This implies that eigenvalues of $E$ are paired up in opposite signs.

Let’s define a particle conjugation operator $C$, which satisfies

$$M^* = MC. \tag{S15}$$

The definition implies

$$C^* = C^{-1}. \tag{S16}$$

From Eq. (S14), we find

$$CE = -EC, \tag{S17}$$

i.e. $C$ exchange modes of opposite energy.

Comparing Eq. (S13) with its complex conjugation, we can show that

$$C^T = C^{-1}. \tag{S18}$$
The new normal modes are given by
\[ v = M^{-1} \zeta. \]  
[S19]

Their commutation relation is given by
\[ K_{ab} = [v_a, v_b], \quad K = M^{-1} iJ (M^T)^{-1}. \]  
[S20]

By construction \( K \) is an antisymmetric matrix.

Multiplying Eq. (S10) with \((iJ)^{-1}\), and contract with \( M^T \), we obtain
\[ K^{-1} E = M^T h M = -E K^{-1}. \]  
[S21]

Therefore \( K \) anticommutes with \( E \). Furthermore, we can relate \( K \) to \( C \) via the normalization condition Eq. (S13):
\[ K = \text{sgn} E C^T. \]  
[S22]

Since \( K \) is antisymmetric, we can derive that
\[ C = C^T = C^* = C^{-1}. \]  
[S23]

Consider the subspace spanned by the two eigenvectors of opposite eigenvalue, in this space \( \text{sgn} E = \sigma^z \) and therefore \( C = \sigma^x \), \( K = i\sigma^y \). Therefore, the normal mode corresponding to positive energy can always be defined as annihilation operator, while the normal mode corresponding to negative energy can be defined as creation operator, and they satisfy the commutation relation.

In terms of the new normal modes, the Hamiltonian reads
\[ \tilde{h} = M^T h M = E K. \]  
[S24]

Expanding in the subspace of conjugate normal modes, the Hamiltonian is equivalent to the standard boson Hamiltonian \((|\omega|/2)(a a^\dagger + a^\dagger a)\).

**B. Free Phonon Green’s Function.** The phonon Green’s function in imaginary time is defined as
\[ D_{ab}(\tau) = -T \langle \zeta_a(\tau) \zeta_b(0) \rangle. \]  
[S25]

This Green’s function can be calculated by using the diagonalization method derived above. Expand \( \zeta \) in terms of the creation and annihilation operators, evaluate the expectations and using Eq. (S20), we obtain
\[ D(i\omega_n) = \frac{1}{i\omega_n - iJ h} iJ. \]  
[S26]

The above result can be alternatively derived from phase space path integral. For a 1D particle with momentum \( p \) and coordinate \( q \), its imaginary-time path integral is given by
\[ \int DpDq \exp \left( - \int \mathrm{d}\tau \left( -ip \frac{\mathrm{d}q}{\mathrm{d}\tau} + H(p, q) \right) \right). \]  
[S27]

Generalizing the above form many variables, we just need to find the canonical momentum \( P_a \) for \( \zeta_a \), which satisfies \([P_a, \zeta_b] = -i\delta_{ab}\). This condition is solved by \( P_a = -(J^{-1} \zeta)_a \). The path integral for the phonon system is therefore
\[ \int D\zeta \exp \left( - \int \mathrm{d}\tau \left( \frac{1}{2} \zeta^T (iJ)^{-1} \frac{\partial \zeta}{\partial \tau} + \frac{1}{2} \zeta^T h \zeta \right) \right), \]  
[S28]

where we have inserted a factor \(1/2\) to avoid double counting. Switching to frequency space, this immediately yields the Green’s function Eq. (S26).

In actual computations of the thermal Hall conductivity, we need the retarded and advanced Green’s functions with dissipation terms put in by hand:
\[ D_{\pm}(z) = \frac{1}{z \pm \frac{\gamma_{\text{ph}}}{2} - iJ h} iJ. \]  
[S29]
C. Acoustic Phonon. For our problem, we assume the Hamiltonian describes acoustic phonons in an isotropic lattice. The elastic matrix $C_{ij}^{pq}$ can be Fourier transformed to momentum space by

$$C_{ij}^{pq}(k) = \frac{1}{N_{\text{cell}}} \sum_p C_{ij}^{pq} e^{-ik(p-q)}$$

where $N_{\text{cell}}$ is the number of unit cells. In momentum representation, we have

$$C_{ij}^{pq}(k) = \frac{mc^2}{T} \delta_{ij} k^2 + mc \left( c_L^2 - c_T^2 \right) k^i k^j,$$  \(\text{[S30]}\)

where $c_L$ is the longitudinal velocity and $c_T$ is the transverse velocity. The momentum space representation of $h$ and $J$ are

$$h^{IJ}(k) = \begin{pmatrix} C_{ij}^{pq}(k) & 0 \\ 0 & 1 \end{pmatrix},$$  \(\text{[S31]}\)

$$J^{IJ}(k) = \begin{pmatrix} 0 & \delta^{ij} \\ -\delta^{ij} & 0 \end{pmatrix}.$$  \(\text{[S32]}\)

The Hamiltonian can now be diagonalized for each individual $k$. An explicit solution for the matrix $M(k)$ is

$$M(k) = \begin{pmatrix} \left( \frac{e^1_k}{\sqrt{m\omega^1_k}} \frac{e^2_k}{\sqrt{m\omega^2_k}} \frac{e^3_k}{\sqrt{m\omega^3_k}} \right) & 0 \\ 0 & \left( e^1_k \sqrt{m\omega^1_k} e^2_k \sqrt{m\omega^2_k} e^3_k \sqrt{m\omega^3_k} \right) \end{pmatrix} \times \begin{pmatrix} 1 \\ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} \otimes I_3 \end{pmatrix}. $$  \(\text{[S33]}\)

The eigenvalues are

$$\mathcal{E} = \text{diag}(\omega^1_k, \omega^2_k, \omega^3_k, -\omega^1_k, -\omega^2_k, -\omega^3_k).$$  \(\text{[S34]}\)

Here $e^a_k$ is a 3 by 1 column vector that describes the polarization vector of the $a$-th mode, and $\omega^a_k$ is the corresponding frequency. $I_3$ is the 3 by 3 identity matrix. From Eq. Eq. (S30) we have one longitudinal mode $\omega^3_k = c_L k$ and two transverse modes $\omega^{1,2}_k = c_T k$.

2. Defect Green’s function

In this part we compute the defect Green’s function which will be used to compute the thermal Hall effect. We assumed the defect-phonon coupling to be of the form

$$H_{\text{ph-def}} = \gamma \pi_o \cdot \delta \dot{V}.$$  \(\text{[S35]}\)

Here we have subtracted off the equilibrium value $\delta \dot{V} = \dot{V} - \langle \dot{V} \rangle$ to fix the equilibrium position of $\pi$ at zero. Since the defect is localized at the site $o$ and couples only to momentum, the defect Green’s function, when written in terms of the index structure of $\zeta^I_p$, is given by

$$S^{IJ}_{pq}(i\omega_n) = \delta_{po} \delta_{qa} \begin{pmatrix} 0 & 0 \\ 0 & S^{ij}(i\omega_n) \end{pmatrix},$$  \(\text{[S36]}\)

where $S^{ij}(i\omega_n)$ is the Green’s function written in the defect Hilbert space

$$S^{ij}(i\omega_n) = -\int_0^\beta d\tau e^{i\omega_n \tau} T_{\tau} \langle V^i(\tau)V^j(0) \rangle.$$  \(\text{[S37]}\)

Here in the definition we have used $V^i$ instead of the subtracted version $\delta V^i = V^i - \langle V^i \rangle$, because ultimately we only need the retarded and the advanced Green’s functions, which are insensitive to variable shifts.
In the continuum limit, it’s convenient to switch to momentum space, then the defect Green’s function becomes

$$\langle k_1 | S^{ij}(i\omega_n) | k_2 \rangle = \frac{1}{N_{\text{sys}}} \begin{pmatrix} 0 & 0 \\ 0 & S^{ij}(i\omega_n) \end{pmatrix}.$$  \[S38\]

Here we have assumed the momentum eigenstates are normalized to one $$\langle k_1 | k_2 \rangle = \delta_{k_1,k_2}$$, and therefore the normalization constant is given by the number of unit cells $$N_{\text{sys}}$$.

We do not include dissipation $$\Gamma_s$$ for the defect Green’s function. Because we found the thermal Hall conductivity is smooth in the $$\Gamma_s \to 0$$ limit, and therefore the effect of $$\Gamma_s$$ will be higher order corrections in terms of the coupling $$\gamma$$.

Now we compute $$S^{ij}$$. The model is a 4-level system with a Zeeman field:

$$H_{\text{def}} = \sum_{l=0}^{1} \sum_{m=-l}^{l} E_{lm} \langle lm | \langle lm | ,$$  \[S39\]

The ground state has energy $$E_{00} = 0$$, and the excited triplet is split by Zeeman field $$E_{1m} = \Delta - m\Delta_Z$$, $$\Delta \gg \Delta_Z$$.

The retarded Green’s function is given by

$$S^{ij}_+(t) = -i\theta(t) \langle [V^i(t), V^j(0)] \rangle.$$  \[S40\]

To compute the Green’s function, it is convenient to switch to the spherical basis

$$\begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} = \begin{pmatrix} \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} V^+ \\ V^- \\ V^0 \end{pmatrix}.$$  \[S41\]

The correlator for the spherical operators can be computed as $$(q, q' = +, -, 0)$$:

$$\langle V^q(0) V^{q'}(0) \rangle = \sum_{l_m, l_m'} \frac{e^{-\beta E_{lm}}}{Z} e^{-i(E_{l_m'} - E_{lm})t} \langle lm | V^q \rangle \langle l_m' | V^{q'} \rangle \langle lm |.$$  \[S42\]

In the second line, we have used the Wigner-Eckart theorem to factorize the matrix elements into Clebsch-Gordon coefficients and the reduced matrix elements $$\langle l_m' | V^{q'} \rangle$$.

For the 4-level model, we find

$$S^{ij}_+(z) = \alpha_R K_1^{ij}(z_\pm) + \alpha_R K_2^{ij}(z_\pm) + \beta_R K_3^{ij}(z_\pm).$$  \[S43\]

The two constants are

$$\alpha_R = \frac{1}{\sqrt{3}} \langle 1 || V || 0 \rangle \langle 0 || V || 1 \rangle,$$  \[S44\]

$$\beta_R = \langle 1 || V || 1 \rangle^2.$$  \[S45\]

The functions involved are

$$K_1^{ij}(z) = - \frac{e^{\beta(\Delta_Z + \Delta)}}{1 + e^{\beta\Delta_Z} + e^{2\beta\Delta_Z} + e^{2\beta(\Delta_Z + \Delta)}} F^{ij}(z, \Delta_Z + \Delta),$$  \[S46\]

$$K_2^{ij}(z) = - \frac{e^{2\beta\Delta_Z} - e^{\beta(\Delta_Z + \Delta)}}{1 + e^{\beta\Delta_Z} + e^{2\beta\Delta_Z} + e^{2\beta(\Delta_Z + \Delta)}} F^{ij}(z, \Delta_Z - \Delta),$$  \[S47\]
\[ K_{3}^{ij}(z) = -\frac{e^{2\beta \Delta z} - 1}{1 + e^{\beta \Delta z} + e^{2\beta \Delta z} + e^{\beta (\Delta z + \Delta)}} F^{ij}(z, \Delta Z), \quad [S48] \]

\[ F^{ij}(z, \epsilon) = \begin{pmatrix} \epsilon z \frac{e^{\beta \Delta Z}}{e^{\epsilon \Delta Z} - 1} & \epsilon z \frac{e^{\beta \Delta Z}}{e^{\epsilon \Delta Z} - 1} & 0 \\ -\epsilon z \frac{e^{\beta \Delta Z}}{e^{\epsilon \Delta Z} - 1} & \epsilon z \frac{e^{\beta \Delta Z}}{e^{\epsilon \Delta Z} - 1} & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad [S49] \]

The contribution of \( K_{3} \) to thermal Hall effect is very similar to the result of the two-level model discussed later. Compared to \( K_{1} \) and \( K_{2} \), \( K_{3} \) is smaller by powers of \( \Delta Z / \Delta (\Delta Z \ll \Delta) \) as well as a thermal weight \( e^{-\beta \Delta} \), therefore we will only keep \( K_{1} \) and \( K_{2} \) in the later calculations.

