Berry curvature and the phonon Hall effect

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We show that an effective magnetic field acting on phonons naturally emerges in the phonon dynamics of magnetic solids, giving rise to the phonon Hall effect. A general formula for the intrinsic phonon Hall conductivity is derived by using the corrected Kubo formula with the energy magnetization contribution incorporated properly. We thus establish a direct connection between the phonon Hall effect and the intrinsic phonon band structure, i.e., the phonon Berry curvature and phonon dispersion. Based on the formalism, we predict that phonons could also display the quantum Hall effect in certain topological phonon systems. In the low-temperature regime, we predict that the phonon Hall conductivity is proportional to T^3 for ordinary phonon systems, while that for the topological phonon system has a linear T dependence with a quantized temperature coefficient.

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I. INTRODUCTION

The phonon Hall effect (PHE) has been discovered recently in $Tb_3Ga_5O_{12}$ (TGG):^{1,2} a magnetized solid can give rise to a temperature difference between two edges of the sample in the direction transverse to both the magnetization and the driving thermal flow. The discovery of the Hall effect in neutral carriers such as phonons has incited great theoretical interest.^{3–7} Most of the theories relate the effect to Raman spin-lattice coupling,⁸ and standard linear response theory, i.e., the Kubo formula^{3,5–7} or its equivalent,⁴ is employed to calculate the thermal Hall coefficient. These investigations, while all focusing on the intrinsic limit, have not yet revealed a simple connection between the phonon Hall effect and the intrinsic phonon band structure for a general system, as has been done in electron systems.⁹ There is also a natural and interesting question: could phonon systems have the quantum (anomalous) Hall effect as well?^{6,10,11}

In this paper, we establish a direct connection between the PHE and the intrinsic phonon band structure, i.e., the phonon Berry curvature and phonon dispersion. To do this, first, we derive the general phonon dynamics applicable for magnetic solids, incorporating the Mead-Truhlar term in the Born-Oppenheimer approximation. 12 The resulting dynamics contains an effective magnetic field acting on phonons, which gives rise to the PHE. It clarifies the microscopic origin of the spin-lattice coupling, and is readily amendable to firstprinciples calculation. Second, we calculate the thermal Hall coefficient of the system using the corrected Kubo formula, incorporating the contribution of the energy magnetization, ^{13,14} which was overlooked in previous calculations. As a result, we obtain a general formula for calculating the intrinsic phonon Hall coefficient. Based on the formalism, we predict that phonons could also have the quantum (anomalous) Hall effect in properly defined topological phonon systems. In the low-temperature regime, we predict that the phonon Hall conductivity is proportional to T^3 for ordinary phonon systems, while that for topological phonon systems has a linear T dependence with a quantized temperature coefficient.

This paper is organized as follow. In Sec. II, we discuss the general phonon dynamics in a magnetic field. In Sec. III, we present our central formula for the phonon Hall conductivity. In

Sec. IV, we give the definition for topological phonon systems and also discussed the possibility of realizing them. In Sec. V, we show the T^3 law in the low-temperature limit for the phonon Hall conductivity. In Sec. VI, we have a brief summary. We also include an Appendix to show details of the derivations.

II. PHONON DYNAMICS OF MAGNETIC SOLIDS

The Hamiltonian for the nuclear motion of a magnetic solid is determined by the complete form of the Born-Oppenheimer approximation: ¹²

$$\hat{H} = \sum_{l_{\kappa}} \frac{\left[-i\hbar \nabla_{l_{\kappa}} - A_{l_{\kappa}} \left(\{\boldsymbol{R}\}\right)\right]^{2}}{2M_{\kappa}} + V_{\text{eff}}(\boldsymbol{R}), \qquad (1)$$

where $\nabla_{l\kappa} = \partial/\partial u_{l\kappa}$, and $V_{\rm eff}(\{R\}) = \tilde{E}_e(\{R\}) + E_i(\{R\})$ is the effective interaction potential for nuclei, including the direct Coulomb interaction between nuclei, $E_i(\{R\})$, as well as the nuclear interaction mediated by electrons: $\tilde{E}_e(\{R\}) = E_0(\{R\}) + (\hbar^2/2M_\kappa) \sum_{l\kappa} [\langle \nabla_{l\kappa} \Phi_0 | \nabla_{l\kappa} \Phi_0 \rangle - |\langle \Phi_0 | \nabla_{l\kappa} \Phi_0 \rangle|^2]$, where $E_0(\{R\})$ is the energy of the ground state $|\Phi_0(\{R\})\rangle$ of the electron subsystem at the instantaneous nuclear positions $\{R\}$. For a crystalline solid, the equilibrium positions of the nuclei form a Bravais lattice, and we use $\{R\} \equiv \{R_{l\kappa}^0 + u_{l\kappa}, l = 1, \dots, N; \kappa = 1, \dots, r\}$ with $R_{l\kappa}^0 \equiv R_l^0 + d_\kappa$, where R_l^0 is the center equilibrium position of the lth unit cell, l0 is the equilibrium position of the l1 nucleus (with mass l1 is the equilibrium position of the l2 th nucleus (with mass l3 is the equilibrium position of the l3 th nucleus (with mass l4 is the equilibrium position of the l5 is the corresponding vibrational displacement, l1 denotes the total number of unit cells, and l2 is the number of atoms in each unit cell.

The most notable feature of Eq. (1) is the presence of the vector potential $A_{l\kappa}(\{R\}) \equiv i\hbar \langle \Phi_0(\{R\})|\nabla_{l\kappa}\Phi_0(\{R\})\rangle \langle \nabla_{l\kappa} \equiv \partial/\partial u_{l\kappa}\rangle$, as first pointed out by Mead and Truhlar. ¹² In modern language, the vector potential is related to the Berry phase. ¹⁵ The corresponding "physical field" at the limit $u_{l\kappa} \rightarrow 0$ is

$$G_{\alpha\beta}^{\kappa\kappa'}(\mathbf{R}_{l}^{0} - \mathbf{R}_{l'}^{0}) = 2\hbar \operatorname{Im} \left\langle \frac{\partial \Phi_{0}}{\partial u_{\beta,l'\kappa'}} \middle| \frac{\partial \Phi_{0}}{\partial u_{\alpha,l\kappa}} \middle\rangle \middle|_{\mathbf{u}_{l\kappa} \to \mathbf{0}}, \quad (2)$$

where $\alpha, \beta = x, y, z$, and the translational symmetry dictates that it must be a function of $\mathbf{R}_{l}^{0} - \mathbf{R}_{l'}^{0}$.

In an external magnetic field, the ion will experience two vector potentials: 16 one from the real magnetic field and the

other from the Berry phase. The role of the latter is crucial here. In a single atom, there is exact cancellation between the two, or the neutral atom would be deflected in the magnetic field. Therefore, it is not correct to deal with the ion in the magnetic field directly by "minimal substitution." In a lattice system, the cancellation is not exact, and the spin-orbit coupling of the electron will give rise to nonzero $G_{\alpha\beta}^{\kappa\kappa'}(R_l^0-R_l^0)$.

To proceed, we adopt the usual harmonic approximation by expanding $V_{\rm eff}(\{R\})$ to the second order of the vibrational displacement $\boldsymbol{u}_{l\kappa}$. For the periodic lattice, it is more convenient to use the Fourier-transformed displacement $\boldsymbol{u}_{\kappa k} = \sqrt{M_{\kappa}/N} \sum_{l} \boldsymbol{u}_{l\kappa} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_{l\kappa}^{0}}$ with \boldsymbol{k} being the quasimomentum, and the Hamiltonian can be written as

$$\hat{H} = \frac{1}{2} \sum_{k} (\hat{P}_k^{\dagger} \hat{P}_k + \hat{u}_k^{\dagger} D_k \hat{u}_k), \tag{3}$$

where \hat{P}_k and \hat{u}_k have 3r components with $\hat{P}_{\kappa\alpha,k} \equiv -i\hbar\partial/\partial u_{\kappa\alpha,-k} - A_{\kappa\alpha,k}$ and $\hat{u}_{\kappa\alpha,k}$, $\alpha = x,y,z$, respectively, $A_{\kappa\alpha,k} = i\hbar\langle\Phi_0|\partial\Phi_0/\partial u_{\kappa\alpha,-k}\rangle$, and D_k is the $3r \times 3r$ dynamical matrix.¹⁸

The momentum $\hat{P}_{\kappa\alpha,k}$ has the commutation relation at the limit $u_{l\kappa} \to 0$

$$[\hat{P}_{\kappa\alpha,k},\hat{P}_{\kappa'\beta,k'}^{\dagger}] = i\hbar G_{\kappa\alpha,\kappa'\beta}(k) \,\delta_{kk'},\tag{4}$$

$$G_{\kappa\alpha,\kappa'\beta}(\mathbf{k}) = \frac{1}{\sqrt{M_{\kappa}M_{\kappa'}}} \sum_{l} G_{\alpha\beta}^{\kappa\kappa'} (R_{l}^{0}) e^{-i\mathbf{k}\cdot(\mathbf{R}_{l}^{0} + \mathbf{d}_{\kappa\kappa'})}, \quad (5)$$

where $d_{\kappa\kappa'} \equiv d_{\kappa} - d_{\kappa'}$. $G_{\kappa\alpha,\kappa'\beta}(k)$ acts like an effective magnetic field for the phonon dynamics. Using Eqs. (2) and (5), the quantity is readily calculable for real materials using a first-principles approach.

