The phonon Hall effect: theory and application

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Abstract

We present a systematic theory of the phonon Hall effect in a ballistic crystal lattice system, and apply it on the kagome lattice which is ubiquitous in various real materials. By proposing a proper second quantization for the non-Hermitian in the polarization-vector space, we obtain a new heat current density operator with two separate contributions: the normal velocity responsible for the longitudinal phonon transport, and the anomalous velocity manifesting itself as the Hall effect of transverse phonon transport. As exemplified in kagome lattices, our theory predicts that the direction of Hall conductivity at low magnetic field can be reversed by tuning the temperatures, which we hope can be verified by experiments in the future. Three phonon-Hall-conductivity singularities induced by phonon-band-topology change are discovered as well, which correspond to the degeneracies at three different symmetric center points, $\Gamma$, $K$, $X$, in the wavevector space of the kagome lattice.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In recent years, phononics, the discipline of science and technology in processing information by phonons and controlling heat flow, has become more and more exciting [1, 2]. Various functional thermal devices such as thermal diodes [3], thermal transistors [4], thermal logic gates [5], thermal memory [6], etc., have been proposed to manipulate and control phonons, the carriers of heat energy and information. And very recently, similarly to the Hall effect of electrons, Strohm \emph{et al} observed the phonon Hall effect (PHE)—the appearance of a temperature difference in the direction perpendicular to both the applied magnetic field and the heat current flowing through an ionic paramagnetic dielectric sample [7], which was confirmed later in [8]. Such an observation of the PHE was really surprising because phonons as charge-free quasiparticles, differently from electrons, cannot directly couple to the magnetic field through the Lorentz force. Since then, several theoretical explanations have been proposed [9–12] to understand this novel phenomenon. From the work of the PHE in four-terminal nano-junctions and phonon Hall conductivity in a two-dimensional periodic crystal lattice, we know that the PHE can exist even in the ballistic system.

Geometric phase effects [13, 14] are fundamentally important in understanding the electrical transport property in the quantum Hall effect [15, 16], the anomalous Hall effect [17, 18], and, as well as in anomalous thermoelectric transport [19] characterizing the underlying mechanism of the quantum spin Hall effect [20, 21]. Such an elegant connection between mathematics and physics provides a broad and deep understanding of the basic material properties. Although there is quite a difference between phonons and electrons, we can still use the topological description to study the underlying properties of the phonon transport, such as the topological phonon modes in the dynamic instability of microtubules [22] and in filamentary structures [23], Berry-phase-induced heat pumping [24], and the Berry-phase contribution of molecular vibrational instability [25].

The topological nature of the PHE was recently studied in [26], where a general expression for the phonon Hall conductivity was obtained in terms of the Berry curvatures of band structures. In [26], the authors found a phase transition in the PHE of a honeycomb lattice, explained from the topological nature and dispersion relations. From the Green–Kubo formula and considering the contributions from all the phonon bands, the authors obtained the general formula for the...
phonon Hall conductivity. Then, by looking at the phases of the polarization vectors of both the displacements and conjugate momenta as a function of the wavevector, a Berry curvature can be defined uniquely for each band. Combining the above two steps, at last the phonon Hall conductivity can be written in terms of Berry curvatures. Such a derivation gives us a clear picture of the contribution to the phonon Hall current from all phonon branches, as well as the relation between the phonon Hall conductivity and the geometrical phase of the polarization vectors, which thus helps us to understand the topological picture of the PHE. However, the process of going from the Berry phase to the heat flux and the phonon Hall conductivity looks to be not very clear and natural.

We know that for the Hall effect of electrons, in addition to the normal velocity from the usual band dispersion contribution, the Berry curvature induces an anomalous velocity always transverse to the electric field, which gives rise to a Hall current; thus the Hall effect occurs [14]. For the recently observed magnon Hall effect [27], the authors also found an anomalous velocity due to the Berry connection which is responsible for the thermal Hall conductivity. Therefore in this article we will derive the theory of the PHE in a more natural way where the Berry-phase effect inducing the anomalous velocity contributes to the extra term of the heat current. Thus it is straightforward for the Berry-phase effect to take responsibility for the PHE.