### 3. Energy Current

In this part, we shall compute the energy current operator. The energy current receives contribution from the quadratic phonon Hamiltonian and the phonon-defect coupling.

#### A. Quadratic Phonon Part.

From Eq. (S3), we can derive the Hamiltonian density to be

\[ H_{p} = \frac{1}{4} \sum_{m} \left( \zeta_{p}^{I} h^{I J} (p, m) \zeta_{m}^{J} + \zeta_{m}^{J} h^{J I} (m, p) \zeta_{p}^{I} \right). \quad [S50] \]

For a local Hamiltonian \( h(p, q) = 0 \) when \( p, q \) are sufficiently separated, therefore \( H_{p} \) represents the local energy density around site \( p \).

Following Ref. (1), the canonical choice for the energy current operator is

\[ J_{pq}^{E} = -i[H_{p}, H_{q}] = \frac{1}{8} \left( \zeta_{p}^{I} h^{I J} J^{J K} (m, q) h^{K L} (q, n) \zeta_{n}^{L} \right). \quad [S51] \]

The first term in the parenthesis is an abbreviation of four different terms. The four terms correspond to four ways of inserting one \( p \) and one \( q \) into the dotted slots, and there are two choices for \( p \) and two choices for \( q \). For example, a term of the form \( \zeta_{p} h_{J} J q h \zeta \) means

\[ \zeta_{p} h_{J} J q h \zeta = \sum_{m, n} \zeta_{p}^{I} h^{I J} (p, m) J^{J K} (m, q) h^{K L} (q, n) \zeta_{n}^{L} \].

That is, at the insertions, the site indices are fixed to be \( p, q \) respectively, and all other indices are contracted.

In later computations, we need to compute the contraction of the chain \( J_{pq}^{E} \) with some coahins. The two contractions we need is

\[ J_{pq}^{E0} (\delta \alpha) = \frac{1}{2} \sum_{pq} J_{pq}^{E} (\alpha(q) - \alpha(p)) = \frac{1}{8} \zeta (2[hJh, \alpha] + h[J, \alpha]h) \zeta. \quad [S52] \]

\[ fJ^{E} g - gJ^{E} f = \sum_{pq} J_{pq}^{E} (f(p) g(q) - g(p) f(q)) = \frac{1}{4} \zeta J^{-1} [h f, h] J (g h + h g)] \zeta \quad [S53] \]

In the final result, the index summations can be absorbed into contractions between matrices and vectors of site index and cartesian index, and \( \alpha \) is understood as a diagonal matrix in both kinds of indices. We will further assume that \( \zeta = (u, \pi) \) consists of canonical coordinates and momenta, such that \( J \) is the standard symplectic form Eq. (S6), and therefore \( J \) commutes with all one-point functions, in particular \( [J, \alpha] = 0 \) in Eq. Eq. (S52).
With the preparations above, we now calculate the thermal Hall conductivity of the phonon-defect system. Since we now express Eq. (S57) in terms of the current-current correlation function

$$\delta J^E_{p,o} = -\delta J^E_{o,p} = \frac{2}{4} \sum_m (\zeta_p h(p, m) J(m, o) \delta V) \quad (p \neq o).$$  

Here we have expanded \( \delta V \) from a 3D vector to 6D vector by filling zeroes. The summation over cartesian indices has the usual matrix multiplication structure and is suppressed.

The relevant contractions are

$$\delta J^E(\delta \alpha) = \frac{\gamma}{2} \zeta [hJ, \alpha] \delta V.$$  

$$f \delta J^E g - g \delta J^E f = \gamma \zeta (fhJg - ghJf) \delta V.$$  

In the above contractions, the operator \( \delta V \) is supported only on \( o \).

4. Thermal Hall conductivity

With the preparations above, we now calculate the thermal Hall conductivity of the phonon-defect system. Since we have assumed that in absence of the coupling \( \gamma \), the phonons are just the usual acoustic phonons in an isotropic crystal, we expect the thermal Hall effect to start at order \( \gamma^2 \). We will first compute the Kubo contribution and next the magnetization contribution.

A. Kubo Contribution. The Kubo contribution to thermal Hall conductance is given by

$$\kappa^{Kubo}(f, g) = \beta^2 \lim_{\tau \to 0} \int_0^\infty dt e^{-st} \langle \langle J^E(t); J^E(\delta g) \rangle \rangle.$$

We now express Eq. (S57) in terms of the current-current correlation function

$$\Pi_{EE}(f, g; \tau) = \langle J^E(f, \tau) J^E(g) \rangle_c,$$

$$\Pi_{EE}(f, g; i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \Pi_{EE}(f, g; \tau).$$

Using spectral representation of \( \Pi_{EE} \), we can show that the Kubo pairing is equivalent to

$$\lim_{\tau \to 0} \int_0^\infty dt e^{-st} \int_0^\beta d\tau \Pi_{EE}(\tau + it) = -i \Pi_{EE,+}(0).$$

Here \( \Pi_{EE,+}(z) = \Pi_{EE}(i\omega_n \to z + i0) \). The Kubo thermal conductivity is then given by

$$\kappa^{Kubo}(f, g) = -i \beta \Pi_{EE,+}(f, g; 0).$$

The current-current correlator \( \Pi_{EE} \) can be calculated using Wick’s theorem*, and there are the following contributions

$$\Pi_{EE}^{(0)}(f, g; i\omega_n) = 2T \sum_{\Omega_n} \text{Tr} \left[ \frac{hJh, f}{4} \frac{D(i\omega_n + i\Omega_n)}{2} G_{V\zeta}(i\Omega_n) \right].$$

$$\Pi_{EE}^{(1)}(f, g; i\omega_n) = 2T \sum_{\Omega_n} \text{Tr} \left[ \frac{hJh, f}{4} \frac{D(i\omega_n + i\Omega_n)}{2} \gamma \frac{hJh, g}{4} G_{V\zeta}(i\Omega_n) \right]$$

$$+ \gamma \frac{hJh, f}{2} G_{V\zeta}(i\Omega_n + i\omega_n) \frac{hJh, g}{4} D(i\Omega_n).$$

*Strictly speaking, Wick’s theorem doesn’t apply to the defect system. However at order \( \gamma^2 \) we only need two-point functions of the defect system, and the correlators do factorize according to Wick’s theorem.
\[
\Pi^{(2)}_{EE}(f, g; i\omega_n) = \frac{\gamma^2}{8} T \sum_{\Omega_n} \text{Tr} \left[ [hJ, f]^T D(i\omega_n + i\Omega_n)[hJ, g]S(i\Omega_n) \right] \\
+ \frac{\gamma^2}{8} T \sum_{\Omega_n} \text{Tr} \left[ [hJ, f]S(i\Omega_n + i\omega_n)[hJ, g]^T D(i\Omega_n) \right] \\
+ \frac{\gamma^2}{4} T \sum_{\Omega_n} \text{Tr} \left[ [hJ, f]G_{V\zeta}(i\omega_n + i\Omega_n)[hJ, g]G_{V\zeta}(i\Omega_n) \right].
\]

Here the superscripts count the power of \( \gamma \) coming from the energy current vertices. The trace is over both site indices and cartesian indices.

In the above expressions, we have ignored vertex corrections due to phonon-defect coupling (which appears at order \( \gamma^4 \)) and dissipation effects. While the ignorance of the latter can’t be rigorously justified, we assume its effect is to renormalize the phonon self-energy lifetime to the transport lifetime, and we account for this by interpreting \( 1/\Gamma_{\text{ph}} \) in the phonon Green’s function as the transport lifetime. Because phonon number is not conserved, we don’t expect vertex corrections to bring qualitative changes.

The Green’s functions \( D, S, G_{V\zeta} \) appearing above are interacting Green’s function defined as the following (we suppressed lattice indices)

\[
D^{IJ}_{\tau} = -T_{\tau} \langle \zeta^I(\tau)\zeta^J(0) \rangle, \quad [S65] \\
G^{IJ}_{\tau} = -T_{\tau} \langle \delta V^I(\tau)\zeta^J(0) \rangle, \quad [S66] \\
S^{IJ}_{\tau} = -T_{\tau} \langle \delta V^I(\tau)\delta V^J(0) \rangle. \quad [S67]
\]

Notice that \( G_{V\zeta} \) is of order \( \gamma \), so the last line of \( \Pi^{(2)} \) can be dropped.

To extract the Hall effects, we need to further antisymmetrize with respect to \( f \leftrightarrow g \).

**B. Magnetization Correction.** The magnetization correction is given by

\[
\mu^E(\delta f \cup \delta g) = \frac{1}{6} \sum_{pq} \mu^E_{pq}(f(q) - f(p))(g(r) - g(q)), \quad [S68] \\
\mu^E_{pq} = -\beta \left[ \langle \langle dH_p; J^E_{qr} \rangle \rangle + \langle \langle dH_r; J^E_{pq} \rangle \rangle + \langle \langle dH_q; J^E_{rp} \rangle \rangle \right].
\]

Here \( dH_p = \frac{\partial H_p}{\partial \tau} \). By simple algebra, we can express \( \mu^E \) in terms of contractions

\[
\mu^E(\delta f \cup \delta g) = -\frac{\beta}{4} \left[ 2 \langle \langle dH(g); J^E(\delta f) \rangle \rangle - 2 \langle \langle dH(f); J^E(\delta g) \rangle \rangle + \langle \langle dH; fJ^E g - gJ^E f \rangle \rangle \right], \quad [S69]
\]

where \( dH_p = \zeta \delta V, \space dH(f) = \zeta f \delta V \). For the final result to be order \( \gamma^2 \), \( \mu_E \) needs to be calculated to linear order in \( \gamma \).