The general phonon dynamics for a magnetic solid can now be determined. From Eq. (3), the linearized canonical equations of motion read

$$\dot{\hat{u}}_k = \hat{P}_k,\tag{6}$$

$$\dot{\hat{P}}_k = -D_k \hat{u}_k + G_k \hat{P}_k,\tag{7}$$

where G_k is a $3r \times 3r$ matrix with the component $G_{\kappa\alpha,\nu\beta}(k)$. The corresponding eigenequation is

$$\omega_{ki}\psi_{ki} = \begin{bmatrix} 0 & i \\ -iD_k & iG_k \end{bmatrix}\psi_{ki} \equiv \tilde{H}_k\psi_{ki}, \tag{8}$$

where ψ_{ki} is the ith eigensolution, and ω_{ki} is the corresponding eigenfrequency. For the non-Hermitian \tilde{H}_k , we define $\bar{\psi}_{ki} = \psi_{ki}^{\dagger} \tilde{D}_k$ with $\tilde{D}_k \equiv \begin{bmatrix} D_k & 0 \\ 0 & I_{3r \times 3r} \end{bmatrix}$ and $I_{3r \times 3r}$ is a unit matrix of dimension $3r \times 3r$, and ψ_{ki} is normalized by $\bar{\psi}_{ki} \psi_{kj} = \delta_{ij}$. Note that the 6r eigensolutions can be divided into two groups of 3r positive- and negative-energy branches, and the two are related by $\omega_{ki}^{(-)} = -\omega_{-ki}^{(+)}$ and $\psi_{ki}^{(-)} = \psi_{-ki}^{(+)*}$ with $1 \le i \le 3r$. This is a result of the symmetries $G_k^* = G_{-k}$ and $D_k^* = D_{-k}$. In the following we use only the positive-energy branches and drop the superscript (+) for brevity.

The Hamiltonian Eq. (3) can be diagonalized with the basis ψ_k . By defining the field operator $\hat{\Psi}_k \equiv (\hat{u}_k, \hat{P}_k)^T$, Eq. (3) can be rewritten as $\hat{H} = (1/2) \sum_k \hat{\Psi}_k \hat{\Psi}_k$ with $\hat{\Psi}_k \equiv \hat{\Psi}_k^{\dagger} \tilde{D}_k$.

Introducing the transformation

$$\hat{\Psi}_{k} = \sum_{i=1}^{3r} \sqrt{\hbar \omega_{ki}} \psi_{ki} \hat{a}_{ki} + \sqrt{\hbar \omega_{-ki}} \psi_{-ki}^* \hat{a}_{-ki}^{\dagger}, \qquad (9)$$

with $[\hat{a}_{ki}, \hat{a}_{kj}^{\dagger}] = \delta_{ij}$, i, j = 1, ..., 3r, we can recover all the commutation relations, and diagonalize the Hamiltonian to

$$\hat{H} = \sum_{k:i=1}^{3r} \hbar \omega_{ki} \left(\hat{a}_{ki}^{\dagger} \hat{a}_{ki} + \frac{1}{2} \right). \tag{10}$$

Similar to the electronic dynamics in magnetic solids, ¹⁹ the intrinsic phonon band structure is determined not only by the phonon dispersion, but also by the Berry connections of the phonon bands. We can define the phonon Berry connection as $\mathcal{A}_{ki} \equiv i \bar{\psi}_{ki} (\partial \psi_{ki} / \partial k)$, and the corresponding Berry curvature as

$$\mathbf{\Omega}_{ki} = -\text{Im}\left[\frac{\partial \bar{\psi}_{ki}}{\partial \mathbf{k}} \times \frac{\partial \psi_{ki}}{\partial \mathbf{k}}\right]. \tag{11}$$

We will show that the phonon Berry curvatures Ω_{ki} and the phonon dispersions ω_{ki} will fully determine the intrinsic phonon Hall conductivity. On the other hand, the interband Berry curvatures proposed in some previous studies are not needed in general.⁶

III. PHONON HALL CONDUCTIVITY

Following the established general procedure, ¹³ we can calculate the thermal Hall coefficient contributed by phonons. For a magnetic system, the transport thermal Hall coefficient includes two contributions: the usual linear response contribution κ^{Kubo} and the contribution from the energy magnetization M_E :

$$\kappa_{xy}^{\text{tr}} = \kappa_{xy}^{\text{Kubo}} + \frac{2M_E^z}{TV},\tag{12}$$

where V is the total volume of the system, and T is the temperature. M_E is the circulation of the phonon energy current, and the reason for the circulation can only be attributed to our effective magnetic field.

A. Kubo contribution $\kappa_{xy}^{\text{Kubo}}$

 $\kappa_{xy}^{\text{Kubo}}$ is determined by the usual Kubo formula²⁰

$$\kappa_{xy}^{\text{Kubo}} = \frac{1}{V k_B T^2} \lim_{s \to 0} \lim_{q \to \mathbf{0}} \int_0^\infty dt e^{-st} \langle \hat{J}_{E,-q}^y; \hat{J}_{E,q}^x(t) \rangle, \quad (13)$$

where $\hat{J}_{E,q}$ is the Fourier-transformed energy current operator in the wave vector q, and $\langle ; \rangle$ denotes the Kubo canonical correlation.²¹ Using the procedure developed by Hardy,²² and with the harmonic approximation and in the small-q limit, we find that (see Appendix A 1):

$$\hat{J}_{E,q} = \frac{1}{8} \sum_{k} \hat{\bar{\Psi}}_{k} (\tilde{V}_{k} + \tilde{V}_{k+q}) \hat{\Psi}_{k+q} + (\text{H.c.}, q \to -q),$$
(14)

where $\tilde{V}_k \equiv \nabla_k \tilde{H}_k$, and (H.c., $q \to -q$) denotes the Hermitian conjugation of the first term after replacing q by -q.

With the phonon current operator $\hat{J}_{E,q}$, we have (see Appendix B)

$$\kappa_{xy}^{\text{Kubo}} = \frac{\hbar}{VT} \sum_{k:i=1}^{3r} \mathcal{M}_{ki}^{z} \omega_{ki} \left(n_{ki} + \frac{1}{2} \right), \tag{15}$$

where $\mathcal{M}_{ki} = \operatorname{Im}\left[\frac{\partial \bar{\psi}_{ki}}{\partial k} \times \tilde{H}_k \frac{\partial \psi_{ki}}{\partial k}\right]$, and $n_{ki} \equiv n_B(\hbar \omega_{ki})$ is the Bose-Einstein distribution. The presence of the "zero-point" contribution (the extra $\frac{1}{2}$ inside the parentheses) is due to the phonon number nonconserving terms (e.g., $a_{ki}a_{k+qj}$ or $a_{ki}^{\dagger}a_{k+qj}^{\dagger}$) in the energy current operator, which were often improperly dropped in many previous calculations. ^{3–5} As a result of the zero-point contribution, $\kappa_{xy}^{\text{Kubo}}$ diverges when $T \to 0$.

B. Phonon energy magnetization M_E^z

The unphysical divergence can be removed by the second term of Eq. (12). The energy magnetization is determined as follows:¹³

$$2M_E^z - T\frac{\partial M_E^z}{\partial T} = \tilde{M}_E^z,\tag{16}$$

$$\tilde{M}_{E}^{z} = \frac{1}{k_{B}T} i \frac{\partial}{\partial q_{y}} \langle \hat{h}_{-q}; \hat{J}_{E,q}^{x} \rangle \bigg|_{q \to 0}, \tag{17}$$

where h_q is the Fourier-transformed energy density operator:

$$\hat{h}_q = \frac{1}{2} \sum_k \hat{\bar{\Psi}}_k \hat{\Psi}_{k+q}. \tag{18}$$

The energy current operator defined in Eq. (14) should satisfy the scaling law necessary for the applicability¹³ of Eqs. (16) and (17) (see Appendix A 2).

For the phonon energy magnetization in Eqs. (16) and (17), we have (see Appendix C)

$$\tilde{M}_{E}^{z} = -\frac{\hbar}{2} \sum_{k;i=1}^{3r} \omega_{ki} \left[\Omega_{ki}^{z} \omega_{ki}^{2} n_{ki}' + \mathcal{M}_{ki}^{z} (2n_{ki} + \omega_{ki} n_{ki}' + 1) \right],$$
(19)

where $n'_{ki} = \partial n_{ki}/\partial \omega_{ki}$. M^z_E is obtained by integrating over the temperature T with the boundary condition that $2M^z_E$ coincides with \tilde{M}^z_E when T=0.