The kagome lattice, composed of interlaced triangles whose lattice points each have four neighboring points [29], has become popular in the magnetic community because the unusual magnetic properties of many real magnetic materials are associated with those characteristic of the kagome lattice [30]. A schematic figure of the kagome lattice is shown in figure 1. In this paper we also apply the PHE theory to the kagome lattice to investigate whether the mechanism of the phase transition found in [26] is general, and find how the phonon Hall conductivity, Chern numbers and the dispersion relation behave and relate to each other.

This paper is organized as follows. In section 2, we give a new systematic derivation of the theory of the PHE in terms of Berry curvatures. In this section, we first introduce the Hamiltonian and the modified second quantization, then derive the heat current density operator which includes both the normal velocity and the anomalous velocity from the Berry-phase effect. Using the Green–Kubo formula, the general formula of the phonon Hall conductivity is obtained. Then we give an application example on the kagome lattice in section 3. In this section the computational details on the dynamic matrix, the Chern numbers and the phonon Hall conductivity are given, and the behaviors and relations between the phonon Hall conductivity, Chern numbers, and the band structures are discussed. Finally, a short conclusion is presented in section 4.

2. The phonon Hall effect theory

In this section, we give the detailed derivation for the PHE theory. We use the Hamiltonian in [26] and [31], which is a positive definite Hamiltonian, to describe the ionic crystal lattice in an applied magnetic field.

2.1. The Hamiltonian and the second quantization

The Hamiltonian for an ionic crystal lattice in a uniform external magnetic field [26, 28, 31] can be written in a compact form as

$$H = \frac{1}{2}(p - \hat{A}u)^T(p - \hat{A}u) + \frac{1}{2}u^T K u$$

$$= \frac{1}{2}p^T p + \frac{1}{2}u^T (K - \hat{A}^2) u + u^T \hat{A}^T p. \quad (1)$$

Here, $u$ is a column vector of displacements from lattice equilibrium positions for all the degrees of freedom, multiplied by the square root of mass, $p$ is the conjugate momentum vector, and $K$ is the force constant matrix. The superscript $T$ stands for the matrix transpose. $\hat{A}$ is an antisymmetric real matrix, which is block diagonal with elements $\Lambda = \begin{pmatrix} 0 & h \\ h & 0 \end{pmatrix}$ (in two dimensions), where $h$ is proportional to the magnetic field, and has the dimension of frequency. For simplicity, we will call $h$ the magnetic field later. According to [9], $h$ is estimated to be 0.1 cm$^{-1} \approx 3 \times 10^8$ rad Hz at a magnetic field $B = 1$ T and a temperature $T = 5.45$ K, which is within the possible range of the coupling strength in ionic insulators [34, 35]. The on-site term, $u^T \hat{A} p$, can be interpreted as the Raman (or spin–phonon) interaction. Based on quantum theory and symmetry considerations, the phenomenological description of the spin–phonon interaction was proposed many years ago [32–39]. From the first line of equation (1), we find that both of the two terms are positive definite, thus the Hamiltonian (1) is positive definite. The origin of the Hamiltonian for the PHE is discussed in detail in the supplementary information of [26].

The Hamiltonian equation (1) is quadratic in $u$ and $p$. We can write the linear equation of motion as

$$\dot{p} = -(K - \hat{A}^2) u - \hat{A} p, \quad (2)$$
\[ \ddot{u} = p - \dot{A}u. \] (3)

The equation of motion for the coordinate is

\[ \ddot{u} + 2\dot{A}\dot{u} + Ku = 0. \] (4)

Since the lattice is periodic, we can apply Bloch’s theorem, \( u_l = e^{i\mathbf{k}\cdot\mathbf{R}}u_0 \). The polarization vector \( \epsilon \) satisfies

\[ \begin{bmatrix} -i\omega + A \end{bmatrix}^2 + D \epsilon = 0, \] (5)

where \( D(k) = -A^2 + \sum_F K_{ll} e^{i\mathbf{k}\cdot\mathbf{R}_l} \) denotes the dynamic matrix and \( A \) is block diagonal with elements \( \Lambda, D, K_{ll}, \) and \( A \) are all \( nd \times nd \) matrices, where \( n \) is the number of particles in one unit cell and \( d \) is the dimension of the vibration.