Expressing everything in terms of Green’s function, we obtain

\[
\mu^E(\delta f \cup \delta g) = -\frac{1}{4} T \sum_{\Omega_n} \text{Tr} \left[ (gG_{V\zeta}[hJh, f]D + \gamma gD[hJ, f]S) - (f \leftrightarrow g) \right] \\
+ \frac{1}{2} G_{V\zeta}^{-1}[J(hf + fh), J(hg + gh)]D \quad [S70] \\
+ \gamma D(fhJg - ghJf)S.
\]

Here all Green’s functions have argument \( i\Omega_n \).
C. Evaluation. We compute the Matsubara sums and analytically continue to real frequency, to obtain

\[ \kappa^{(0)}_{\text{Kubo}}(f, g) = \frac{\beta}{16\pi} \int d\Omega_B(z) \text{Tr} \left[ [h Jh, f](-D'_+) [h Jh, g](D_+ - D_-) \right] \]

\[ - [h Jh, f](D_+ - D_-)[h Jh, g](-D'_-) \],

\[ \kappa^{(1)}_{\text{Kubo}}(f, g) = \frac{\beta \gamma}{8\pi} \int d\Omega_B(z) \text{Tr} \left[ [h Jh, f](-D'_+) [h Jh, g](G_{V\zeta, +} - G_{V\zeta, -}) \right. \]

\[ - [h Jh, f](D_+ - D_-)[h Jh, g](-D'_-) \] + \left. [h Jh, f](-G_{V\zeta, +}'h Jh, g)(D_+ - D_-) \right],

\[ \kappa^{(2)}_{\text{Kubo}}(f, g) = \frac{\beta \gamma^2}{16\pi} \int d\Omega_B(z) \text{Tr} \left[ [h Jh, f](-D'_+) [h Jh, g](S_+ - S_-) \right. \]

\[ - [h Jh, f](D_+ - D_-)[h Jh, g](-S'_-) \] + \left. [h Jh, f](-S'_+) [h Jh, g](D_+ - D_-) \right],

\[ \mu^E(\delta f \cup \delta g) = -\frac{1}{8\pi i} \int d\Omega_B(z) \text{Tr} \left[ \gamma D_+ [h Jh, f] D_+ [h Jh, g] S_+ \right. \]

\[ + G_{V\zeta, +} [h Jh, f] D_+ [h Jh, g] D_+ + \frac{1}{2} G_{V\zeta, +} [h Jh, f] J J [h Jh, g] D_+ \]

\[ - (f \leftrightarrow g) - (+ \rightarrow -) \].

Here \( D_{\pm} = D(i\Omega_n \to z \pm i0) \) and similarly for \( G_{V\zeta} \) and \( S \). Prime means derivative with respect to \( z \).

Next, we should antisymmetrize with respect to \( f, g \), and also transform the Green’s functions into a more convenient form, using the following substitutions

\[ \tilde{h} = iJh \] \[ \tilde{D} = D(iJ)^{-1} \]

\[ \tilde{S} = iJS \]

\[ \tilde{G}_{V\zeta} = iJG_{V\zeta}(iJ)^{-1} \]

We can now get rid of \( J \) and obtain

\[ \kappa_H^{(0)}(f, g) = -\frac{\beta}{32\pi} \int d\Omega_B(z) \text{Tr} \left[ [\tilde{h}^2, f](-\tilde{D}'_+) [\tilde{h}^2, g](-\tilde{D}_-) \right] \]

\[ - [\tilde{h}^2, f](-\tilde{D}_-)[\tilde{h}, g](-\tilde{D}'_-) \] - \( (f \leftrightarrow g) \),

\[ \kappa_H^{(1)}(f, g) = -\frac{\beta \gamma}{16\pi} \int d\Omega_B(z) \text{Tr} \left[ [\tilde{h}^2, f](-\tilde{D}'_+) [\tilde{h}, g](-\tilde{G}_{V\zeta, +} - \tilde{G}_{V\zeta, -}) \right. \]

\[ - [\tilde{h}^2, f](-\tilde{G}_{V\zeta, +})[\tilde{h}, g](-\tilde{G}_{V\zeta, -}) \] + \left. [\tilde{h}, f](-\tilde{G}_{V\zeta, +})[\tilde{h}, g](-\tilde{G}_{V\zeta, -}) \right],

\[ - [\tilde{h}, f](-\tilde{G}_{V\zeta, +})[\tilde{h}, g](-\tilde{D}_-) \] - \( (f \leftrightarrow g) \).
\begin{align*}
\kappa_{H}^{\text{Kubo},(2)} &= -\frac{\beta\gamma^2}{32\pi} \int \text{d}z \text{n}_B(z) \text{Tr} \left[ [\hbar, f](-\hat{D}_+)[\hbar, g](\hat{S}_+ - \hat{S}_-) \right. \\
&\quad - [\hbar, f](\hat{D}_+ - \hat{D}_-)[\hbar, g](\hat{S}_+ - \hat{S}_-) + \left. [\hbar, f](\hat{S}_+ - \hat{S}_-) [\hbar, g](\hat{D}_+ - \hat{D}_-) - (f \leftrightarrow g) \right] \\
&\quad + \hat{G}_{\nu\zeta} [\hbar^2, f] [\hat{D}_+, \hat{D}_+] [\hbar, g] + \frac{1}{2} \hat{G}_{\nu\zeta} [\hbar, f] [\hbar, g] \hat{D}_+ + (f \leftrightarrow g) - (\rightarrow \rightarrow) \right]
\end{align*}

In the above equations, all Green’s functions are written using the interacting Green’s function, which are subject to perturbation expansion in $\gamma$ that we carry out now.

To second order in $\gamma$, we have
\begin{align*}
\hat{D} &= \hat{D}_0 + \gamma^2 \frac{\hat{D}_0 \hat{S}_0 \hat{D}_0}{K_0}, \quad \text{[S83]} \\
\hat{G}_{\nu\zeta} &= \gamma \frac{\hat{S}_0 \hat{D}_0}{G_0}, \quad \text{[S84]} \\
\hat{S} &= \hat{S}_0, \quad \text{[S85]}
\end{align*}
Here $\hat{D}_0$ and $\hat{S}_0$ denote the free Green’s function. All Green’s function appearing below refer to the free Green’s function, and for notational simplicity, we will now suppress the subscript 0.

The full thermal Hall conductance is given by the differential equation with respect to $\gamma$.
\begin{align*}
d\kappa_H(f, g) &= d\kappa_{H}^{\text{Kubo}}(f, g) - 2\beta\mu^E (\delta f \cup \delta g), \quad \text{[S86]}
\end{align*}
and the boundary condition is that $\kappa_A(f, g) = 0$ when $\gamma = 0$. To order $\gamma^2$, we have
\begin{align*}
\kappa_H(f, g) &= \kappa_{H}^{\text{Kubo}}(f, g) - \gamma\beta\mu^E (\delta f \cup \delta g).
\end{align*}

The above expression contains several pieces which are all of order $\gamma^2$, explicitly written below:
\begin{align*}
\kappa_{H}^{\text{Kubo},(0)}(f, g) &= -\frac{\beta\gamma^2}{32\pi} \int \text{d}z \text{n}_B(z) \text{Tr} \left[ [\hbar^2, f](-\hat{D}_+ - \hat{D}_-) [\hbar, g] (\hat{K}_+ - \hat{K}_-) \\
&\quad + [\hbar, f](-\hat{K}_+ - \hat{K}_-) [\hbar^2, g] (\hat{D}_+ - \hat{D}_-) - (f \leftrightarrow g) \right] \\
&\quad + [\hbar, f](-\hat{G}_+ - \hat{G}_-) [\hbar^2, g] (\hat{D}_+ - \hat{D}_-) - (f \leftrightarrow g), \quad \text{[S88]}
\end{align*}
\begin{align*}
\kappa_{H}^{\text{Kubo},(1)} &= -\frac{\beta\gamma^2}{16\pi} \int \text{d}z \text{n}_B(z) \text{Tr} \left[ [\hbar^2, f](-\hat{D}_+ - \hat{D}_-) [\hbar, g] (\hat{G}_+ - \hat{G}_-) \\
&\quad + [\hbar, f](-\hat{G}_+ - \hat{G}_-) [\hbar^2, g] (\hat{D}_+ - \hat{D}_-) - (f \leftrightarrow g), \quad \text{[S89]}
\end{align*}
\begin{align*}
\kappa_{H}^{\text{Kubo},(2)} &= -\frac{\beta\gamma^2}{32\pi} \int \text{d}z \text{n}_B(z) \text{Tr} \left[ [\hbar, f](-\hat{D}_+ - \hat{D}_-) [\hbar, g] (\hat{S}_+ - \hat{S}_-) \\
&\quad + [\hbar, f](-\hat{S}_+ - \hat{S}_-) [\hbar, g] (\hat{D}_+ - \hat{D}_-) - (f \leftrightarrow g). \quad \text{[S90]}
\end{align*}
\[-\beta \gamma \mu^E(\delta f \cup \delta g) = -\frac{\beta \gamma^2}{8\pi} \int dz n_B(z) \text{Tr} \left[ \left( \tilde{G} + [\tilde{h}, f] \tilde{D}_+ [\tilde{h}, g] + \frac{1}{2} \tilde{K}_+ [\tilde{h}, f] [\tilde{h}, g] - (f \leftrightarrow g) \right) - (+ \rightarrow -) \right] \tag{S91}\]

The evaluation of the above integrals are done using Mathematica. The intermediate results are quite complicated so we just describe the algorithm.

The above integrals Eq. Eq. (S88)-Eq. (S91) are written as a trace over the single-particle indices (site index + cartesian index). The trace over site indices can be transformed into a momentum sum, according to

\[\text{Tr} \to L^d \int \frac{d^d k}{(2\pi)^d} \text{tr}.\tag{S92}\]

Here \(\text{tr}\) denote the trace over cartesian indices \((2d \text{ by } 2d)\). \(L\) is the system size and \(d = 3\) is the spatial dimension. The phonon Green's function is given by Eq. (S29) with a \(k\)-dependent \(\tilde{h}\), and the defect Green's function is given by Eq. (S38) with \(k_1 = k_2 = k\). Notice that although momentum does not have to conserve at the defect, the momentum trace naturally sets all momenta in the Green’s functions to be equal. To further simplify, we switch to the band basis where \(\tilde{h}\) and \(\tilde{D}_\pm\) become diagonal. This can be done by diagonalizing the matrix \(\tilde{h}(k) = iJ\tilde{h}(k)\):

\[\tilde{h}(k) = M(k) \mathcal{E}(k) M(k)^{-1}, \tag{S93}\]

where \(\mathcal{E}(k)\) is a diagonal matrix with entries \(\pm c_F k\) and \(\pm c_L k\).

As discussed in the main text, the function \(f(p) = -x(p)/L\) and \(g(p) = -y(p)/L\). In the continuum limit they should be replaced by momentum derivatives, which reads

\[[\tilde{h}, f] = \frac{i}{L} \frac{\partial \tilde{h}(k)}{\partial k_x}, \quad [\tilde{h}, g] = \frac{i}{L} \frac{\partial \tilde{h}(k)}{\partial k_y}, \tag{S94}\]

and similarly for \([\tilde{h}^2, f]\) and \([\tilde{h}^2, g]\). We see that overall the thermal Hall conductance scales with system size as \(L^{d-2}\), as expected, and by dividing out the \(L^{d-2}\) factor we obtain the thermal Hall conductivity.

By conjugating every term in Eq. (S88)-Eq. (S91) by \(M(k)\), we arrive at a form where the phonon Green’s function \(\tilde{D}_\pm\) is diagonal. The energy current vertices \(M(k)^{-1}[\tilde{h}, \cdot] M(k), \ M(k)^{-1}[\tilde{h}^2, \cdot] M(k)\) and the defect Green’s function will contain both diagonal and off-diagonal components. Notice that the energy current vertices have no matrix element between the two degenerate transverse bands.