C. Phonon Hall conductivity

We are in a position to present our central result for the phonon Hall conductivity.

$$\kappa_{xy}^{\text{tr}} = -\frac{(\pi k_B)^2}{3h} Z_{\text{ph}} T - \frac{1}{T} \int d\epsilon \epsilon^2 \sigma_{xy}(\epsilon) \frac{dn(\epsilon)}{d\epsilon}, \quad (20)$$

where

$$\sigma_{xy}(\epsilon) = -\frac{1}{V\hbar} \sum_{\hbar \omega_{ki} \le \epsilon} \Omega_{ki}^{z}$$
 (21)

and

$$Z_{\rm ph} = \frac{2\pi}{V} \sum_{k:i=1}^{3r} \Omega_{ki}^{z}.$$
 (22)

Equation (20) gives the general formula of the intrinsic phonon Hall conductivity for a magnetic solid. As expected, the

intrinsic phonon Hall conductivity is fully determined by the dispersions and the Berry curvatures.

In the following, we show how the topological term emerges naturally in Eq. (20). First, we express $\kappa_{xy}^{\text{Kubo}}$, $\tilde{M}_E^{z,\text{inter}}$, and $\tilde{M}_E^{z,\text{intra}}$ as

$$\kappa_{xy}^{\text{Kubo}} = \frac{1}{2T} \int d\epsilon \epsilon m_{1z}^{6r}(\epsilon) n(\epsilon), \qquad (23)$$

$$\tilde{M}_{E}^{z,\text{inter}} = -\frac{1}{2} \int d\epsilon \epsilon m_{1z}^{6r}(\epsilon) n(\epsilon), \qquad (24)$$

$$\tilde{M}_{E}^{z,\text{intra}} = -\frac{1}{4} \int d\epsilon \left(m_{1z}^{6r}(\epsilon) - \frac{1}{\hbar} \epsilon \tilde{\sigma}_{xy}^{6r}(\omega) \right) \epsilon^{2} \frac{\partial n(\epsilon)}{\partial \epsilon}, \tag{25}$$

where

$$m_{1z}^{6r}(\epsilon) = \frac{1}{V} \sum_{k,i=1}^{6r} \mathcal{M}_{ki}^{z} \delta\left(\epsilon - \hbar\omega_{ki}\right), \tag{26}$$

$$\tilde{\sigma}_{xy}^{6r}(\epsilon) = -\frac{1}{V\hbar} \sum_{k,i=1}^{6r} \Omega_{ki}^{z} \delta\left(\epsilon - \hbar\omega_{ki}\right). \tag{27}$$

So the real energy magnetization M_E^z is

$$M_{E}^{z} = -\frac{V}{4} \int d\epsilon \epsilon m_{1z}^{6r}(\epsilon) \frac{1}{\beta^{2}} \int^{\beta} d\beta' \beta' \left(2n(\epsilon) + \epsilon \frac{\partial n(\epsilon)}{\partial \epsilon} \right) + \frac{V}{4} \int d\epsilon \epsilon^{3} \tilde{\sigma}_{xy}^{6r}(\epsilon) \frac{1}{\beta^{2}} \int^{\beta} d\beta' \beta' \frac{\partial n(\epsilon)}{\partial \epsilon},$$
(28)

where the boundary condition is that $2M_E^z$ coincides with \tilde{M}_E^z when T=0. There is no indefiniteness in Eq. (28), for the thermodynamic quantity $M_s=M_E/T$ should be zero in the high-temperature limit. We can change the integration over β' into integration over ϵ and we have

$$\kappa_{xy}^{\text{tr}} = \kappa_{xy}^{\text{Kubo}} + \frac{2M_E^z}{TV} \tag{29}$$

$$=\frac{1}{2T}\int d\epsilon \tilde{\sigma}_{xy}^{6r}(\epsilon)\left(-2\int^{\epsilon}dxxn\left(x\right)+\epsilon^{2}n\left(\epsilon\right)\right). \quad (30)$$

We can define $\tilde{\sigma}_{xy}^{6r}(\epsilon) = \frac{d\sigma_{xy}^{6r}(\epsilon)}{d\epsilon}$, so we have

$$\kappa_{xy}^{\text{tr}} = \frac{1}{2T} \sigma_{xy}^{6r}(\epsilon) \left(-2 \int_{-\infty}^{\epsilon} dx x n(x) + \epsilon^{2} n(\epsilon) \right) \Big|_{-\infty}^{\infty}
- \frac{1}{2T} \int_{-\infty}^{\infty} d\epsilon \sigma_{xy}^{6r}(\epsilon) \epsilon^{2} \frac{dn(\epsilon)}{d\epsilon}.$$
(31)

The first term in Eq. (31) is zero, for the following reasons:

$$\sigma_{xy}^{6r}(\epsilon) = \int_{-\infty}^{\epsilon} dx \tilde{\sigma}_{xy}^{6r}(x), \qquad (32)$$

$$\sigma_{xy}^{6r}(\infty) = 0, \tag{33}$$

$$\sigma_{xy}^{6r}(-\infty) = 0. \tag{34}$$

We can show Eq. (33) using the properties of the phonon Berry curvature: $\Omega_{ki}^{(-)} = -\Omega_{-ki}^{(+)}$ where $1 \le i \le 3r$, because of the symmetry properties of ψ_{ki} . Equation (34) is zero because of the integration limit. Therefore,

$$\kappa_{xy}^{\text{tr}} = -\frac{1}{2T} \int d\epsilon \epsilon^2 \sigma_{xy}^{6r}(\epsilon) \frac{dn(\epsilon)}{d\epsilon}.$$
 (35)

Next, we express κ_{xy}^{tr} using the 3r positive-energy bands:

$$\sigma_{xy}^{6r}(\epsilon) = \int_{-\infty}^{0} dx \tilde{\sigma}_{xy}^{6r}(x) + \int_{0}^{\epsilon} dx \tilde{\sigma}_{xy}^{6r}(x)$$
 (36)

$$= -\frac{Z_{\rm ph}}{2\pi\hbar} + \int_0^\epsilon dx \,\tilde{\sigma}_{xy}^{6r}(x). \tag{37}$$

Using our definition in Eq. (21), we can write Eq. (37) as

$$\sigma_{xy}^{6r}(\epsilon) = \begin{cases} -\frac{Z_{\text{ph}}}{2\pi\hbar} + \sigma_{xy}(\epsilon), & \epsilon > 0, \\ -\frac{Z_{\text{ph}}}{2\pi\hbar} + \sigma_{xy}(-\epsilon), & \epsilon < 0. \end{cases}$$
(38)

Therefore.

$$\kappa_{xy}^{\text{tr}} = -\frac{1}{2T} \int_{0}^{\infty} d\epsilon \epsilon^{2} \left(-\frac{Z_{\text{ph}}}{2\pi\hbar} + \sigma_{xy}(\epsilon) \right) \frac{dn(\epsilon)}{d\epsilon} - \frac{1}{2T} \int_{-\infty}^{0} d\epsilon \epsilon^{2} \left(-\frac{Z_{\text{ph}}}{2\pi\hbar} + \sigma_{xy}(-\epsilon) \right) \frac{dn(\epsilon)}{d\epsilon}.$$
(39)

Finally, after some simple algebra we obtain the phonon Hall conductivity in Eq. (20) and the topological term emerges naturally.

IV. TOPOLOGICAL PHONON SYSTEM

The first term in Eq. (20) is of topological nature, determined by the global phonon band structures. This is different from the second term which is determined only by the low-energy sectors of the phonon bands limited by k_BT . For two-dimensional (2D) systems, $Z_{\rm ph}$ is the Chern number, quantized as an integer. For three-dimensional (3D) systems, $Z_{\rm ph}$ is quantized²³ in units of $G_z/2\pi$, where G_z is the z component of the reciprocal lattice vector \mathbf{G} . As the result, the phonon Hall conductivity has a topological contribution with a quantized linear temperature coefficient in units of $(\pi k_B)^2/3h$ (2D) or $\pi k_B^2 G_z/6\pi h$ (3D).

Not surprisingly, most phonon systems have $Z_{\rm ph}=0$. It is natural to define the topological phonon systems as those with

$$Z_{\rm ph} \neq 0. \tag{40}$$

This puts a stringent constraint on the definition of a real topological phonon system: it requires that the sum of the Chern numbers of all phonon bands must be nonzero. Previous theoretical studies have had success in constructing phonon systems with nonzero Chern numbers of individual bands. 6,10,11 However, these models rely on the reorganization of the phonon bands within the positive-energy branches, so still have zero Z_{ph} . They are not topological phonon systems in the stringent sense, nor will they manifest unusual phonon Hall conductivity. To realize a real topological phonon system, we need to look for insulating materials with spin-orbit coupling so strong that the resulting effective magnetic field can intermix and reorganize the phonon bands between the positive- and negative-energy branches. A realistic lattice model for realizing the topological phonon system is an interesting topic for future investigation.

We note that the value of the topological contribution to the thermal Hall conductivity is actually the same as the longitudinal thermal conductivity of a dielectric quantum wire with $Z_{\rm ph}$ acoustic phonon modes. ^{24–26} This is because topological phonon systems have chiral edge phonon modes

that behave just like the 1D acoustic phonon modes. The edge-bulk correspondence picture in the topological phonon system is very similar to that in quantum Hall systems. On the other hand, unlike the phonons in a quantum wire, phonons in the chiral edge modes cannot be backscattered without coupling to the bulk. This will make the topological phonon Hall effect more robust against imperfections than the quantized thermal conduction in a 1D quantum wire. The latter has been observed experimentally.²⁵

V. LOW-TEMPERATURE LIMIT

At low temperatures, only the low-energy phonon modes are relevant for ordinary systems. It is thus sufficient to consider the long-wave acoustic phonon modes.