From equation (5), we can require the following relations:

\[ \epsilon_k^* = \epsilon_k; \quad \omega_{\pm k} = \omega_{\mp k}. \] (6)

Here, we use the short-hand notation \( k = (\mathbf{k}, \sigma) \) to specify both the wavevector and the phonon branch, and \( -k \) means \( (-\mathbf{k}, -\sigma) \). In normal lattice dynamic treatment, we usually take \( \sigma, \omega \geq 0 \) as a convention, and require \( \omega_{\pm k} = \omega_{\mp k} \).

For the current problem, this is not true [26, 31]. It is more convenient to have the frequency taking both positive and negative values and require the above equation (6). And from equation (3), the momentum and displacement polarization vectors are related through

\[ \mu_k = -i\omega_k \epsilon_k + A\epsilon_k. \] (7)

Equation (5) is not a standard eigenvalue problem. However, we can describe the system by the polarization vector \( x = (\mu, \epsilon)^T \), where \( \mu \) and \( \epsilon \) are associated with the momenta and coordinates, respectively. Using Bloch’s theorem, equations (2) and (3) can be recast as

\[ \frac{\partial}{\partial t} x = H_{\text{eff}} x, \quad H_{\text{eff}} = i \begin{pmatrix} -A & -D \\ N_{nd} & -A \end{pmatrix}. \] (8)

Here the \( I_{nd} \) is the \( nd \times nd \) identity matrix. Therefore, the eigenvalue problem of the equation of motion (8) reads

\[ H_{\text{eff}} x_k = \omega_k x_k, \quad x_k^T H_{\text{eff}} = \omega_k x_k^T, \] (9)

where the right eigenvector \( x_k = (\mu_k, \epsilon_k)^T \), the left eigenvector \( x_k^T = (\epsilon_k^*, -\mu_k^*)/(-2i\omega_k) \), and with such a choice the second quantization of the Hamiltonian equation (1) holds, which will be proved later. Because the effective Hamiltonian \( H_{\text{eff}} \) is not Hermitian, the orthonormal condition then holds between the left and right eigenvectors, as

\[ x_{\sigma, k}^T x_{\sigma', k} = \delta_{\sigma, \sigma'}. \] (10)

We also have the completeness relation

\[ \sum_{\sigma} x_{\sigma, k} \otimes x_{\sigma, k}^T = I_{2nd}. \] (11)

The normalization of the eigenmodes is equivalent to [11]

\[ \epsilon_k^* \epsilon_k + \frac{i}{\omega_k} \epsilon_k^* A \epsilon_k = 1. \] (12)

From the eigenvalue problem (9), we know that the completed set contains the branch of the negative frequency. And from the topological nature of the PHE [26], the formula of the phonon Hall conductivity can be written in a form comprising the contribution of all the branches including both positive and negative frequency branches. In order to simplify the notation, for all the branches, we define

\[ a_{-k} = a_k^*. \] (13)

The time dependence of the operators is given by

\[ a_k(t) = a_k e^{-i\omega_k t}, \]

\[ a_k^*(t) = a_k^* e^{i\omega_k t}. \] (15)

The commutation relation is

\[ [a_k, a_{k'}^*] = \delta_{k, k'} \text{sign}(\sigma). \] (16)

And we can get

\[ (a_k^* a_k) = f(\omega_k) \text{sign}(\sigma); \]

\[ (a_k a_{k'}^*) = [1 + f(\omega_k)] \text{sign}(\sigma). \] (18)

Here, \( f(\omega_k) = (e^{i\omega_k/\hbar} - 1)^{-1} \) is the Bose distribution function.