Next, we compute the \(z\) integral in Eq. (S88)-Eq. (S91). We first use \texttt{Apart} [] in Mathematica to decompose all rational functions in \(z\) into simple fractions. All the \(z\) integrals can be calculated using the formula

\[\int_{-\infty}^{\infty} dz n_B(z) \frac{1}{(z - a)^n} = \frac{1}{(n - 1)!} \theta^n \left[ \frac{i\pi}{\beta a} - \psi^{(0)} \left( \frac{i\beta a}{2\pi} \right) + 2\pi i n_B(a) \theta(\text{Im} a) \right], \tag{S95}\]

where \(\theta\) is the step function and \(\psi^{(0)}\) is the digamma function. The derivative doesn’t act on the step function. Here, the pole of \(n_B(z)\) at \(z = 0\) is resolved with principal value. The formula can be derived using a rectangular integral between \(\text{Im} z = 0\) and \(\text{Im} z = 2\pi i/\beta\). Notice that when \(n = 1\) the integral is logarithmically divergent, and we regulate the integral by ignoring the contribution from the path \(z = -\infty \to z = -\infty + 2\pi i/\beta\). In the actual evaluation, the whole integral is UV convergent, so the result is independent of regularization.
The last step is to evaluate the $k$-integral. We first perform the angular integral of $k$. The integral over the magnitude of $k$ can't be performed analytically, and it is UV divergent. We are interested in the most singular part in the $\Gamma_{ph} \to 0$ limit. According to discussion in the main text, this should come from the side-jump effects and we expect it to scale as $1/\Gamma_{ph}$. This $1/\Gamma_{ph}$ enhancement comes from integrating pairs of retarded and advanced phonon Green's function of the same band over $z$. The integrand can then be classified into three types

1. $1/\Gamma_{ph}$ enhanced resonance: These terms have the $1/\Gamma_{ph}$ prefactor, and have resonant denominators $1/(c_T k - \epsilon \pm i\Gamma_{ph})$ or $1/(c_T k - \epsilon \pm i\Gamma_{ph})$ with $\epsilon > 0$. This is the resonant side-jump effect. This type of integrals can be calculated using the Sokhotski–Plemelj theorem and its derivatives. It turns out that only the $\delta$-function piece of Sokhotski–Plemelj theorem contributes, and the principal value parts cancelled out.

2. $1/\Gamma_{ph}$ enhanced non-resonant terms: These terms have the $1/\Gamma_{ph}$ prefactor, but doesn't have resonance at positive $k$. It can be shown explicitly that such terms are purely imaginary in the $\Gamma_{ph} \to 0$ limit, but it can be checked numerically that the total integrand is real, so these terms don't contribute

3. The rest terms are not enhanced by $1/\Gamma_{ph}$. These terms classified as the intrinsic contribution to thermal Hall conductivity. There is no simple formula to evaluate these terms and some of them are UV divergent. However, because of the absence of $1/\Gamma_{ph}$ factor, we expect these terms are subdominant to the side-jump effects.

Therefore, the resonant side-jump effect dominates the thermal Hall conductivity, and we obtain

$$
\kappa_{H}^{sj} = \frac{1}{N_{sys}} \frac{\alpha R \beta^2 \gamma^2 \Delta m \epsilon_0^3}{12 \pi \Gamma_{ph} (e^{\beta \epsilon_0} + 3) \sinh^2(\beta \Delta/2)}. \tag{S96}
$$

Some remarks:

1. Despite that the full integral is UV divergent, the contribution from the resonant peaks is UV finite, and it vanishes exponentially at low temperature, in agreement with the consistency requirement of thermal Hall conductance in Ref. (1).

2. By attaching a labelling variable to the diagonal parts of the vertex functions, we can show that this result exactly corresponds to the case where one vertex is intra-band and the other one is inter-band. The result is also enhanced by the phonon lifetime by $1/\Gamma_{ph}$. Both features are consistent with the side-jump effects studied in Ref. (2).

3. Again by using labelling variables, we can show that only Eq. (S88) and Eq. (S89) contribute to the final result. In particular the magnetization correction doesn’t contribute. This can be understood as the following: The $1/\Gamma_{ph}$ enhancement essentially arises from a product of retarded and advanced phonon Green’s function $D_+D_-$ of the same band. In Eq. (S90), there is only one phonon Green’s function. In Eq. (S91), the Green’s functions are either all retarded or all advanced. This is an example showing that magnetization correction is unimportant for the extrinsic contributions.

4. The last factor $(c_L^{-1} + c_T^{-1})$ looks unnatural because there are two transverse bands but they only contribute only half the contribution of a longitudinal band. This is an artifact of using the isotropic phonon band structure, as the side-jump coordinate shift between two degenerate transverse bands should vanish due to gauge-invariance (see Sec.7). In a realistic model where the two transverse bands slightly split, we expect the answer should be $(c_L^{-1} + 2c_T^{-1})$. 

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5. Absence of Magnetization Correction in Extrinsic Effects

In this part we try to give an argument of why magnetization correction is unimportant for extrinsic effects. According to the diagrammatic study in Ref. (2), the $1/\Gamma_{ph}$ enhancement of extrinsic contributions (side jump or skew scattering) comes from a product of retarded and advanced phonon Green’s function of the same band $(z - \omega_k + i\Gamma_{ph}/2)^{-1}(z - \omega_k - i\Gamma_{ph}/2)^{-1}$ that are attached to the energy current vertex, which after integrating over $z$ produces a factor of $1/\Gamma_{ph}$.

The magnetization correction, however, can’t produce such a configuration of Green’s functions. According to Eq. Eq. (S68), the correction term is a linear combination of Kubo correlation function, which is the $i\omega_n = 0$ case of a two-point function of bilinear operators, which has the generic form

$$\Pi(i\omega_n) \sim T \sum_{\Omega_n} D_1(i\omega_n + i\Omega_n) D_2(i\Omega_n) P(i\Omega_n, i\omega_n) D_3(i\omega_n + i\Omega_n) D_4(i\Omega_n).$$

[S97]

Here we have only schematically written down the frequency sum and ignored other summations. In the complex $z = i\Omega_n$ plane, the integrand only has branch cut when $\text{Im} z = 0$ or $\text{Im} z = -i\omega_n$. Therefore, when $i\omega_n = 0$, all Green’s functions are evaluated above the cut or below the cut, i.e. they are either all retarded or all advanced, and this is not a configuration for the $1/\Gamma_{ph}$ enhancement.

\section*{Part II}

\section*{Models A and B}

In this part we consider models A and B which have a more complicated structure in phonon-defect coupling. We will also derive a semiclassical expression for the thermal Hall effect.

\section*{6. General Phonon-Defect Coupling}

The calculation of the first model assumes the phonon-defect coupling to be of a special inner product form. In this section we generalize the coupling to accommodate for more complex structure. The coupling between the phonon and the defect system can be written as

$$\delta H = \gamma \sum_q \zeta^K q_B \zeta^K q_o V^\alpha_0,$$

[S98]

where $V^\alpha_0$ is some operator of the defect, the coupling coefficients are encoded in $B$. Here $\gamma$ only serves as a power-counting parameter and will be set to one in the final result. We assume the matrix $B$ is translational invariant in its site indices, and therefore it has a well-defined fourier transform. We also assume $B^K q_0 \alpha$ is quasi-diagonal, meaning that it vanishes when $q$ and $o$ are far apart.

Using the freedom of redefining Hamiltonian density (1), we can distribute all of $\delta H$ to $H_\alpha$, and from this we can compute

$$\delta J^E_{p o} = -\delta J^E_{o p} = \gamma \left( \zeta^T hJ p B V + \zeta^T \phi h J B V \right),$$

[S99]

for $p \neq o$.

The contractions are then

$$f \delta J^E f - g \delta J^E g = \gamma \zeta^T (hJ(fB - gBf) + (hJ B g - g h J B f)) V,$$

[S100]

$$f \delta J^E f - g \delta J^E g = \gamma \zeta^T (hJ(fB - gBf) + (hJ B g - g h J B f)) V.$$

[S101]
To second order in phonon-defect coupling, the phonon Green’s function is now
\[ D = D^{(0)} + D^{(0)} \gamma^2 BSB^T D^{(0)}. \]  

We have also defined the phonon self energy \( \Pi \). Note that in momentum space \( (B^T)(k) = B(-k)^T \).

The crossed Green’s function is
\[ G = \gamma S B^T D. \]

For notational simplicity we have dropped \( V\zeta \) in the subscript. This expression is valid to all orders in \( \gamma \) provided that \( S \) and \( D \) are the full defect Green’s function and phonon Green’s function respectively.

7. Semiclassical Expression for Phonon Thermal Hall Effect

In the computation of model C, we have shown that the side-jump thermal Hall effect comes from diagrams that exactly contains one pair of retarded and advanced phonon Green’s function \( D_+D_- \) which has identical argument, and is therefore enhanced by a factor of \( 1/\Gamma_{ph} \). In this section we take advantage of this to derive a semiclassical expression for the thermal Hall effect. In what follows we set \( \gamma = 1 \).

Only the Kubo part contributes to side jump, and the current-current correlation functions we need are
\[ \Pi^{(0)}_{EE}(f, g; i\omega_n) = 2T \sum_{\Omega_n} \text{Tr} \left[ \left( \frac{hJh}{4} \right) D(i\omega_n + i\Omega_n) \left( \frac{hJh}{4} \right) D(i\Omega_n) \right], \]
\[ \Pi^{(1)}_{EE}(f, g; i\omega_n) = 2T \sum_{\Omega_n} \text{Tr} \left[ \left( \frac{hJh}{4} \right) D(i\omega_n + i\Omega_n) \left( \frac{hJh}{4} \right) \left( \frac{hJh}{4} \right) D(i\Omega_n) \right]. \]

We first compute \( \Pi^{(0)}_{EE} \). Retain only terms with a pair of \( D_+D_- \), we obtain
\[ \kappa^{(0)}_H(f, g) = \frac{\beta}{2\pi} \int dz(-n'_B(z)) \text{Tr} \left[ \left( \frac{hJh}{4} \right) D_+(z) \left( \frac{hJh}{4} \right) D_-(z) \right] - (f \leftrightarrow g). \]

To facilitate evaluation, we use change of variables slightly different from that in model C
\[ D = M \tilde{D} M^{-1}(iJ) \]
\[ \Pi = (iJ)^{-1} M \tilde{\Pi} M^{-1}. \]

Here \( M = M(k) \) is a momentum-dependent matrix that diagonalizes the Hamiltonian
\[ M^{-1}(k)iJh(k)M(k) = \mathcal{E}(k), \]
where \( \mathcal{E}(k) \) is a diagonal matrix in band indices which encodes the phonon dispersion. In this basis the self energy reads
\[ \tilde{\Pi} = M^{-1}iJBSB^TM. \]

Then Eq. Eq. (S106) becomes
\[ \kappa^{(0)}_H(f, g) = \frac{-\beta}{2\pi} \int dz(-n'_B(z)) \text{Tr} \left[ V^{(0)}_f \tilde{D}_+ V^{(0)}_g \tilde{D}_- \right] - (f \leftrightarrow g), \]
and the vertex function is
\[ V_f^{(0)} = \frac{M^{-1}[(ifJh)^2, f]M}{4} = \frac{1}{4} \left( [\mathcal{E}^2, f] + [\mathcal{E}^2, A_f] \right), \]  
where we have separated it into band-diagonal and band-off diagonal parts. The off-diagonal part is given by the connection \( A_f \):
\[ A_f = -M^{-1}[M, f]. \]
We recall that the formula for converting commutator to derivative is \( [H(k), f] = i\partial_k H(k), [H(k), g] = i\partial_k H(k) \).

Now expanding Eq. Eq. (S111) to first order in self energy, we obtain
\[ \kappa_H^{(0)} = \frac{-\beta}{2\pi} \int dz (-n_B'(z)) \text{Tr} \left[ V_f^{(0)} \bar{D}^{(0)}_+ \bar{D}^{(0)}_g V_g^{(0)} \bar{D}^{(0)}_+ + V_f^{(0)} \bar{D}^{(0)}_g V_g^{(0)} \bar{D}^{(0)}_+ \bar{D}^{(0)}_g \right] - (f \leftrightarrow g). \]  
We proceed to pick out the side-jump contribution, using the formula
\[ \bar{D}^{(0),a}(z) \bar{D}^{(0),a}(z) = \frac{2\pi}{\Gamma_a(z)} \delta(z - \mathcal{E}_a), \]
where \( a \) here denotes an eigenstate of the quadratic phonon Hamiltonian \( iJh \) and \( \Gamma_a \) is its decay rate.