A. Constraint for the effective magnetic field

An important constraint for this case is

$$\sum_{l \nu \nu'} G_{\alpha\beta}^{\kappa\kappa'} (\mathbf{R}_l^0) = 0. \tag{41}$$

This can be verified directly by using the effective magnetic field in Eq. (2). As we will show, this is still true even when we explicitly consider the external magnetic field because of the overall charge neutrality. It is easy to see that

$$\sum_{l\kappa\kappa'} G_{\alpha\beta}^{\kappa\kappa'}(\mathbf{R}_{l}^{0})$$

$$= \frac{2\hbar}{N} \operatorname{Im} \left\langle \frac{\partial \Phi_{0}(\{\mathbf{R}^{0} + \mathbf{u}_{0}\})}{\partial u_{0\beta}} \middle| \frac{\partial \Phi_{0}(\{\mathbf{R}^{0} + \mathbf{u}_{0}\})}{\partial u_{0\alpha}} \middle\rangle \middle|_{\mathbf{u}_{0} \to \mathbf{0}} + Z_{\operatorname{tot}} e \epsilon_{\alpha\beta\gamma} B_{\gamma}, \tag{42}$$

where $\Phi_0(\{R^0 + u_0\})$ is the ground-state wave function of the electron subsystem when the whole system is displaced by u_0 , and Z_{tot} is the total charge number of the nuclei in an unit cell. We have assumed that there is an external magnetic field B. Since the displacement is equivalent to a redefinition of the origin, we have

$$\Phi_0(\{\mathbf{R}^0 + \mathbf{u}_0\}, \{\mathbf{r}\}) = \exp\left[-i\frac{e}{2\hbar}(\mathbf{B} \times \mathbf{u}_0) \cdot \left(\sum_i \mathbf{r}_i\right)\right]$$

$$\cdot \Phi_0(\{\mathbf{R}^0\}, \{\mathbf{r} - \mathbf{u}_0\}), \tag{43}$$

where $\{r\} \equiv \{r_1, r_2, \dots, r_{N_e}\}$ denotes the coordinates of the electron. We have

$$\frac{\partial \Phi_0(\{\mathbf{R}^0 + \mathbf{u}_0\}, \{\mathbf{r}\})}{\partial \mathbf{u}_0}$$

$$= -\frac{i}{\hbar} \exp \left[-i \frac{e}{2\hbar} (\mathbf{B} \times \mathbf{u}_0) \cdot \left(\sum_i r_i \right) \right]$$

$$\cdot \sum_i \left(\hat{\mathbf{p}}_i - \frac{e}{2} \mathbf{B} \times \mathbf{r}_i \right) \Phi_0(\{\mathbf{R}^0\}, \{\mathbf{r} - \mathbf{u}_0\}). \tag{44}$$

Substituting Eq. (44) into (42), one can easily verify that the first and second terms of the right-hand side of Eq. (42) exactly cancel each other due to the overall charge neutrality.

B. T^3 law

It is easy to see that the phonon dynamics with the constraint always has three acoustic modes that have zero energy at k = 0, consistent with the general requirement of global translational symmetry. This remedies an important issue of the widely adopted phenomenological model of Raman spinlattice coupling, which has nonvanishing coupling constant even in the long-wave limit, inducing nonzero acoustic phonon energies at k = 0. We will see that the constraint will change the theoretical expectation of the low-temperature behavior of the phonon Hall conductivity.

With this constraint in mind, we can write down the general Hamiltonian for the long-wave acoustic phonons of an isotropic continuous medium:²⁷

$$\hat{H} = \int d\mathbf{x} \left[\frac{\hat{\mathbf{P}}(\mathbf{x})^2}{2\rho} + \frac{\mu_1}{2} \nabla \hat{\mathbf{u}} \cdot \nabla \hat{\mathbf{u}} + \frac{\mu_2}{2} (\nabla \cdot \hat{\mathbf{u}})^2 \right], \quad (45)$$

where $\hat{P}(x) = -i\hbar\delta/\delta\hat{u}(x) - A[\hat{u}]$, u(x) is the vibrational displacement, μ_1 and μ_2 are elastic constants, and ρ is the mass density. The symmetry dictates that $A[\hat{u}] = \gamma_1 \nabla \nabla \cdot (M \times \hat{u}) + \gamma_2 \nabla^2 (M \times \hat{u})$, where M is the magnetization of the system, and γ_1 and γ_2 are coupling constants characterizing the spin-lattice coupling. After Fourier transformation, we can identify $D_{\alpha\beta}(k) = (1/\rho)(\mu_1\delta_{\alpha\beta}k^2 + \mu_2k_{\alpha}k_{\beta})$ and $G_{\alpha\beta}(k) = (1/\rho)\sum_{\gamma}\epsilon_{\alpha\beta\gamma}[-\gamma_1k_{\gamma}k\cdot M + (\gamma_1+2\gamma_2)k^2M_{\gamma}]$ with k=|k| and $\alpha,\beta,\gamma=x,y,z$. We can then adopt our general formula for calculating the phonon Hall conductivity.

To the first order in the magnetization M, we obtain the phonon dispersions $\omega_{k1} = c_L k$ and $\omega_{k2(3)} = c_T k \pm \gamma_2 k k \cdot M$, where $c_T = \sqrt{\mu_1/\rho}$ and $c_L = \sqrt{(\mu_1 + 2\mu_2)/\rho}$ are the transverse and longitudinal phonon velocities, respectively. The phonon Berry curvatures are

$$\mathbf{\Omega}_{k1} = -\frac{g_1(k^2 \mathbf{M} + \mathbf{k} \mathbf{k} \cdot \mathbf{M})}{k^3},\tag{46}$$

$$\Omega_{k2(3)} = \pm \frac{k}{k^3} + \frac{g_2(k^2 M + kk \cdot M)}{k^3},\tag{47}$$

where $g_1 = (\gamma_1 + 2\gamma_2)(1 + 3\delta^2)/[2c_T\delta(\delta^2 - 1)],$ $g_2 = g_1\delta(3 + \delta^2)/[2(1 + 3\delta^2)],$ and $\delta = c_L/c_T$.

Using Eq. (20), we determine the phonon Hall conductivity:

$$\kappa_{xy}^{\text{tr}} = \frac{4\pi^2 k_B^4}{45c_T^3 \hbar^3} \left[1 - \frac{\gamma_1 + 2\gamma_2}{2\gamma_2} \frac{4\delta^3 + \delta^2 + \delta + 1}{\delta^3 (\delta^2 + \delta + 1)} \right] \gamma_2 M_z T^3, \tag{48}$$

where we assume M is along the z direction and the Debye energy $\hbar\omega_D\gg k_BT$. We can see that at low temperature, $\kappa_{xy}^{\rm tr}$ is proportional to T^3 , instead of T as proposed in previous studies.³

We can obtain insights from the above calculation into how the phonon would be deflected by the effective magnetic field. We can see from Eqs. (46) and (47) that, on different branches, the phonon will experience different "reciprocal-space magnetic fields." The corresponding anomalous velocity of the phonon is proportional to $\Omega_{ki} \times \nabla T$, similar to that for electrons. The net deflection direction will be perpendicular to the directions of both the magnetization and the temperature gradient.

We make a few comments concerning the disorder effect:²⁸ In analogy to the anomalous Hall effect of electron systems,²⁹

we generally expect that the total phonon Hall coefficient can be decomposed into $\kappa_{xy}^{\rm tr} = \kappa_{xy}^{\rm in} + \kappa_{xy}^{\rm sj} + \kappa_{xy}^{\rm skew}$, where $\kappa_{xy}^{\rm in}$ is the intrinsic phonon Hall conductivity we calculate in Eq. (20), and the disorder will introduce the side jump contribution $\kappa_{xy}^{\rm sj}$ and the skew scattering contribution $\kappa_{xy}^{\rm skew}$. However, there is an important difference between the phonon and electron systems: the mean free path of phonons in TGG had been determined to be ~ 1 mm, 30 much longer than its electron counterpart. Moreover, in the low-temperature limit, the dominant contribution to the thermal conductivity is from the long-wave phonons which are not affected by the disorder. 31 We thus expect that the disorder correction is less important in phonon systems, and the T^3 law of the phonon Hall conductivity will survive.

VI. SUMMARY

In summary, we establish the general phonon dynamics for magnetic solids. Based on the dynamics, we propose a general theory of the PHE. Using the corrected Kubo formula, we link the intrinsic phonon Hall conductivity to the phonon Berry curvature. The general formula suggests that the phonons could also experience the quantum Hall effect, and our theory presents a rigorous definition of the topological phonon system. We predict that the phonon Hall conductivity of the ordinary phonon system is proportional to T^3 at low temperature, while that for the topological phonon system has a linear T dependence with a quantized temperature coefficient.