The displacement and momentum operators can be written in the following second quantization forms:

\[ u_l = \sum_k \epsilon_k e^{i\mathbf{k}\cdot\mathbf{R}_l} \sqrt{\frac{2\hbar}{N|\omega_k|}} a_k; \]

\[ p_l = \sum_k \mu_k e^{i\mathbf{k}\cdot\mathbf{R}_l} \sqrt{\frac{2\hbar}{N|\omega_k|}} a_k. \] (20)

Here, \( |\omega_k| = \omega_k \text{sign}(\sigma) \). We can verify that the canonical commutation relations are satisfied, \( [u_l, p_{l'}] = i\hbar \delta_{ll'} \), by using the completeness equation (11) and the commutation relation (16). The Hamiltonian equation (1) then can be written as [31]

\[ H = \hbar \sum_{l, l'} \chi_l^T \begin{pmatrix} A\delta_{l, l'} & K_{l, l'} \omega_{l, l'}^2 \omega_{l, l'}^2 \end{pmatrix} \chi_{l'}. \] (21)

where

\[ \chi_l = \begin{pmatrix} p_l \\ u_l \end{pmatrix} = \sqrt{\frac{\hbar}{N}} \sum_k x_k e^{i\mathbf{k}\cdot\mathbf{R}_l} a_k; \]

\[ \chi_{l'} = \begin{pmatrix} u_{l'} \\ -p_{l'} \end{pmatrix} = \sqrt{\frac{\hbar}{N}} \sum_k x_k^* e^{-i\mathbf{k}\cdot\mathbf{R}_l} a_k^*. \] (23)

Here, \( c_k = \sqrt{\frac{\hbar}{2\omega_k}} \) and \( \tilde{c}_k = (-2i\omega_k)^{-1/2} \). It is easy to verify that \( [\chi_l, \chi_{l'}^T] = -i\hbar \delta_{ll'} \). Because of \( e^{i\mathbf{R}_l\cdot\mathbf{k}} e^{i\mathbf{R}_l'\cdot\mathbf{k}} = e^{i\mathbf{R}_l\cdot(\mathbf{k}-\mathbf{k}')} + e^{i\mathbf{R}_l\cdot(\mathbf{k}'+\mathbf{k})} \) and the definition of the dynamic matrix \( D \), then the Hamiltonian can be written as

\[ H = \frac{\hbar}{2N} \sum_{k, k', \ell} e^{i\mathbf{R}_l\cdot(\mathbf{k}-\mathbf{k}')} c_k c_{k'} \chi_l^T \begin{pmatrix} A \delta_{\ell, \ell'} & D(k') \\ -D(k) \omega_{\ell, \ell'}^2 \end{pmatrix} \chi_{l'} a_k a_{k'}^* \]

\[ = \frac{\hbar}{2N} \sum_{k, k', \ell} e^{i\mathbf{R}_l\cdot(\mathbf{k}-\mathbf{k}')} c_k c_{k'} \chi_l^T H_{\text{eff}} \chi_{l'} a_k a_{k'}^* \]

\[ = \frac{1}{2} \sum_k \hbar |\omega_k| a_k a_{k}^*. \] (24)
which contains the identity \( \sum_k e^{i\mathbf{R}_k \cdot (\mathbf{k} - \mathbf{k}')} = N \delta_{kk'} \) and the eigenvalue problem (9). Using the relations (13) and (16), it is easy to prove that equation (24) is equivalent to the form \( H = \sum_{\sigma, \sigma' \rightarrow k} \hbar \omega_{\sigma} (a_\sigma^\dagger a_\sigma + 1/2) \), which only includes the nonnegative branches.

2.2. The heat current operator

The heat current density can be computed as [40]

\[
J = \frac{1}{2V} \sum_{i,j,\sigma} (\mathbf{R}_i - \mathbf{R}_j) \mathbf{u}_i^T \mathbf{K}_{ij} \mathbf{u}_j,
\]

where \( V \) is the total volume of \( N \) unit cells. Because of the equation of motion (3), we can rewrite the heat current as

\[
J = \frac{1}{4V} \sum_{i,j,\sigma} \tilde{\chi}_i M_{ij} \mathbf{X}_j.
\]

Inserting equations (22) and (23), we obtain

\[
J = \frac{\hbar}{4VN} \sum_{k,k',l,j} \tilde{c}_k c_{k'} e^{i(\mathbf{R}_k - \mathbf{R}_k') \mathbf{k} - \mathbf{R}_j) \mathbf{k}'} \tilde{\chi}_k \mathbf{M}_{ij} \mathbf{X}_j a_{k'}^\dagger a_{k'},
\]