We obtain
\[ \kappa_H^{(0)} = \sum_{a,b; \mathcal{E}_a \neq \mathcal{E}_b} \beta n_B'(\mathcal{E}_a) \mathcal{E}_a \mathcal{E}_b \frac{[\mathcal{E}_a, f] \mathcal{E}_b}{4} \left( [\bar{\Pi}^{ab}_+(\mathcal{E}_a) - \bar{\Pi}^{ab}_+(\mathcal{E}_a)] A_g^{ba} + (\bar{\Pi}^{ab}_+(\mathcal{E}_a) - \bar{\Pi}^{ab}_+(\mathcal{E}_a)) A_g^{ab} \right) - (f \leftrightarrow g). \]
Here the summation indices \( a, b \) are general, which include both momentum and band indices. Here we notice that the off-diagonal component of the vertex function is \( V_f^{(0),ab} = A_f^{ab}(\mathcal{E}_a^2 - \mathcal{E}_b^2)/4 \), which vanishes when the two bands are degenerate, and therefore the summation should be restricted to bands with distinct energy.

The above result can be simplified by noting that the two terms in the bracket are actually equal. To show this we need the transpose properties of the connection \( A_f \) and the self energy \( \bar{\Pi} \), which are
\[ A_f^T = -K^{-1} A_f K, \]
\[ \bar{\Pi}^{T}_\pm(z) = -K^{-1} \bar{\Pi}^{T}_\pm(-z) K, \]
where \( K \) is defined in Eq. (S20). Eq. (S117) follows from its definition Eq. (S113) and Eq. (S118) can be derived from the symmetry of the Green’s function \( D^{ab}(\tau) = -T_v (\zeta^a(\tau) \zeta^b(0)) = D^{ba}(-\tau) \) under \( a \leftrightarrow b \). Following the discussion in the section of phonon diagonalization \( A \), we know that the matrix \( K \) only has matrix element \( K_{\bar{a}\bar{b}} = \pm 1 \) between mode \( a \) and mode \( \bar{a} \) of opposite eigenvalue \( \mathcal{E}_a = -\mathcal{E}_a \). We can therefore eliminate \( K \) by changing the summation variables to \( \bar{a}, \bar{b} \) for the second term in the bracket, which flips the sign of \( \mathcal{E} \) in the summand, and the result is equal to the first term.

We proceed by writing out the momentum summation explicitly:
\[ \kappa_H^{(0)} = \sum_{a,b; \mathcal{E}_a \neq \mathcal{E}_b} \frac{d^3k}{(2\pi)^3} \frac{\beta n_B'(\mathcal{E}_a(k)) \mathcal{E}_a(k)}{2\Gamma_a(k)} \left( \mathcal{E}_a(k) A_g^{ba}(k) \mathcal{E}_b(k) + \mathcal{E}_b(k) A_g^{ab}(k) \mathcal{E}_a(k) \right) \frac{1}{2} \left( [\bar{\Pi}^{ab}_+(\mathcal{E}_a(k)) - \bar{\Pi}^{ab}_+(\mathcal{E}_a(k))] \right) - (f \leftrightarrow g). \]
Now the indices \( a, b \) are only over band indices. The commutator \( [\mathcal{E}_a(k), f] \) is equivalent to \( i\partial_{k_a} \mathcal{E}_a(k) \) and the connection \( A_g \) is \( A_g(k) = -iM(k)^{-1} \partial_{k_a} M(k) \).
where we have used the fact that spin Green’s function are evaluated at

Next we evaluate the contribution from $\Pi^{(1)}_{EE}$ which can be decomposed as $\kappa^{(1)}_H = \kappa^{(1a)}_H + \kappa^{(1b)}_H$:

$$
\kappa^{(1a)}_H \equiv \frac{\beta}{2\pi} \int dz (-n_B'(z)) \text{Tr} \left[ \frac{[hJ_h,f]}{4} D_+ \left[ \frac{[h,g] J_B G_- + \frac{[h,f] J_B G_+ + [hJ_h,g]}{4} D_-}{} \right] \right] - (f \leftrightarrow g),
$$

$$
\kappa^{(1b)}_H \equiv \frac{\beta}{2\pi} \int dz (-n_B'(z)) \text{Tr} \left[ \frac{[hJ_h,f]}{4} D_+ h[jB,g] G_- + h[jB,f] G_+ \frac{[hJ_h,g]}{4} D_- \right] - (f \leftrightarrow g).
$$

To make contact of $\kappa^{(1a)}_H$ to $\kappa^{(0)}_H$, we substitute Eq. (S103) into Eq. (S120) and take transpose within the trace:

$$
\kappa^{(1a)}_H = \frac{\beta}{2\pi} \int dz (-n_B'(z)) \text{Tr} \left[ \frac{[hJ_h,f]}{4} D_+ B S_+ \frac{B^T [h,g]}{2} D_- + \frac{B^T [h,f]}{2} D_+ \frac{[hJ_h,g]}{4} D_- B S_- \right] - (f \leftrightarrow g),
$$

where we have used the fact that $D_\pm(z)^T = D_\mp(-z), S_\pm(z)^T = S_\mp(-z), n_B'(z) = n_B'(z)$. Using the expression for phonon self energy, we have

$$
\kappa^{(1a)}_H = \sum_{a,b,\xi \neq \xi_a} \int \frac{d^3k}{(2\pi)^3} \frac{\beta n_B'(\xi_a(k))}{2 \Gamma_a(k)} \xi_a(k) \xi_a(k,f) A_{ab} \frac{\xi_a(k) - \xi_b(k)}{2} (\tilde{\Pi}_{ab}(\xi_a(k)) - \tilde{\Pi}_{ab}^+(\xi_a(k)))
$$

$$
- (f \leftrightarrow g).
$$

The other term $\kappa^{(1b)}_H$ is

$$
\kappa^{(1b)}_H = \sum_a \int \frac{d^3k}{(2\pi)^3} \frac{\beta n_B'(\xi_a(k))}{2 \Gamma_a(k)} \xi_a(k)^2 \xi_a(k,f) (M^{-1}[iJ_B,g](S_- - S_+)) B^T M^a = (f \leftrightarrow g).
$$

The total side-jump thermal Hall effect is therefore

$$
\kappa^{(s)}_H = \kappa^{(0)}_H + \kappa^{(1a)}_H + \kappa^{(1b)}_H.
$$

This result has a very clear semiclassical interpretation. It can be rewritten into a form similar to the solution of a semiclassical Boltzmann equation:

$$
\kappa^{(s)}_H = \frac{1}{2} \sum_a \int \frac{d^3k}{(2\pi)^3} \frac{(-\beta n_B'(\xi_a))}{\Gamma_a(k)} j^{E}_{\text{off-shell}}(f) j^{E}_{\text{side-jump}}(g) - (f \leftrightarrow g).
$$

Here $j^{E}_{\text{off-shell}}$ denotes the energy current of an on-shell phonon, which takes the form

$$
j^{E}_{\text{off-shell}}(f) = -i \xi_a(\xi_a,f).
$$

Converting the commutator to momentum derivative, this is exactly energy times velocity. The other part is the side-jump energy current, which is

$$
\xi_a(\xi_a,f) = (v_{aa}^a(g) + \sum_{b, \xi \neq \xi_a} v_{ab}^a(g)) \xi_a.
$$

and the side-jump velocities are

$$
v_{aj}^{ab}(g) = (M^{-1}[iJ_B,g](-i)(S_- - S_+)) B^T M^a,
$$

$$
v_{aj}^{ab}(g) = A^a_{bj}(-i) (\tilde{\Pi}^{ab}(\xi_a) - \tilde{\Pi}^{ab}_{+}(\xi_a)).
$$

In the above equations, both $M$ and $\xi_a$ are functions of the phonon momentum $k$. The phonon self energy $\tilde{\Pi}$ and spin Green’s function are evaluated at $z = \xi_a$. The expression for $\kappa_H$ in the main text is obtained by converting commutators to derivatives according to Eq. (S94).

Several remarks are in order:
1. Eq. (S126) takes the form as a solution to a semiclassical Boltzmann equation: $-\beta n'_B(E_a)$ is the boson thermal weight, and $1/\Gamma_a$ is the phonon lifetime. Because our phonon band contains both positive and negative energy modes, there is an overall $1/2$ factor in the front. There are two energy currents $j^E_{\text{on-shell}}$ and $j^E_{\text{side-jump}}$. One couples to the temperature gradient and the other one is measured as an observable, and the two configurations are both included via the $f \leftrightarrow g$ antisymmetrization.

2. The first side-jump velocity $v^{a\alpha}_{ij}$ occurs when the phonon-defect coupling $B$ has momentum dependence, which reflects the fact that a momentum-dependent coupling $B$ renormalizes phonon velocity.

3. The second side-jump velocity $v^{b\alpha}_{ij}$ appears for arbitrary phonon-defect coupling. It appears as a product of the coordinate shift $A^{ab}_{g}$ and the scattering rate $(-i)(\Pi^{ab}_+(E_a) - \Pi^{ab}_+(E_a))$. The coordinate shift we have derived is the inter-band berry connection Eq. (S113) which is automatically gauge invariant for $a \neq b$, while the semiclassical result in Ref. (3) is the difference of intra-band berry connections plus the argument of T-matrix to restore gauge invariance.

4. The coordinate shift $A^{ab}_f(k)$ is gauge invariant when $E_a(k) \neq E_b(k)$. The gauge degrees freedom of the diagonalization matrix $M(k)$ is $M(k) \rightarrow M(k)U(k)$ where $[U(k),E(k)] = 0$. This condition requires $U(k)$ to be a block-diagonal matrix with nonzero elements only between degenerate bands. The corresponding change of $A^{ab}_f(k)$ will be $A^{ab}_f(k) \rightarrow (U(k)^{-1}A_f(k)U(k))^\alpha\beta - (U^{-1}(k)[U(k),f])^{\alpha\beta}$ where the commutator is proportional to some momentum derivative. Therefore, the change of $A^{ab}_f(k)$ will also be block-diagonal, meaning the components between non-degenerate bands are non-zero. However, components of $A^{ab}_f(k)$ between degenerate bands are not gauge-invariant, but it has been naturally excluded in the calculation.

5. The inclusion of the phonon-spin coupling into energy current (i.e. including $\Pi^{(1)}_{\text{EE}}$) is crucial for energy conservation. Without this term, the side-jump energy current will look like

$$j^{E,(0)}_{\text{side-jump}}(g) = \sum_{b \neq a} v^{ba}_{ij}(g)\frac{E_b + E_a}{2}.$$ 

The energy transported by the phonon during the jump is wrong.

6. Since one of the phonon in the side jump is off shell, one may wonder whether high energy optical phonons can contribute. The answer is no for the following reason: Assuming the acoustic branches are non topological (zero total Chern number), the Hamiltonian can then be written in a block diagonal form $H = H_{\text{acoustic}} \oplus H_{\text{optical}}$. The coordinate shift $A^{ab}_f(k)$ between two bands is proportional to $M^{-1}(k)\partial_k M(k)$ and $M(k)$ must also take a block diagonal form $M(k) = M_{\text{acoustic}}(k) \oplus M_{\text{optical}}(k)$, implying that $A_f$ between the acoustic and the optical branch is zero.