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APPENDIX A: PHONON ENERGY CURRENT OPERATOR AND ITS SCALING LAW

1. Phonon energy current operator

We follow Hardy²² in deriving the phonon energy current operator. The Hamiltonian density is

$$\hat{h}(x) = \frac{1}{2} \sum_{l_{\kappa}} \{ \Delta (x - R_{l_{\kappa}}) \hat{H}_{l_{\kappa}} + \text{H.c.} \},$$
 (A1)

where $\hat{H}_{l\kappa} = \frac{\hat{P}_{l\kappa}^2}{2M_{\kappa}} + \hat{V}_{l\kappa}$ and $\hat{P}_{l\kappa} = -i\hbar\nabla_{l\kappa} - A_{l\kappa}$, and $\Delta(x)$ is a localized function near x = 0 with $\int dx \Delta(x) = 1$. We adopt the harmonic approximation for $\hat{V}_{l\kappa}$: $\hat{V}_{l\kappa} = \frac{1}{2} \sum_{l'\kappa'\alpha\beta} \hat{u}_{l\kappa\alpha} D_{\alpha\beta}^{\kappa\kappa'}(R_l^0 - R_{l'}^0) \hat{u}_{l'\kappa'\beta}$ where $D_{\alpha\beta}^{\kappa\kappa'}(R_l^0 - R_{l'}^0)$ is the dynamical matrix. The Hamiltonian is $\hat{H} = \int dx \hat{h}(x) = \sum_{l\kappa} H_{l\kappa}$. The energy current operator is defined by the energy conservation equation:

$$\hat{h}(x) + \nabla \cdot \hat{J}_E(x) = 0, \tag{A2}$$

where $\hat{J}_E(x)$ is the phonon energy current operator, and $\hat{h}(x) = (1/i\hbar)[\hat{h}(x),\hat{H}]$.

We can express $[\hat{h}(x), \hat{H}]$ as a divergence. We have

$$\frac{i}{\hbar}[\hat{h}(\mathbf{x}),\hat{H}] = \frac{i}{2\hbar} \sum_{l\kappa,l'\kappa'} \Delta(\mathbf{x} - \mathbf{R}_{l\kappa})[\hat{H}_{l\kappa},\hat{H}_{l'\kappa'}] + \text{H.c.} + \cdots,$$

(A3)

where "···" denotes higher-order terms such as $[\Delta(x - R_{l\kappa}), \frac{\hat{P}_{l'\kappa'}^2}{2M_{\kappa'}}]\hat{H}_{l\kappa}$, which will be a cubic product of $\hat{u}_{l\kappa}$ and $\hat{P}_{l'\kappa'}$. Noting that

$$[\hat{H}_{l\kappa}, \hat{H}_{l'\kappa'}] = \left[\frac{\hat{\boldsymbol{P}}_{l\kappa}^{2}}{2M_{\kappa}}, \hat{V}_{l'\kappa'}\right] + \left[\hat{V}_{l\kappa}, \frac{\hat{\boldsymbol{P}}_{l'\kappa'}^{2}}{2M_{\kappa'}}\right] + \frac{i\hbar}{2M_{\kappa}M_{\kappa'}}$$

$$\times \sum_{\alpha\beta} G_{\alpha\beta}^{\kappa\kappa'} \left(\boldsymbol{R}_{l}^{0} - \boldsymbol{R}_{l'}^{0}\right) \left(\hat{P}_{l\kappa}^{\alpha} \hat{P}_{l'\kappa'}^{\beta} + \hat{P}_{l'\kappa'}^{\beta} \hat{P}_{l\kappa}^{\alpha}\right), \tag{A4}$$

and interchanging subscripts $l\kappa$ and $l'\kappa'$, we have

$$\frac{i}{\hbar} [\hat{h}(\mathbf{x}), \hat{H}]
= \frac{i}{2\hbar} \sum_{l\kappa, l'\kappa'} \left[\Delta \left(\mathbf{x} - \mathbf{R}_{l\kappa} \right) - \Delta \left(\mathbf{x} - \mathbf{R}_{l'\kappa'} \right) \right] \left(\left[\frac{\hat{\mathbf{P}}_{l\kappa}^2}{2M_{\kappa}}, \hat{V}_{l'\kappa'} \right] \right)
+ \frac{i\hbar}{2M_{\kappa} M_{\kappa'}} \sum_{\alpha\beta} G_{\alpha\beta}^{\kappa\kappa'} \left(\mathbf{R}_{l}^0 - \mathbf{R}_{l'}^0 \right) \hat{P}_{l\kappa}^{\alpha} \hat{P}_{l'\kappa'}^{\beta} \right) + \text{H.c.} \quad (A5)$$

Inserting the expansion

$$\Delta (\mathbf{x} - \mathbf{R}_{l\kappa}) - \Delta (\mathbf{x} - \mathbf{R}_{l'\kappa'})$$

$$\approx \frac{1}{2} \left(\mathbf{R}_{l'\kappa'}^{0} - \mathbf{R}_{l\kappa}^{0} \right) \cdot \left(\frac{\partial \Delta (\mathbf{x} - \mathbf{R}_{l'\kappa'}^{0})}{\partial \mathbf{x}} + \frac{\partial \Delta (\mathbf{x} - \mathbf{R}_{l\kappa}^{0})}{\partial \mathbf{x}} \right)$$
(A6)

into Eq. (A5), we obtain

$$\frac{i}{\hbar}[\hat{h}(\mathbf{x}), \hat{H}] = \nabla \cdot \hat{J}_{E}(\mathbf{x}), \tag{A7}$$

where

$$\hat{\boldsymbol{J}}_{E}(\boldsymbol{x}) = \frac{i}{4\hbar} \sum_{l\kappa,l'\kappa'} (\boldsymbol{R}_{l'\kappa'}^{0} - \boldsymbol{R}_{l\kappa}^{0}) \left[\Delta \left(\boldsymbol{x} - \boldsymbol{R}_{l'\kappa'}^{0} \right) + \Delta \left(\boldsymbol{x} - \boldsymbol{R}_{l\kappa}^{0} \right) \right] \left(\left[\frac{\hat{\boldsymbol{P}}_{l\kappa}^{2}}{2M_{\kappa}}, \hat{V}_{l'\kappa'} \right] + \frac{i\hbar}{2M_{\kappa}M_{\kappa'}} \right)$$

$$\times \sum_{\alpha\beta} G_{\alpha\beta}^{\kappa\kappa'} (\boldsymbol{R}_{l}^{0} - \boldsymbol{R}_{l'}^{0}) \hat{P}_{l\kappa}^{\alpha} \hat{P}_{l'\kappa'}^{\beta} + \text{H.c.} \quad (A8)$$

Doing the Fourier transformation $\hat{J}_{E,q} = \int dx \hat{J}_{E}(x)e^{-iq\cdot x}$, we have

$$\hat{\boldsymbol{J}}_{E,q} = -\frac{i}{8} \Delta_q \sum_{k} [\hat{\boldsymbol{P}}_{k}^{\dagger} \nabla_k \left(D_k + D_{k+q} \right) \hat{\boldsymbol{u}}_{k+q} - \hat{\boldsymbol{P}}_{k}^{\dagger} \nabla_k (G_k + G_{k+q}) \hat{\boldsymbol{P}}_{k+q}], \tag{A9}$$

where $D_{\pmb{k}}$ is the dynamical matrix with components $D_{\kappa\alpha,\kappa'\beta}(\pmb{k}) = \frac{1}{\sqrt{M_{\kappa}M_{\kappa'}}} \sum_{l} D_{\alpha\beta}^{\kappa\kappa'}(R_l^0) e^{-i\pmb{k}\cdot(\pmb{R}_l^0+\pmb{d}_{\kappa\kappa'})}$. In the small- \pmb{q} limit, $\Delta_{\pmb{q}} \to 1$. We obtain

$$\hat{\boldsymbol{J}}_{E,q} = \frac{1}{8} \sum_{k} \hat{\Psi}_{k}^{\dagger} [\nabla_{k} (\tilde{H}_{k} + \tilde{H}_{k+q}) + \nabla_{k} (\tilde{H}_{k}^{\dagger} + \tilde{H}_{k+q}^{\dagger})] \hat{\Psi}_{k+q}.$$
(A10)

Using the identities $\nabla_k \tilde{H}_k = \tilde{D}_k \nabla_k \tilde{H}_k$ and $\nabla_k \tilde{H}_k^{\dagger} = (\nabla_k \tilde{H}_k^{\dagger}) \tilde{D}_k$, we obtain Eq. (14).