Because of

\[
\sum_i \mathbf{R}_i = \sum_i \mathbf{R}_i - \mathbf{k} = \sum_i \mathbf{R}_i - \mathbf{R}_j = \mathbf{0},
\]

the heat current can be written as

\[
J = \frac{\hbar}{4V} \sum_{\sigma,\sigma',k} \tilde{c}_{\sigma,k} c_{\sigma',k} \tilde{\chi}_k \mathbf{M}_{ij} \mathbf{X}_j a_{\sigma'}^\dagger a_{\sigma},
\]

where we use

\[
\frac{\partial H^2_{\text{eff}}}{\partial \mathbf{k}} = \left( \begin{array}{cc} \frac{\partial D}{\partial \mathbf{k}} & (\frac{3}{2} A) \\ 0 & -\frac{12}{5} \frac{\partial D}{\partial \mathbf{k}} + \frac{3}{5} A \end{array} \right)
\]

by making the first derivative of the square of the effective Hamiltonian (8) with respect to the wavevector \( \mathbf{k} \), we have

\[
H_{\text{eff}} X = \Omega \tilde{X}; \quad \tilde{X}^T H_{\text{eff}} = \Omega \tilde{X}^T,
\]

where the \( 2nd \times 2nd \) matrices \( X = (x_1, x_2, \ldots, x_{2nd}) = \{ x_\sigma \} \) (the system has 2nd phonon branches), \( \tilde{X} = \{ \tilde{x}_\sigma \} \), and \( \Omega = \text{diag}(\omega_1, \omega_2, \ldots, \omega_{2nd}) = \{ \omega_\sigma \} \). Because of the completeness relation (11), \( X X^T = 2nd \), we get

\[
H_{\text{eff}}^2 = \Omega^2 \tilde{X}^T.
\]

By calculating the derivative of the above equation, and using the definition of Berry connection,

\[
\mathbf{A} = \tilde{X}^T \frac{\partial X}{\partial \mathbf{k}},
\]

taking the first derivative of equation (33) with respect to \( \mathbf{k} \), we obtain

\[
\frac{\partial H^2_{\text{eff}}}{\partial \mathbf{k}} = X \left( \frac{\partial \Omega^2}{\partial \mathbf{k}} + [\mathbf{A}, \Omega^2] \right) \tilde{X}^T.
\]

Because of the orthogonality relation between the left and right eigenvectors, i.e., equation (10), at last we obtain the heat current as

\[
J = \frac{i\hbar}{4V} \sum_{\sigma,\sigma',k} \tilde{c}_{\sigma,k} c_{\sigma',k} \tilde{\chi}_k \left( \frac{\partial \Omega^2}{\partial \mathbf{k}} + [\mathbf{A}, \Omega^2] \right) a_{\sigma',k}.
\]

The first term in the brackets, \( \frac{\partial \Omega^2}{\partial \mathbf{k}} \), is a diagonal one corresponding to \( \omega_\sigma \frac{\partial \mathbf{R}_\sigma}{\partial \mathbf{k}} \) relating the group velocity. The second term in the brackets, \( [\mathbf{A}, \Omega^2] \), gives the off-diagonal elements of the heat current density, which can be regarded as the contribution from anomalous velocities similar to the one in the intrinsic anomalous Hall effect. The Berry connection \( \mathbf{A} \) or we can call it Berry vector potential matrix (the Berry vector potential defined in [26], \( \mathbf{A}^0(k) \), is equal to \( i \mathbf{A}^{\sigma \sigma'} = i \mathbf{X}^{\sigma \sigma'} \)), takes the anomalous velocities to the heat current, which will take responsibility for the PHE. Therefore, the Berry vector potential comes naturally into the heat current and the PHE. Such a picture is clearer than that in [26].