8. Application to the Models A and B

Now we apply the above formalism to the first two models in the main text. For model A, we have

$$B^{I\alpha}(k) = K_{i\alpha}, \quad [S131]$$

where $i$ means momentum components.

In model B the continuum limit of $B$ should be

$$B^{I\alpha}(k) = -ik^j K_{i\alpha}, \quad [S132]$$
where now \( i \) denotes displacement components.

In both models, the spin-spin correlation function is

\[
S_{\pm}^{x\beta}(z) = 2 \tanh \left( \frac{\beta \Delta}{2} \right) \left[ \begin{array}{ccc}
\frac{\Delta}{z_\pm^2 - \Delta^2} & \frac{i \Delta}{z_\pm^2 - \Delta^2} & 0 \\
\frac{i \Delta}{z_\pm^2 - \Delta^2} & \frac{i \Delta}{z_\pm^2 - \Delta^2} & 0 \\
0 & 0 & 0
\end{array} \right],
\]  

[S133]

where \( z_\pm = z \pm i 0 \).

The integrals in Eq. (S119), Eq. (S123), Eq. (S124) are easy to evaluate since they are all proportional to a delta function at resonance. We obtain for model A

\[
\kappa^x_{H} = \frac{1}{N_{\text{sys}}} \frac{\beta^2 \Delta^4 m (c_L^{-1} + c_T^{-1}) \text{csch}(\beta \Delta)}{6 \pi \Gamma_{\text{ph}}} (K_{x1} K_{y2} - K_{x2} K_{y1}),
\]  

[S134]

The last factor of Eq. (S134) can be understood from symmetry considerations: The thermal Hall conductivity \( \kappa_{xy} \) is invariant under spatial SO(2)\( z \) along the \( z \) axis, and it is odd under spatial reflections \( R_x, R_y \). These two conditions require a quadratic combination of \( K_{\alpha} \) with exactly one \( x \) and one \( y \) index, and is invariant under SO(2)\( z \), yielding \( K_{xy} K_{\alpha} + K_{xy} K_{\beta} \) or \( K_{xy} K_{\alpha} - K_{xy} K_{\beta} \). Next, notice that the choice of the spin frame has a redundancy because we only fix the ‘3’ direction to align with the polarization of the defect, and then the remaining ‘1’ and ‘2’ axes can rotate freely around the ‘3’ axis. Physical observables should be independent of this free rotating angle, and only the coupling combination \( K_{x1} K_{y2} + K_{x2} K_{y1} \) satisfies the requirement.

For model B, we obtain

\[
\kappa^x_{H} = \frac{1}{N_{\text{sys}}} \frac{\beta^2 \Delta^4 \text{csch}(\beta \Delta)}{30 \pi \Gamma_{\text{ph}} m} (c_L^{-3} K_L + c_T^{-3} K_T),
\]  

[S135]

where

\[
K_L = \frac{5}{2} \left[ (K_{xy} + K_{yx}) (K_{xx1} - K_{yy1}) - (K_{xy} + K_{yx}) (K_{xx2} - K_{yy2}) \right] + K_{xx1} K_{zy2} - K_{xx2} K_{zy1} + K_{xx1} K_{zy2} - K_{xx2} K_{zy1} - K_{xz1} K_{zy2} + K_{xz1} K_{zy2},
\]  

[S136]

\[
K_T = - \frac{5}{2} \left[ (K_{xy} + K_{yx}) (K_{xx1} + K_{yy1}) - (K_{xy} + K_{yx}) (K_{xx1} + K_{yy1}) \right] + K_{xx1} K_{zy2} - K_{xx2} K_{zy1} + 4 K_{xx1} K_{yx2} - 4 K_{xx2} K_{yx1} + K_{xz1} (K_{yx2} - K_{yx1}) \right) + K_{xz2} (K_{yx1} - K_{yx2}).
\]  

[S137]

The above result for model B has several features: First, same as model A, the spin-spin correlation function requires the coupling constants appear in antisymmetric combinations under \( 1 \leftrightarrow 2 \), and the 3 component is absent. Second, the invariance of \( \kappa_{xy} \) under SO(2)\( z \) and its covariance under \( R_x, R_y \) require the couplings form SO(2)\( z \) invariant combinations with odd number of \( x \) and \( y \) indices. Each line of Eq. (S136) and Eq. (S137) satisfies the above conditions.
9. Model B from a lattice antiferromagnet

Let us consider a coupled-ladder Heisenberg antiferromagnet in a transverse field (see Fig. (S1)), thereby leading to canting of the moments. There is also a vacancy leading to a spin defect. We have the following Hamiltonian:

$$H = \sum_{\langle pq \rangle \in \mathcal{D}} J_{pq} \vec{S}_p \cdot \vec{S}_q + \sum_{\langle pq \rangle \notin \mathcal{D}} K^\alpha_{pq} S^\alpha_p S^\alpha_q + h \sum_p S^3_p. \quad [S138]$$

Here $\mathcal{D}$ denotes a dimer unit cell (see Fig. (S1)). The real-space cartesian coordinates are $x, y, z$, while the spin-space indices are labelled as $1, 2, 3$. For the inter-dimer couplings we have considered an anisotropic exchange both in the spin space as well as the real space. The exchange interaction along the $\hat{x}$-direction is $K^\alpha$, while that in the $\hat{y}$-direction is $K^{\beta}$. We are interested in spin-phonon interaction. Such an interaction has been considered earlier in the context of magnetization plateaus in quantum magnets (4). Here our interest is to study the effect of such interactions on thermal-Hall conductivity. Spin-phonon coupling arises naturally if we consider that the spin-exchange interactions depend on the bond distances, $J_{pq} \equiv J(|\vec{R}_p - \vec{R}_q|)$ and $K_{pq} \equiv K(|\vec{R}_p - \vec{R}_q|)$. Let $\vec{u}_p$ be the small displacement of the lattice site at $\vec{R}_p$ from its equilibrium position. We can then expand the coupling constants in terms of $\vec{u}_p$ to linear order,

$$J_{pq} = J(|\vec{R}_p - \vec{R}_q|) + \frac{dJ}{d\vec{R}} \hat{x} \cdot (\vec{u}_p - \vec{u}_q) \equiv J (1 + \alpha \hat{x} \cdot (\vec{u}_p - \vec{u}_q)), \quad [S139]$$

$$K^\alpha_{pq} = K^\alpha (|\vec{R}_p - \vec{R}_q|) + \frac{dK^\alpha}{d\vec{R}} \hat{\epsilon}_{pq} \cdot (\vec{u}_p - \vec{u}_q) \equiv K^\alpha (1 + \beta^\alpha \hat{\epsilon}_{pq} \cdot (\vec{u}_p - \vec{u}_q)), \quad [S140]$$

$$K^{\beta \alpha}_{pq} = K^{\beta \alpha} (|\vec{R}_p - \vec{R}_q|) + \frac{dK^{\beta \alpha}}{d\vec{R}} \hat{\epsilon}_{pq} \cdot (\vec{u}_p - \vec{u}_q) \equiv K^{\beta \alpha} (1 + \beta^{\beta \alpha} \hat{\epsilon}_{pq} \cdot (\vec{u}_p - \vec{u}_q)). \quad [S141]$$

We will label the defect site by the index $o$. Using the notation, $u^i_o - u^i_{o \pm \hat{z}} = \pm \partial_i u^j$, with $i, j = x, y, z$, the defect spin Hamiltonian is

$$H_o = \sum_{\alpha = 1, 2, 3} \left[ K^{\alpha \alpha} \langle S^\alpha_o \rangle S^\alpha_o + K^\alpha \left( \langle S^\alpha_{o+y} \rangle + \langle S^\alpha_{o-y} \rangle \right) S^\alpha_o \right] + h S^3_o$$

$$+ K^\alpha \beta^\alpha \langle S^1_{o+x} \rangle \partial_x u^x S^1_o + K^\alpha \beta^\alpha \langle S^2_{o+x} \rangle \partial_x u^x S^2_o + K^\alpha \beta^\alpha \langle S^3_{o+x} \rangle \partial_x u^x S^3_o$$

$$+ K^\alpha \beta^\alpha \langle \langle S^1_{o+y} \rangle + \langle S^1_{o-y} \rangle \rangle \partial_y u^y S^1_o + K^\alpha \beta^\alpha \langle \langle S^2_{o+y} \rangle + \langle S^2_{o-y} \rangle \rangle \partial_y u^y S^2_o$$

$$+ K^\alpha \beta^\alpha \langle \langle S^3_{o+y} \rangle + \langle S^3_{o-y} \rangle \rangle \partial_y u^y S^3_o. \quad [S142]$$

We identify the coefficient of the term $\partial_i u^j S^\alpha_o$ by $K_{ij\alpha}$, with $ij = x, y, z$ and $\alpha = 1, 2, 3$. Thus we have,

$$K_{xx1} = K^\alpha \beta^\alpha \langle S^1_{o+y} \rangle, \quad K_{xx2} = K^\alpha \beta^\alpha \langle S^2_{o+y} \rangle, \quad K_{xx3} = K^\alpha \beta^\alpha \langle S^3_{o+y} \rangle$$

$$K_{yy1} = K^\alpha \beta^\alpha \langle \langle S^1_{o+y} \rangle + \langle S^1_{o-y} \rangle \rangle, \quad K_{yy2} = K^\alpha \beta^\alpha \langle \langle S^2_{o+y} \rangle + \langle S^2_{o-y} \rangle \rangle, \quad K_{yy3} = K^\alpha \beta^\alpha \langle \langle S^3_{o+y} \rangle + \langle S^3_{o-y} \rangle \rangle. \quad [S143]$$
We therefore have the following additional terms in the defect-spin Hamiltonian:

\[ K_{o,o+x+y}^{\alpha} = K_{o}^{\alpha} \left[ 1 + \beta K \right] \left( \hat{u}_o - \hat{u}_{o+x+y} \right), \]

\[ K_{o,o-x-y}^{\alpha} = K_{o}^{\alpha} \left[ 1 + \beta K \right] \left( \hat{u}_o - \hat{u}_{o-x-y} \right), \]

\[ K_{o,o-(x+y)}^{\alpha} = K_{o}^{\alpha} \left[ 1 - \beta K \right] \left( \hat{u}_o - \hat{u}_{o-(x+y)} \right), \]

\[ K_{o,o+x-y}^{\alpha} = K_{o}^{\alpha} \left[ 1 + \beta K \right] \left( \hat{u}_o - \hat{u}_{o+x-y} \right) \].