2. Scaling law for the energy current operator

In order to calculate the energy magnetization, we need to verify that the energy current satisfies the scaling law^{13}

$$\hat{J}_{E}^{\psi}(x) = [1 + \psi(x)]^{2} \hat{J}_{E}(x) + O(\nabla^{(2)}\psi(x))$$
 (A11)

in the presence of the gravitational field $\psi(r)$ which modifies the local Hamiltonian density by

$$\hat{h}^{\psi}(\mathbf{x}) = \frac{1}{2} \sum_{l_{\kappa}} \{ (1 + \psi(\mathbf{x})) \Delta(\mathbf{x} - \mathbf{R}_{l_{\kappa}}) \, \hat{H}_{l_{\kappa}} + \text{H.c.} \}.$$
(A12)

Similar to the derivation in Appendix A1, we have

$$\nabla \cdot \hat{\boldsymbol{J}}_{E}^{\psi}(\boldsymbol{x}) = \frac{i}{\hbar} [\hat{h}^{\psi}(\boldsymbol{x}), \hat{H}^{\psi}]$$
 (A13)

and

$$\frac{i}{\hbar} [\hat{h}^{\psi}(\mathbf{x}), \hat{H}^{\psi}] = \frac{i}{4} \int d\mathbf{x}' [1 + \psi(\mathbf{x})] [1 + \psi(\mathbf{x}')] \Gamma(\mathbf{x}, \mathbf{x}')
\approx \frac{i}{4} \int d\mathbf{x}' \left[[1 + \psi(\mathbf{x})]^2 \Gamma(\mathbf{x}, \mathbf{x}') + [1 + \psi(\mathbf{x})] (\mathbf{x}' - \mathbf{x}) \cdot \frac{\partial \psi(\mathbf{x})}{\partial \mathbf{x}} \Gamma(\mathbf{x}, \mathbf{x}') \right]
+ \frac{1}{2} [1 + \psi(\mathbf{x})] \sum_{\mu\nu} (x'_{\mu} - x_{\mu}) (x'_{\nu} - x_{\nu}) \frac{\partial^2 \psi(\mathbf{x})}{\partial x_{\mu} \partial x_{\nu}} \Gamma(\mathbf{x}, \mathbf{x}') + O(\nabla^{(3)} \psi(\mathbf{x})) \right]$$
(A14)

with

$$\Gamma(\mathbf{x}, \mathbf{x}') = \frac{1}{\hbar} \sum_{l_{k', l', k'}} \Delta(\mathbf{x} - \mathbf{R}_{l_{k}}) \{ \Delta(\mathbf{x}' - \mathbf{R}_{l'_{k'}}), [\hat{H}_{l_{k}}, \hat{H}_{l'_{k'}}] \} + \text{H.c.} + \cdots.$$
(A16)

In Eq. (A16), we also ignore the terms which will lead to the cubic products of $\hat{u}_{l\kappa}$ and $\hat{P}_{l'\kappa'}$ in the energy current operator. For the first term in Eq. (A15), after the integration over x' and repeating the derivation from Eq. (A3) to Eq. (A7), we can show

$$\frac{i}{4} \int d\mathbf{x}' \left[1 + \psi(\mathbf{x})\right]^2 \Gamma(\mathbf{x}, \mathbf{x}') = \left[1 + \psi(\mathbf{x})\right]^2 \nabla \cdot \hat{\mathbf{J}}_E(\mathbf{x}). \tag{A17}$$

For the second term in Eq. (A15):

$$\frac{i}{4} \int d\mathbf{x}' \left[1 + \psi(\mathbf{x})\right] (\mathbf{x}' - \mathbf{x}) \cdot \frac{\partial \psi(\mathbf{x})}{\partial \mathbf{x}} \Gamma(\mathbf{x}, \mathbf{x}') = \frac{i}{4\hbar} \left[1 + \psi(\mathbf{x})\right] \frac{\partial \psi(\mathbf{x})}{\partial \mathbf{x}} \cdot \sum_{l\kappa, l'\kappa'} \Delta(\mathbf{x} - \mathbf{R}_{l\kappa}) \left\{ \mathbf{R}_{l'\kappa'}^0 - \mathbf{R}_{l\kappa}^0, [\hat{H}_{l\kappa}, \hat{H}_{l'\kappa'}] \right\}$$

$$= 2 \left[1 + \psi(\mathbf{x})\right] \frac{\partial \psi(\mathbf{x})}{\partial \mathbf{x}} \cdot \hat{\mathbf{J}}_E(\mathbf{x}). \tag{A18}$$

For the third term in Eq. (A15), we have

$$\frac{i}{4} \int d\mathbf{x}' \left[1 + \psi(\mathbf{x}) \right] \sum_{\mu\nu} (x'_{\mu} - x_{\mu}) (x'_{\nu} - x_{\nu}) \frac{\partial^{2} \psi(\mathbf{x})}{\partial x_{\mu} \partial x_{\nu}} \Gamma(\mathbf{x}, \mathbf{x}')$$

$$= \frac{i}{2\hbar} \left[1 + \psi(\mathbf{x}) \right] \sum_{l\kappa, l'\kappa', \mu\nu} \frac{\partial^{2} \psi(\mathbf{x})}{\partial x_{\mu} \partial x_{\nu}} \Delta\left(\mathbf{x} - \mathbf{R}_{l\kappa}\right) \left(R_{l'\kappa'\mu}^{0} - R_{l\kappa\mu}^{0} \right) \left(R_{l'\kappa'\nu}^{0} - R_{l\kappa\nu}^{0} \right) \left[\hat{H}_{l\kappa}, \hat{H}_{l'\kappa'} \right] + \text{H.c.}, \tag{A19}$$

$$= \frac{i}{4\hbar} \left[1 + \psi(\mathbf{x}) \right] \sum_{l\kappa, l'\kappa', \mu\nu} \frac{\partial^{2} \psi(\mathbf{x})}{\partial x_{\mu} \partial x_{\nu}} \left[\Delta\left(\mathbf{x} - \mathbf{R}_{l\kappa}\right) - \Delta\left(\mathbf{x} - \mathbf{R}_{l'\kappa'}\right) \right] \left(R_{l'\kappa'\mu}^{0} - R_{l\kappa\mu}^{0} \right) \left(R_{l'\kappa'\nu}^{0} - R_{l\kappa\nu}^{0} \right) \left[\hat{H}_{l\kappa}, \hat{H}_{l'\kappa'} \right] + \text{H.c.}. \tag{A20}$$

Noting the expansion in Eq. (A6), Eq. (A20) does not have a contribution to the current in the long-wave limit.

Combining Eqs. (A17) and (A18), we obtain Eq. (A11).

APPENDIX B: DERIVATION DETAILS FOR $\kappa_{xy}^{\text{Kubo}}$ IN Eq. (15)

Direct calculation of the Kubo formula leads to

$$\kappa_{xy}^{\text{Kubo}} = \frac{\hbar}{32VT} \sum_{k;i,j=1}^{6r} \frac{\text{Im}(\mathcal{V}_{kij}^x \mathcal{V}_{kji}^y - \mathcal{V}_{kij}^y \mathcal{V}_{kji}^x) \omega_{ki} \omega_{kj} n_{ki}}{(\omega_{ki} - \omega_{kj})^2},$$
(B1)

where $V_{kij} \equiv 2(\bar{\psi}_{ki} \frac{\partial \tilde{H}_k}{\partial k} \psi_{kj} + \psi_{ki}^{\dagger} \frac{\partial \tilde{H}_k^{\dagger}}{\partial k} \bar{\psi}_{kj}^{\dagger})$. It is easy to verify that

$$\bar{\psi}_{ki}\frac{\partial \tilde{H}_k}{\partial k_x}\psi_{kj} = (\omega_{kj} - \omega_{ki})\bar{\psi}_{ki}\frac{\partial \psi_{kj}}{\partial k_x} + \frac{\partial \omega_{ki}}{\partial k_x}\delta_{ij}, \quad (B2)$$

so

$$\mathcal{V}_{kij}^{x} = 4 \frac{\partial \omega_{ki}}{\partial k_{x}} \delta_{ij} + 2(\omega_{kj} - \omega_{ki}) \left(\bar{\psi}_{ki} \frac{\partial \psi_{kj}}{\partial k_{x}} + \psi_{ki}^{\dagger} \frac{\partial \bar{\psi}_{kj}^{\dagger}}{\partial k_{x}} \right).$$
(B3)

Note that here $i \neq j$, so we have

$$\sum_{j=1}^{6r} \frac{\mathcal{V}_{kij}^{x} \mathcal{V}_{kji}^{y} \omega_{ki} \omega_{kj}}{(\omega_{ki} - \omega_{kj})^{2}}$$

$$= 4\omega_{ki} \left(\frac{\partial \bar{\psi}_{ki}}{\partial k_{x}} \tilde{H}_{k} \frac{\partial \psi_{ki}}{\partial k_{y}} + \frac{\partial \psi_{ki}^{\dagger}}{\partial k_{x}} \tilde{H}_{k}^{\dagger} \frac{\partial \bar{\psi}_{ki}^{\dagger}}{\partial k_{y}} \right)$$

$$+ \frac{\partial \psi_{ki}^{\dagger}}{\partial k_{x}} \tilde{H}_{k}^{\dagger} \tilde{D}_{k} \frac{\partial \psi_{ki}}{\partial k_{y}} + \frac{\partial \bar{\psi}_{ki}}{\partial k_{x}} \tilde{H}_{k} \tilde{D}_{k}^{-1} \frac{\partial \bar{\psi}_{ki}^{\dagger}}{\partial k_{y}}, \quad (B4)$$