2.3. The phonon Hall conductivity

Inserting the coefficients \( \tilde{c} \) and \( c \) into equation (36), we get

\[
J = \frac{\hbar}{4V} \sum_{\sigma,\sigma',k} \frac{\omega_{\sigma,k}}{\sqrt{\omega_{\sigma,k} \omega_{\sigma',k}}} a_{\sigma',k} \left( \frac{\partial \Omega^2}{\partial \mathbf{k}} + [\mathbf{A}, \Omega^2] \right) a_{\sigma,k}.
\]

This expression is equivalent to that given in [26] and [31].

Based on such an expression of the heat current, the phonon Hall conductivity can be obtained through the Green–Kubo formula [41]:

\[
\kappa_{xy} = \frac{V}{h T} \int_0^{h/(kT)} d\lambda \int_0^{\infty} dt \left[J^x (-i\lambda) J^y(t)\right]_{\text{eq}},
\]

where the average is taken over the equilibrium ensemble with Hamiltonian \( H \). The time dependences of the creation and annihilation operators are given as equations (14) and (15), which are also true if \( t \) is imaginary. From the Wick theorem, we have

\[
\langle a_{\sigma',k} a_{\sigma,k} a_{\sigma',k} a_{\sigma,k} \rangle = \langle a_{\sigma',k} a_{\sigma,k} \rangle \langle a_{\sigma',k} a_{\sigma,k} \rangle + \langle a_{\sigma',k} a_{\sigma,k} \rangle \langle a_{\sigma',k} a_{\sigma,k} \rangle + \langle a_{\sigma',k} a_{\sigma,k} \rangle \langle a_{\sigma',k} a_{\sigma,k} \rangle.
\]

Using the properties of the operators \( a^\dagger \) and \( a \) as in equation (17), we have

\[
\langle a_{\sigma',k} a_{\sigma,k} \rangle \langle a_{\sigma',k} a_{\sigma,k} \rangle = \langle a_{\sigma',k} a_{\sigma,k} \rangle \langle a_{\sigma',k} a_{\sigma,k} \rangle + \langle a_{\sigma',k} a_{\sigma,k} \rangle \langle a_{\sigma',k} a_{\sigma,k} \rangle + \langle a_{\sigma',k} a_{\sigma,k} \rangle \langle a_{\sigma',k} a_{\sigma,k} \rangle.
\]

(39)

By taking the first derivative of equation (33) with respect to \( \mathbf{k} \), we obtain

\[
\frac{\partial H^2_{\text{eff}}}{\partial \mathbf{k}} = X \left( \frac{\partial \Omega^2}{\partial \mathbf{k}} + [\mathbf{A}, \Omega^2] \right) \tilde{X}^T.
\]

(35)

Because of the orthogonality relation between the left and right eigenvectors, i.e., equation (10), at last we obtain the heat current as

\[
J = \frac{i\hbar}{4V} \sum_{\sigma,\sigma',k} \tilde{c}_{\sigma,k} c_{\sigma',k} \tilde{\chi}_k \left( \frac{\partial \Omega^2}{\partial \mathbf{k}} + [\mathbf{A}, \Omega^2] \right) a_{\sigma',k}.
\]
Similarly to [26], the diagonal term in the brackets $\frac{\partial^2 \Omega}{\partial \omega \partial \epsilon}$ corresponding to $\omega_0 \neq \omega_2$ has no contribution to the phonon Hall conductivity because it is an odd function of $\bm{k}$. Because of the off-diagonal term

$$[A_{k_x}, \Omega^2]_{\sigma, \sigma'} = (\omega_0^2 - \omega_2^2) A^{\sigma\sigma'}_{k_x}$$  \hspace{1cm} (41)$$
and $A^{\sigma\sigma'}_{k_x} = \tilde{x}_{\sigma}^x \frac{\partial \epsilon_0}{\partial k_x} \tilde{x}_{\sigma'}^x \frac{\partial \epsilon_0}{\partial k_x}$ from the definition, the phonon Hall conductivity can be written as

$$\kappa_{xy} = \frac{\hbar}{8 V T} \sum_{\bm{k}, \sigma, \sigma' \neq \sigma} \left[ f(\omega_{\sigma'}) - f(\omega_{\sigma}) \right] (\omega_{\sigma} + \omega_{\sigma'})^2 \frac{\epsilon_0^2}{4 \omega_0 \omega_2} (\omega_{\sigma} - \omega_{\sigma'})^2$$ \hspace{1cm} (42)$$
Here, we simplify the notation of the subscripts of $\omega, \epsilon$ which have the same wavevector $\bm{k}$. We can prove $\kappa_{xy} = -\kappa_{yx}$, such that