We therefore have the following additional terms in the defect-spin Hamiltonian:

\[ H_{o,2n} = \sum_{\alpha=1,2,3} K_{o}^{\alpha} P_{o}^{\alpha} S_{o}^{\alpha} + \sum_{\alpha=1,2,3} K_{o}^{\alpha} \beta K^{\alpha} P_{o}^{\alpha} (\partial_x u^x + \partial_y u^y) S_{o}^{\alpha} + \sum_{\alpha=1,2,3} K_{o}^{\alpha} \beta K^{\alpha} M_{\alpha} (\partial_x u^y + \partial_y u^x) S_{o}^{\alpha}, \]

where

\[ P_{o}^{\alpha} = \sum_{i=x,y,j=x,y} (S_{o+1}^{\alpha}), \quad M_{\alpha} = \sum_{j=\pm 1} (S_{o+3}^{\alpha}) + \sum_{\eta=\pm 1} (S_{o+\eta}^{\alpha}). \]

In terms of the convention introduced above we have the following couplings:

\[ K_{xx1} = K_{yy1} = K_{o}^{\alpha} \beta K^{\alpha} P_{1}, \quad K_{xx2} = K_{yy2} = K_{o}^{\alpha} \beta K^{\alpha} P_{2}, \quad K_{xx3} = K_{yy3} = K_{o}^{\alpha} \beta K^{\alpha} P_{3} \]

\[ K_{xy1} = K_{yx1} = K_{o}^{\alpha} \beta K^{\alpha} M_{1}, \quad K_{xy2} = K_{yx2} = K_{o}^{\alpha} \beta K^{\alpha} M_{2}, \quad K_{xy3} = K_{yx3} = K_{o}^{\alpha} \beta K^{\alpha} M_{3}. \]

The thermal-Hall conductivity is proportional to terms like \((K_{xx\alpha} - K_{yy\alpha})(K_{yx\beta} + K_{yx\beta})\) and \((K_{xx\alpha} + K_{yy\alpha})(K_{yx\beta} - K_{yx\beta})\). If we consider only nearest neighbors then we can not generate terms like \(K_{xy\alpha}\) etc. Hence the thermal-Hall conductivity vanishes trivially for any spin ordering. Whereas if we consider only second nearest neighbors we always have \(K_{xx\alpha} = K_{yy\alpha}\) as well as \(K_{xy\alpha} = K_{yx\alpha}\). Thus, there is no thermal-Hall in this case as well, irrespective of the spin ordering. However, if we have both first neighbor and the second neighbor interactions then

\[ K_{xx1} = K_{o}^{\alpha} \beta K^{\alpha} \langle S_{o+1}^{\alpha} \rangle + K_{o}^{\alpha} \beta K^{\alpha} P_{1}, \quad K_{xx2} = K_{o}^{\alpha} \beta K^{\alpha} \langle S_{o+2}^{\alpha} \rangle + K_{o}^{\alpha} \beta K^{\alpha} P_{2}, \]

\[ K_{xx3} = K_{o}^{\alpha} \beta K^{\alpha} \langle S_{o+3}^{\alpha} \rangle + K_{o}^{\alpha} \beta K^{\alpha} P_{3} \]

\[ K_{yy1} = K_{o}^{\alpha} \beta K^{\alpha} \langle S_{o+1}^{\alpha} \rangle + K_{o}^{\alpha} \beta K^{\alpha} P_{1}, \quad K_{yy2} = K_{o}^{\alpha} \beta K^{\alpha} \langle S_{o+2}^{\alpha} \rangle + K_{o}^{\alpha} \beta K^{\alpha} P_{2}, \]

\[ K_{yy3} = K_{o}^{\alpha} \beta K^{\alpha} \langle S_{o+3}^{\alpha} \rangle + K_{o}^{\alpha} \beta K^{\alpha} P_{3} \]

\[ K_{xy1} = K_{o}^{\alpha} \beta K^{\alpha} M_{1}, \quad K_{xy2} = K_{o}^{\alpha} \beta K^{\alpha} M_{2}, \quad K_{xy3} = K_{o}^{\alpha} \beta K^{\alpha} M_{3}. \]

In this case, for a non-trivial spin ordering we may have a non-zero thermal-Hall conductivity. In particular, for a spin-glass order we may generically obtain a non-zero thermal-Hall. Additionally, this will most likely be independent
Fig. S1. Solid lines, i.e., in the notation of the Hamiltonian in Eq. (S138) those bonds connecting sites within a $D$ have interaction $J_{pq}$, while dashed lines have interaction $K_{pq}$. Horizontal direction is $\hat{x}$ and vertical is $\hat{y}$. The inter-dimer interactions are different along the $\hat{x}$ and $\hat{y}$ bonds. These are $K'$ and $K$ respectively.

of the field direction - as soon as the defect is polarized by the field in it’s direction there should be a non-zero signal. Furthermore, this may also be a possible mechanism for an anomalous thermal-Hall effect.

We may also have a thermal-Hall effect in the case when the spin order is coplanar in the absence of an external magnetic field, provided the above conditions are satisfied. In this case, suppose the spins are coplanar in the 1 – 3 plane then an external field in the 2 direction will lead to a non-zero spin component in the 2 direction that is proportional to the field. Thus, this will lead to a thermal-Hall conductivity that is proportional the applied magnetic field.

B. Presence of spin-orbit coupling. Let us now consider spin-orbit coupling leading to a DM interaction. Such a term is another route to generate spin-phonon interaction. Recently, spin-phonon interaction mediated by spin-orbit coupling was reported in certain transition metal oxides (5), and the influence of such a term on thermal-Hall has been recently investigated in Ref. (6). We will consider out-of-plane mirror symmetry breaking. This results in the following term,

$$H_{DM} = \sum_{(pq)} D_{pq} \cdot (\hat{s}_p \times \hat{s}_q),$$  \[S152\]

where $D_{pq} = D\hat{R}_{pq} \times \hat{z}$ is in the $x-y$ plane, with $\hat{R}_{pq}$ being the vector connecting the sites $p$ and $q$ and $\hat{R}_{pq} = \hat{R}_{pq}/|\hat{R}_{pq}|$. We will restrict ourselves to nearest neighbors only. Let us denote the equilibrium lattice positions by $\hat{R}_{pq}$, thus $\hat{R}_{pq}^0$ is the equilibrium value of vector connecting different sites. We will denote the displacement away from these equilibrium positions by $\hat{u}_p$. Let us first expand the DM term,

$$D(\hat{R}_{pq} \times \hat{z}) \cdot (\hat{s}_p \times \hat{s}_q) = D \left[ \hat{R}_{pq} \cdot (\hat{s}_p \times \hat{s}_q) - (\hat{z} \cdot \hat{s}_p)(\hat{R}_{pq} \cdot \hat{s}_q) \right]$$  \[S153\]

Let us denote the defect site by index $o$, then the nearest neighbors are at $o + \hat{x}$, $o + \hat{y}$ and $o - \hat{y}$. Now the spin-space and real-space are not independent. The spin-space directions 1, 2, 3 now align along $x, y, z$ respectively. So, at the
mean-field level the DM term contribution at the defect site is

\[ H_{\alpha,DM} = \sum_{i=x,y} D \hat{R}_{o,o+i} \cdot \left[ \hat{S}_\alpha \langle S^3_{o+i} \rangle - S^3_o \langle \hat{S}^3_o \rangle \right] \]

\[ = \sum_{i=x,y} \frac{D}{\hat{R}_{o,o+i}} \left( \hat{R}_{o,o+i} + \hat{u}_o - \hat{u}_{o+i} \right) \cdot \left[ \hat{S}_\alpha \langle S^3_{o+i} \rangle - S^3_o \langle \hat{S}^3_o \rangle \right]. \]

The DM coupling \( D \) is a function of the bond distances and direction. We can expand it as follows:

\[ \frac{D}{\hat{R}_{o,o+i}} = \frac{D}{\hat{R}_{o,o+i}} \left( 1 - \frac{\partial D}{\partial R} \frac{1}{D/R} \right) \frac{D}{\hat{R}_{o,o+i}} \left( \hat{R}_{o,o+i} \cdot (\hat{u}_o - \hat{u}_{o+i}) \right), \]

\[ \equiv \frac{D}{\hat{R}_{o,o+i}} \left( 1 - \frac{\gamma}{\hat{R}_{o,o+i}} \hat{R}_{o,o+i} \cdot (\hat{u}_o - \hat{u}_{o+i}) \right). \]

where we used the notation, \( R \equiv |\hat{R}|. \) We will substitute this in the \( H_{\alpha,DM} \) and collect all terms to linear order in \( u. \) We therefore have

\[ H_{\alpha,DM} = \sum_{i=x,y} \frac{D}{\hat{R}_{o,o+i}} \left[ (\hat{u}_o - \hat{u}_{o+i}) \cdot \left[ \hat{S}_\alpha \langle S^3_{o+i} \rangle - S^3_o \langle \hat{S}^3_o \rangle \right] \right] \]

\[ - \gamma \left[ \hat{R}_{o,o+i} \cdot (\hat{u}_o - \hat{u}_{o+i}) \right] \hat{R}_{o,o+i} \cdot \left[ \hat{S}_\alpha \langle S^3_{o+i} \rangle - S^3_o \langle \hat{S}^3_o \rangle \right]. \]

Thus we have,

\[ H_{\alpha,DM} = \frac{D}{\hat{R}^3} \left[ (u_o^x - u_{o+x}^x)(\langle S^3_{o+x} \rangle S^1_o - S^3_o \langle S^1_{o+x} \rangle) + (u_o^y - u_{o+y}^y)(\langle S^3_{o+y} \rangle S^2_o - S^3_o \langle S^2_{o+y} \rangle) \right] \]

\[ + (u_o^z - u_{o+z}^z)(\langle S^3_{o+z} \rangle S^3_o - S^3_o \langle S^3_{o+z} \rangle) \]

\[ - \gamma \frac{D}{\hat{R}^3} \left[ (u_o^x - u_{o+x}^x)(\langle S^3_{o+x} \rangle S^1_o - S^3_o \langle S^1_{o+x} \rangle) \right] \]

\[ + (u_o^y - u_{o+y}^y)(\langle S^3_{o+y} \rangle S^2_o - S^3_o \langle S^2_{o+y} \rangle) \]

\[ + (u_o^z - u_{o+z}^z)(\langle S^3_{o+z} \rangle S^3_o - S^3_o \langle S^3_{o+z} \rangle) \].

where we used the fact that \( \hat{R}_{o,o-x} = \hat{x}, \hat{R}_{o,o+y} = \pm \hat{y}, \) with the lattice constant being set to unity, \( a = 1. \) This also means \( R^3 = 1. \)

In the continuum limit, \( u_o^i - u_{o+i}^i = \pm \partial_i u^i, \) with \( i, j = x, y, z. \) Using this notation we have

\[ H_{\alpha,DM} = D \left[ \partial_x u^x S^1_o \langle S^3_{o+x} \rangle (1 - \gamma) - \partial_x u^x S^3_o \langle S^1_{o+x} \rangle (1 - \gamma) \right] \]

\[ + \partial_y u^y S^2_o \langle S^3_{o+y} \rangle - \partial_y u^y S^3_o \langle S^2_{o+y} \rangle \]

\[ + \partial_y u^y S^2_o \langle S^3_{o+y} \rangle - \partial_y u^y S^3_o \langle S^2_{o+y} \rangle \]

\[ + \partial_y u^y S^2_o \langle S^3_{o+y} \rangle - \partial_y u^y S^3_o \langle S^2_{o+y} \rangle \].
Further we identify the coefficient of the term $\partial_i u^j S^\alpha_o$ by $K_{ij\alpha}$. So from the above Hamiltonian it is clear that $K_{xx1} = D(1 - \gamma)\langle S^3_{o+\hat{z}} \rangle$, $K_{xx3} = -D(1 - \gamma)\langle S^3_{o+\hat{x}} \rangle$, $K_{xy2} = D\langle S^3_{o+\hat{y}} \rangle$, and so on. As a simple case, if we consider an in-plane Neel ordering with canting in $\hat{z}$ direction then $\langle \vec{S}_o + \hat{z} \rangle = \langle \vec{S}_{o-\hat{z}} \rangle$, then the last two lines in Eq. (S159) vanish. Even in this simple case, the thermal-Hall conductivity is non-vanishing. This may also be a possible mechanism for anomalous thermal-Hall effect.

C. Spin-Orbit Coupling or Non-coplanar Order. In this section, we argue for the necessity of spin-orbit coupling or non-coplanar spin order in model B.