where we have used $\bar{\psi}_{ki} \frac{\partial \psi_{kj}}{\partial k_x} = -\frac{\partial \bar{\psi}_{ki}}{\partial k_x} \psi_{kj}$, $\psi^{\dagger}_{kj} \frac{\partial \bar{\psi}^{\dagger}_{ki}}{\partial k_x} = -\frac{\partial \psi^{\dagger}_{kj}}{\partial k_x} \bar{\psi}^{\dagger}_{ki}$, and $\tilde{H}_k = \sum_j \omega_{kj} \psi_{kj} \bar{\psi}_{kj}$ and its Hermitian conjugate. We can further simplify the last two terms in Eq. (B4) using $\tilde{D}_k \frac{\partial \psi_{ki}}{\partial k_y} = \frac{\partial \bar{\psi}^{\dagger}_{ki}}{\partial k_y} - \frac{\partial \tilde{D}_k}{\partial k_y} \psi_{ki}$ and $\tilde{D}_k^{-1} \frac{\partial \bar{\psi}^{\dagger}_{ki}}{\partial k_y} = \frac{\partial \psi_{ki}}{\partial k_y} - \frac{\partial \tilde{D}_k^{-1}}{\partial k_y} \bar{\psi}^{\dagger}_{ki}$,

and we obtain

$$\frac{\partial \psi_{ki}^{\dagger}}{\partial k_{x}} \tilde{H}_{k}^{\dagger} \tilde{D}_{k} \frac{\partial \psi_{ki}}{\partial k_{y}} + \frac{\partial \bar{\psi}_{ki}}{\partial k_{x}} \tilde{H}_{k} \tilde{D}_{k}^{-1} \frac{\partial \bar{\psi}_{ki}^{\dagger}}{\partial k_{y}}$$

$$= \frac{\partial \psi_{ki}^{\dagger}}{\partial k_{x}} \tilde{H}_{k}^{\dagger} \frac{\partial \bar{\psi}_{ki}^{\dagger}}{\partial k_{y}} + \frac{\partial \bar{\psi}_{ki}}{\partial k_{x}} \tilde{H}_{k} \frac{\partial \psi_{ki}}{\partial k_{y}}$$

$$- \frac{\partial \psi_{ki}^{\dagger}}{\partial k_{x}} \tilde{H}_{k}^{\dagger} \frac{\partial \tilde{D}_{k}}{\partial k_{y}} \psi_{ki} - \frac{\partial \bar{\psi}_{ki}}{\partial k_{x}} \tilde{H}_{k} \frac{\partial \tilde{D}_{k}^{-1}}{\partial k_{y}} \bar{\psi}_{ki}^{\dagger}.$$
(B6)

The second term in Eq. (B6), $\frac{\partial \bar{\psi}_{ki}}{\partial k_x} \tilde{H}_k \frac{\partial \bar{D}_k^{-1}}{\partial k_y} \bar{\psi}_{ki}^{\dagger} = \psi_{ki}^{\dagger} \frac{\partial D_k}{\partial k_x} \tilde{H}_k \frac{\partial \bar{D}_k^{-1}}{\partial k_y} \bar{\psi}_{ki}^{\dagger} - \frac{\partial \psi_{ki}^{\dagger}}{\partial k_x} \tilde{D}_k \tilde{H}_k \tilde{D}_k^{-1} \frac{\partial \bar{D}_k}{\partial k_y} \psi_{ki} = -\frac{\partial \psi_{ki}^{\dagger}}{\partial k_x} \tilde{H}_k^{\dagger} \frac{\partial \bar{D}_k}{\partial k_y} \psi_{ki}$ and $\frac{\partial \bar{D}_k}{\partial k_x} \tilde{H}_k \frac{\partial \bar{D}_k^{-1}}{\partial k_y} = 0$ for $\frac{\partial \bar{D}_k}{\partial k_x} = \begin{bmatrix} \frac{\partial D_k}{\partial k_x} & 0 \\ 0 & 0 \end{bmatrix}$, and then the two terms in Eq. (B6) vanish. Substituting Eq. (B5) into Eq. (B4), we have

$$\sum_{j=1}^{6r} \frac{\operatorname{Im}(\mathcal{V}_{kij}^{x} \mathcal{V}_{kji}^{y}) \omega_{ki} \omega_{kj}}{(\omega_{ki} - \omega_{kj})^{2}}$$

$$= 8\omega_{ki} \operatorname{Im}\left(\frac{\partial \bar{\psi}_{ki}}{\partial k_{x}} \tilde{H}_{k} \frac{\partial \psi_{ki}}{\partial k_{y}} - \frac{\partial \bar{\psi}_{ki}}{\partial k_{y}} \tilde{H}_{k} \frac{\partial \psi_{ki}}{\partial k_{x}}\right). \quad (B7)$$

Finally, we obtain

$$\kappa_{xy}^{\text{Kubo}} = \frac{\hbar}{2VT} \text{Im} \sum_{k,i=1}^{6r} \left(\frac{\partial \bar{\psi}_{ki}}{\partial k_x} \tilde{H}_k \frac{\partial \psi_{ki}}{\partial k_y} - \frac{\partial \bar{\psi}_{ki}}{\partial k_y} \tilde{H}_k \frac{\partial \psi_{ki}}{\partial k_x} \right) \\
\times \omega_{ki} n_{ki}, \tag{B8}$$

$$= \frac{\hbar}{2VT} \text{Im} \sum_{k,i=1}^{3r} \left(\frac{\partial \bar{\psi}_{ki}}{\partial k_x} \tilde{H}_k \frac{\partial \psi_{ki}}{\partial k_y} - \frac{\partial \bar{\psi}_{ki}}{\partial k_y} \tilde{H}_k \frac{\partial \psi_{ki}}{\partial k_x} \right) \\
\times \omega_{ki} (2n_{ki} + 1). \tag{B9}$$

From Eq. (B8) to Eq. (B9), we have used the symmetry properties of ω_{ki} and ψ_{ki} , so we come to Eq. (15).

APPENDIX C: DERIVATION DETAILS FOR \tilde{M}_E^z IN Eq. (19)

After a direct calculation of the canonical correlation function in Eq. (17), we obtain

$$\tilde{M}_{E}^{z} = \frac{i\hbar}{16} \frac{\partial}{\partial q_{y}} \sum_{k;i,j=1}^{6r} S_{k+q,kji} \left(\mathcal{V}_{k,k+qij}^{x} + \mathcal{V}_{k+q,kji}^{x*} \right) \times \omega_{ki} \omega_{k+qj} \frac{n_{k+qj} - n_{ki}}{\omega_{ki} - \omega_{k+qj}} \bigg|_{q \to 0},$$
(C1)

 $\bar{\psi}_{ki} \frac{\partial (\bar{H}_k + \bar{H}_{k+q})}{\partial k} \psi_{k+qj} + \psi_{ki}^{\dagger} \frac{\partial (\bar{H}_k^{\dagger} + \bar{H}_{k+q}^{\dagger})}{\partial k} \bar{\psi}_{k+qj}^{\dagger}.$ First, we calculate the interband contribution from the terms

with $i \neq j$ in Eq. (C1). When $q \rightarrow 0$, we have

$$\tilde{M}_{E}^{z,\text{inter}} = -\frac{\hbar}{8} \sum_{k;i,j=1}^{6r} \frac{\operatorname{Im}\left(\frac{\partial \bar{\psi}_{kj}}{\partial k_{y}} \psi_{ki} \mathcal{V}_{kij}^{x}\right) \omega_{ki} \omega_{kj} (n_{kj} - n_{ki})}{\omega_{ki} - \omega_{kj}}. \qquad \frac{\frac{\partial \left(\mathcal{V}_{k,k+qi}^{x} + \mathcal{V}_{k+q,ki}^{x*}\right)}{\partial q_{y}}\Big|_{q \to 0}}{\partial q_{y}}$$

$$= 2\left(2\bar{\psi}_{ki} \frac{\partial \tilde{H}_{k}}{\partial d_{x}} \frac{\partial \psi_{ki}}{\partial d_{x}} + \frac{\partial \tilde{H}_{k}}{\partial d_{x}} \frac{\partial \tilde{H}_{k}}{\partial d_{x}} \frac{\partial \psi_{ki}}{\partial d_{x}} + \frac{\partial \tilde{H}_{k}}{\partial d_{x}} \frac{\partial \psi_{ki}}{\partial d_{x}} \frac{\partial \psi_{ki}}{\partial d_{x}} + \frac{\partial \tilde{H}_{k}}{\partial d_{x}} \frac{\partial \psi_{ki}}{\partial d_{x}} \frac{\partial \psi_{ki}}{\partial d_{x}} + \frac{\partial \tilde{H}_{k}}{\partial d_{x}} \frac{\partial \psi_{ki}}{\partial d_{x}} \frac{\partial \psi_{ki}}{\partial d_{x}} + \frac{\partial \tilde{H}_{k}}{\partial d_{x}} \frac{\partial \psi_{ki}}{\partial d_{x}} \frac{\partial \psi_{ki}}{\partial d_{x}} + \frac{\partial \tilde{H}_{k}}{\partial d_{x}} \frac{\partial \psi_{ki}}{\partial d_{x}} \frac{\partial \psi_{ki}}{$$