Suppose there is no spin-orbit coupling, the microscopic Hamiltonian for the defect must be SU(2) invariant in the absence of external magnetic field, which can be written as

$$H_{micro} = \sum_p J_{op} \vec{S}_o \cdot \vec{S}_p.$$  \[S160\]

Here the defect sits at site $o$ and the summation is over neighboring lattice sites $p$. Introducing phonons by modifying the exchange interaction, and assume lattice translation symmetry is preserved, we have

$$H_{micro+ph} = \sum_p J^p_{op} \partial_i u^j_{op} \vec{S}_o \cdot \vec{S}_p.$$  \[S161\]

In the mean-field theory, we can replace treat neighboring spins $\vec{S}_p$ as frozen and replace them by the average $\langle \vec{S}_p \rangle$, so we have

$$H_{def} = \vec{S}_o \cdot \sum_p J_{op} \langle \vec{S}_p \rangle,$$  \[S162\]

and

$$H_{ph-def} = \partial_i u^j_{op} \vec{S}_o \cdot \sum_p J^j_{op} \langle \vec{S}_p \rangle.$$  \[S163\]

The information we learn from Eq. (S135) is that we need one coupling to polarize the defect spin, and two other couplings to couple the remaining two perpendicular components to phonons. From Eq. (S162) and Eq. (S163), all these couplings involve some linear combinations of the neighboring spin orders. When the spin order is collinear, we can always choose a frame (this is only allowed without SOC) to make the couplings align in one direction zero, and therefore the thermal Hall effect vanishes. Non-coplanar spin order is a sufficient condition for nonzero thermal Hall effect as there is no frame to make couplings to all three spin directions vanish. There is no definite answer for the case of coplanar magnetic order as it depends on the lattice configuration.

In summary, non-coplanar spin order or spin-orbit coupling are sufficient to give rise to a thermal Hall effect.

10. Order-of-Magnitude Estimate for Model B

In this part we present an order-of-magnitude estimate of the ratio $|\kappa_H/\kappa_{xx}|$ within model B.

Assuming that there are $N_i$ defects in the system, our result for model $B$ reads

$$\kappa^{sj}_H = \frac{N_i}{N_{sys}} \frac{\beta^2 \Delta^4 \text{csch}(\beta \Delta)}{30 \pi \Gamma_{ph} m} \left( c_L^{-3} K_L + c_T^{-3} K_T \right).$$  \[S164\]

By dimensional analysis, $K_{ij\alpha}$ has the dimension of energy. Microscopically, it comes from expanding the exchange coupling $J(a)$ as a function of inter-atomic distance $a$: $K_{ij\alpha} \sim a \partial_a J(a)$. Assuming, $\partial_a J(a) \approx J(a)/a$, we conclude that $K_{ij\alpha} \sim J(a)$. Notice that the local splitting the spin defect also comes from exchange, we therefore assume $K_{ij\alpha} \sim \Delta$. 


To have a linear-in-field thermal Hall effect, we consider a scenario where coplanar spin-order at zero field is cantled by external field. We choose the spin frame such that when external field \( B = 0 \), the couplings are such that \( K_{ij1} \sim \Delta, \ K_{ij2} = 0 \). Due to canting of the spins, we would expect \( K_{ij2} \sim \Delta \theta_B \), with the canting angle \( \theta_B \sim \Delta_B/\Delta \ll 1 \). Here \( \Delta_B \approx 2\mu_B B \) is the splitting due to external magnetic field. The quadratic combinations of couplings therefore scales as \( K_L, K_T \sim \Delta \Delta_B \). So the thermal Hall effect scales as

\[
\kappa_{ij} = \frac{N_i}{N_{sys}} \frac{\Delta^3 \Delta_B}{T^2 \sinh (\frac{\Delta}{k_B T})} \frac{A_H}{m \Gamma_{ph} c^3 k_B \hbar^3}.
\]

Here \( A_H \) is a numerical coefficient depending on the detailed expressions of \( K_L \) and \( K_T \), \( c \) is some averaged sound velocity and we have restored \( k_B \) and \( \hbar \).

We compare this with the simple kinetic model for longitudinal thermal conductivity

\[
\kappa_{xx} \approx \frac{1}{3} \frac{c^2}{\Gamma_{ph}} C_V,
\]

where the heat capacity \( C_V \) follows the Debye model

\[
C_V = \frac{12\pi^4}{5} \left( \frac{T}{T_D} \right)^3 k_B \rho \frac{\rho}{m}.
\]

Here \( \rho \) is the mass density and \( m \) is the ion mass and \( T_D \) is the Debye temperature.

The ratio is therefore

\[
\frac{\kappa_H}{\kappa_{xx}} = \frac{5\Delta_B k_B^3 T_D^3}{4\pi^4 c^2 \rho \hbar^3} \frac{A_H}{N_{sys}} \frac{\Delta}{k_B T} \Phi \left( \frac{\Delta}{k_B T} \right), \quad \Phi(x) = \frac{x^5}{\sinh(x)}.
\]

Plugging in values of \( \rho = 6000 \text{kg/m}^3, \ c = 5000 \text{m/s}, \ T_D = 400 \text{K}, \ \Delta_B = 2\mu_B B \) where \( B = 15 \text{T} \), we have

\[
\frac{\kappa_H}{\kappa_{xx}} = 2.7 \times 10^{-5} A_H \frac{N_i}{N_{sys}} \Phi \left( \frac{\Delta}{k_B T} \right).
\]

Remarkably, the maximum of this function is independent of value of \( \Delta \), which is also a measure of the phonon-spin coupling. The function \( \Phi \) is peaked at \( k_B T \approx 0.2\Delta \), where we have

\[
\frac{\kappa_H}{\kappa_{xx}} = 1.2 \times 10^{-3} A_H \frac{N_i}{N_{sys}}.
\]

Experimentally, the peak occurs at around 20K, and therefore \( \Delta \) is about 100K.

If the thermal Hall effect in cuprate is due to phonons scattering on spin glass, essentially every spin participates in phonon scattering and we can set \( N_i/N_{sys} = 1 \). Then the ratio is indeed close to the experiment, provided that \( A_H \) is around order one.

**Part III**

**Intrinsic contribution in Quadratic System**

**11. Berry Curvature Formula for Intrinsic Contribution**

To demonstrate the lattice formalism, we show that it agree with the Berry curvature formula for phonon Hall effect derived in Ref. (7). We assume there is only a quadratic phonon system with no dissipation \( \Gamma_{ph} = 0 \), and there is no defect present.
A. Kubo contribution to Thermal Hall Conductance. The Kubo contribution is the same as Eq. (S71), we reproduce it here without antisymmetrizing $f, g$:

$$\kappa_{xy}^{\text{Kubo}}(f, g) = \frac{\beta}{16\pi} \int \, dz n_B(z) \text{Tr} \left[ \left\{ [hJh, f] \right\} (D_+ - D_-) \right]$$

[B171]

$\kappa$ the same algebra that lead to (F23) in Ref. (1) we conclude that times (F18) and (F19) of Ref. (C. Berry Curvature formula.

B. Magnetization Correction. We now consider arbitrary variation of the quadratic Hamiltonian. The expression for magnetization correction is again given by

$$\mu^E(\delta f \cup \delta g) = -\frac{\beta}{4} \left[ 2 \left\{ \langle dH(g); J^E(\delta f) \rangle \right\} - 2 \left\{ \langle dH(f); J^E(\delta g) \rangle \right\} + \langle dH(fJ^Eg - gJ^Ef) \rangle \right] .$$

[S172]

where

$$dH(f) = \sum_p f_p dH_p = \frac{1}{4} \zeta (f dh + dh f) \zeta,$$

[S173]

$$dH = \sum_p dH_p = \frac{1}{2} \zeta dh \zeta.$$  

[S174]

The formula we need is

$$-\beta \left\langle \langle \zeta A \zeta; \zeta B \zeta \rangle \right\rangle$$

$$= -2 \int \frac{dz}{2\pi i} n_B(z) \text{Tr} \left[ AD_+B(D_+ - D_-) + A(D_+ - D_-)BD_- \right] .$$

[S175]

We obtain

$$\mu^E(\delta f \cup \delta g) = \frac{-1}{32\pi i} \int dz n_B(z) \text{Tr} \left[ D_+ dhD_+^{-1}([[hJh, f], [Jh, g]]) + [[hJh, g]D_+J_+^{-1}Jh, f] - [Jh, g]D_+J_+^{-1}[(hJh)^2, f] + [Jh, f]D_+J_+^{-1}[(hJh)^2, g]) - (D_+ \to D_-) \right] .$$

[S176]

C. Berry Curvature formula. We now follow Ref. (1) choose a scaling variation $dh = h$ which will yield derivative of $\kappa_{xy}$ with respect to temperature. By inspection, the algebraic form of Eq. (S171) and Eq. (S176) are exactly 1/2 times (F18) and (F19) of Ref. (1), given that we substitute $G_{\pm} \to D_{\pm}(iJ)^{-1}$, $h \to iJh$, $f \to n_B$. Therefore, following the same algebra that lead to (F23) in Ref. (1) we conclude that

$$\frac{d}{dT} \left( \frac{\kappa_{xy}(f, g)}{T} \right) = -\frac{i}{4\pi T^3} \int_{-\infty}^{\infty} dz n'_B(z) \text{Tr} \left[ [hJh, f]D_+J_+^{-1}D_+[hJh, g])z^3(D_+ + D_-) - [hJh, g]D_+J_+^{-1}D_+[hJh, f])z^3(D_+ - D_-) \right]$$

[S177]

$$= \frac{1}{4\pi T^3} \int_{-\infty}^{\infty} dz n'_B(z) \text{Tr} \left[ iJh, f \right] (-iD_+J_+^{-1}[iJh, g])z^3(D_+ - D_-)(iJ)^{-1}$$

$$- [iJh, g](iD_+J_+^{-1})^2[iJh, f])z^3(D_+ - D_-)(iJ)^{-1} .$$

We can now evaluate Eq. (S177) in the continuum limit. We set $f = -x/L$ (the average of $\theta$ functions) and $g = -y/L$. In the continuum limit we therefore have

$$[iJh, f] = \frac{i}{L} \frac{\partial iJh(k)}{\partial k_x} , \quad [iJh, g] = \frac{i}{L} \frac{\partial iJh(k)}{\partial k_y} .$$  

[S178]

Switching to the basis where $iJh$ is diagonal, we have

$$iJh(k) = M(k)E(k)M(k)^{-1}.$$  

[S179]
The Green’s functions are

\[
D_{\pm}(z,k)(iJ)^{-1} = \frac{1}{z \pm i0 - iJh(k)} = M(k)\frac{1}{z \pm i0 - \mathcal{E}(k)}M(k)^{-1}.
\]  

[S180]

The trace factorizes into momentum sum and band trace:

\[
\text{Tr} \ X = L^d \int \frac{d^dk}{(2\pi)^d} \sum_i X_{ii}(k).
\]  

[S181]

The thermal conductivity is therefore

\[
\frac{d(\kappa_{xy}/T)}{dT} = \frac{1}{2T^3} \int \frac{d^dk}{(2\pi)^d} \sum_i n_i'(\mathcal{E}_{ik})\mathcal{E}_{ik}^3\Omega_{z}^\mathcal{E}_{ik}.
\]  

[S182]

Here the sum is over both positive and negative energy modes, both of which contribute equally.

The Berry curvature is defined as

\[
\Omega_{z}^\mathcal{E}_{ik} = -i[A_x, A_y]_{ii},
\]  

[S183]

where the connection is

\[
A_{\mu,ij} = \left(M^{-i} \frac{\partial M}{\partial k^\mu}\right)_{ij}.
\]  

[S184]

It can be checked that Eq. (S182) agrees with Ref. (7).
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