We further have

$$\operatorname{Im}\left(\frac{\partial \bar{\psi}_{kj}}{\partial k_{y}}\psi_{ki}\mathcal{V}_{kij}^{x}\right) = \frac{1}{2}\operatorname{Im}\left(\frac{\partial \bar{\psi}_{kj}}{\partial k_{y}}\psi_{ki}\mathcal{V}_{kij}^{x} - \psi_{ki}^{\dagger}\frac{\partial \bar{\psi}_{kj}^{\dagger}}{\partial k_{y}}\mathcal{V}_{kij}^{x*}\right),\tag{C3}$$

Noting that $V_{kij}^* = V_{kji}$ and inserting Eq. (C3) into Eq. (C2),

$$\tilde{M}_{E}^{z,\text{inter}} = -\frac{\hbar}{16} \sum_{k;i,j=1}^{6r} \text{Im} \left[\left(\frac{\partial \bar{\psi}_{kj}}{\partial k_{y}} \psi_{ki} - \psi_{kj}^{\dagger} \frac{\partial \bar{\psi}_{ki}^{\dagger}}{\partial k_{y}} \right) \mathcal{V}_{kij}^{x} \right] \times \frac{\omega_{ki} \omega_{kj} (n_{kj} - n_{ki})}{\omega_{ki} - \omega_{kj}}, \tag{C4}$$

where we have interchanged i and j of the second term in Eq. (C3). Using Eq. (B3), we have

$$\tilde{M}_{E}^{z,\text{inter}} = \frac{\hbar}{32} \sum_{k;i,j=1}^{6r} \frac{\operatorname{Im}(\mathcal{V}_{kji}^{y} \mathcal{V}_{kij}^{x}) \omega_{ki} \omega_{kj} (n_{kj} - n_{ki})}{(\omega_{ki} - \omega_{kj})^{2}}$$

$$= -\frac{\hbar}{32} \sum_{k;i,j=1}^{6r} \frac{\operatorname{Im}(\mathcal{V}_{kij}^{x} \mathcal{V}_{kji}^{y} - \mathcal{V}_{kij}^{y} \mathcal{V}_{kji}^{x}) \omega_{ki} \omega_{kj} n_{ki}}{(\omega_{ki} - \omega_{kj})^{2}}.$$
(C5)

Comparing Eqs. (C5) and (B1), we finally obtain

$$\tilde{M}_{E}^{z,\text{inter}} = -\frac{\hbar}{2} \text{Im} \sum_{k;i=1}^{3r} \left(\frac{\partial \bar{\psi}_{ki}}{\partial k_{x}} \tilde{H}_{k} \frac{\partial \psi_{ki}}{\partial k_{y}} - \frac{\partial \bar{\psi}_{ki}}{\partial k_{y}} \tilde{H}_{k} \frac{\partial \psi_{ki}}{\partial k_{x}} \right) \times \omega_{ki} (2n_{ki} + 1) \qquad (C6)$$

$$= -\frac{\hbar}{2} \sum_{i=1}^{3r} \mathcal{M}_{ki}^{z} \omega_{ki} (2n_{ki} + 1) . \qquad (C7)$$

Second, we calculate the intraband contribution from the term with i = j in Eq. (C1):

$$\tilde{M}_{E}^{z,\text{intra}} = -\frac{\hbar}{16} \frac{\partial}{\partial q_{y}} \sum_{k;i=1}^{6r} \text{Im} \left[S_{k+q,ki} \left(\mathcal{V}_{k,k+qi}^{x} + \mathcal{V}_{k+q,ki}^{x*} \right) \right]$$

$$\times \frac{\omega_{ki} \omega_{k+qi} (n_{k+qi} - n_{ki})}{\omega_{ki} - \omega_{k+qi}} \bigg|_{q \to 0}.$$
(C8)

For further simplification, note that

$$\frac{\partial S_{k+q,ki}}{\partial q_y} \bigg|_{q \to 0} = \frac{\partial \bar{\psi}_{ki}}{\partial k_y} \psi_{ki},$$

$$\frac{\partial (\mathcal{V}_{k,k+qi}^x + \mathcal{V}_{k+q,ki}^{x*})}{\partial q_y} \bigg|_{q \to 0}$$

$$= 2 \left(2 \bar{\psi}_{ki} \frac{\partial \tilde{H}_k}{\partial k_x} \frac{\partial \psi_{ki}}{\partial k_y} + 2 \psi_{ki}^{\dagger} \frac{\partial \tilde{H}_k^{\dagger}}{\partial k_x} \frac{\partial \bar{\psi}_{ki}^{\dagger}}{\partial k_y} + \bar{\psi}_{ki} \frac{\partial^2 \tilde{H}_k}{\partial k_x \partial k_y} \psi_{ki} + \psi_{ki}^{\dagger} \frac{\partial^2 \tilde{H}_k^{\dagger}}{\partial k_x \partial k_y} \bar{\psi}_{ki}^{\dagger} \right), \tag{C9}$$

$$\frac{n_{k+qi} - n_{ki}}{\omega_{k+qi} - \omega_{ki}} \bigg|_{q \to 0} = n'_{ki}.$$

One can show that the sum of the last two terms in Eq. (C9) is real, so it makes no contribution. So we can write

$$\tilde{M}_{E}^{z,\text{intra}} = \frac{\hbar}{4} \sum_{k;i=1}^{6r} \text{Im} \left[2 \frac{\partial \bar{\psi}_{ki}}{\partial k_{y}} \psi_{ki} \frac{\partial \omega_{ki}}{\partial k_{x}} + \bar{\psi}_{ki} \frac{\partial \tilde{H}_{k}}{\partial k_{x}} \frac{\partial \psi_{ki}}{\partial k_{y}} + \psi_{ki} \frac{\partial \tilde{H}_{k}}{\partial k_{x}} \frac{\partial \psi_{ki}}{\partial k_{y}} \right] \omega_{ki}^{2} n_{ki}'.$$
(C10)

With $\operatorname{Im}\left[\frac{\partial \bar{\psi}_{ki}}{\partial k_{y}}\psi_{ki}\right] = -\operatorname{Im}\left[\bar{\psi}_{ki}\frac{\partial \psi_{ki}}{\partial k_{y}}\right] = \operatorname{Im}\left[\frac{\partial \psi_{ki}^{\dagger}}{\partial k_{y}}\bar{\psi}_{ki}^{\dagger}\right]$, we come

$$\tilde{M}_{E}^{z,\text{intra}} = \frac{\hbar}{4} \sum_{k;i=1}^{6r} \text{Im} \left[\bar{\psi}_{ki} \frac{\partial (\tilde{H}_{k} - \omega_{ki})}{\partial k_{x}} \frac{\partial \psi_{ki}}{\partial k_{y}} + \psi_{ki}^{\dagger} \frac{\partial (\tilde{H}_{k}^{\dagger} - \omega_{ki})}{\partial k_{x}} \frac{\partial \bar{\psi}_{ki}^{\dagger}}{\partial k_{y}} \right] \omega_{ki}^{2} n_{ki}'. \quad (C11)$$

Using $\bar{\psi}_{ki} \frac{\partial (\tilde{H}_k - \omega_{ki})}{\partial k_x} = -\frac{\partial \bar{\psi}_{ki}}{\partial k_x} (\tilde{H}_k - \omega_{ki})$ and $\psi_{ki}^{\dagger} \frac{\partial (\tilde{H}_k^{\dagger} - \omega_{ki})}{\partial k_x} =$ $-\frac{\partial \psi_{ki}^{\dagger}}{\partial k}(\tilde{H}_{k}^{\dagger}-\omega_{ki})$, we obtain

$$\tilde{M}_{E}^{z,\text{intra}} = -\frac{\hbar}{4} \sum_{k;i=1}^{6r} \text{Im} \left[\frac{\partial \bar{\psi}_{ki}}{\partial k_{x}} (\tilde{H}_{k} - \omega_{ki}) \frac{\partial \psi_{ki}}{\partial k_{y}} - \frac{\partial \bar{\psi}_{ki}}{\partial k_{y}} (\tilde{H}_{k} - \omega_{ki}) \frac{\partial \psi_{ki}}{\partial k_{x}} \right] \omega_{ki}^{2} n'_{ki}. \quad (C12)$$

Using the definitions for \mathcal{M}_{ki}^z and Ω_{ki}^z , we have

$$\tilde{M}_{E}^{z,\text{intra}} = -\frac{\hbar}{4} \sum_{k;i=1}^{6r} \left(\mathcal{M}_{ki}^{z} + \omega_{ki} \Omega_{ki}^{z} \right) \omega_{ki}^{z} n_{ki}'$$

$$= -\frac{\hbar}{2} \sum_{k'i=1}^{3r} \left(\mathcal{M}_{ki}^{z} + \omega_{ki} \Omega_{ki}^{z} \right) \omega_{ki}^{z} n_{ki}'.$$
(C13)

$$= -\frac{\hbar}{2} \sum_{k:i=1}^{3r} \left(\mathcal{M}_{ki}^z + \omega_{ki} \Omega_{ki}^z \right) \omega_{ki}^2 n'_{ki}. \tag{C14}$$

Finally, combining Eqs. (C7) and (C14), we come to Eq. (19).

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