$$\kappa_{xy} = \frac{\hbar}{16 V T} \sum_{\bm{k}, \sigma, \sigma' \neq \sigma} \left[ f(\omega_{\sigma}) - f(\omega_{\sigma'}) \right] (\omega_{\sigma} + \omega_{\sigma'})^2 B^\sigma_{k_x, k_y}$$ \hspace{1cm} (43)$$

In the last step we use the relation $\tilde{x}_{\sigma}^x \frac{\partial \epsilon_0}{\partial k_x} \tilde{x}_{\sigma'}^x \frac{\partial \epsilon_0}{\partial k_x} \approx (\omega_{\sigma} - \omega_{\sigma'}) \tilde{x}_{\sigma}^x \frac{\partial \epsilon_0}{\partial k_x} \tilde{x}_{\sigma'}^x \frac{\partial \epsilon_0}{\partial k_x}$ and the definition of $\mathcal{A}$ in equation (34). And the Berry curvature is

$$B^\sigma_{k_x, k_y} = \sum_{\sigma' \neq \sigma} B^\sigma'_{k_x, k_y} = -i \sum_{\sigma'} (\mathcal{A}^\sigma'_{k_x} \mathcal{A}^{\sigma'}_{k_y} - (k_x \leftrightarrow k_y))$$ \hspace{1cm} (45)$$

The definition of Berry curvature here is the same as that of [26]; that is, $B^\sigma_{k_x, k_y} = \frac{\partial}{\partial k_x} \mathcal{A}^\sigma_{k_y} - \frac{\partial}{\partial k_y} \mathcal{A}^\sigma_{k_x}$. From the above derivation, we find that a Berry curvature can be defined uniquely for each band by looking at the phases of the polarization vectors of both the displacements and conjugate momenta as functions of the wavevector. If we only look at the polarization vector $\epsilon$ of the displacement, a Berry curvature cannot properly be defined. We need both $\epsilon$ and $\mu$. The nontrivial Berry vector potential takes responsibility for the PHE. The associated topological Chern number is obtained through integrating the Berry curvature over the first Brillouin zone as

$$C^\sigma = \frac{1}{2\pi} \int_{BZ} dk_x dk_y B^\sigma_{k_x, k_y} = \frac{2\pi}{L^2} \sum_{k} B^\sigma_{k_x, k_y}$$ \hspace{1cm} (46)$$
where $L$ is the length of the sample.

### 3. Application on the kagome lattice

In [26], we provide a topological understanding of the PHE in dielectrics with Ramon spin–phonon coupling for the honeycomb lattice structure. Because of the nature of phonons, the phonon Hall conductivity, which is not directly proportional to the Chern number, is not quantized. We observed a phase transition in the PHE, which corresponds to a sudden change of band topology, characterized by the altering of integer Chern numbers. Such PHE can be explained by touching and splitting of the phonon bands. To check whether the mechanism of the PHE is universal, in the following we apply the theory to the kagome lattice, which has been used to model many real materials [30].

#### 3.1. Calculation of the dynamic matrix $D$

In order to calculate the phonon Hall conductivity, we first need to calculate the dynamic matrix $D(k)$, for the two-dimensional kagome lattice. As shown in figure 1, each unit cell has three atoms, thus $n = 3$. We only consider the nearest neighbor interactions. The spring-constant matrix along the $x$ direction is assumed as

$$K_x = \begin{pmatrix} K_{11} & 0 & -K_{02} \\ 0 & K_{33} & 2K_{03} \\ -K_{02} & 2K_{03} & -K_{03} \end{pmatrix}.$$ \hspace{1cm} (47)$$

$K_L = 0.144 \text{ eV/\AA}^{-2}$ is the longitudinal spring constant and the transverse one $K_T$ is four times smaller. The unit cell lattice vectors are $(a, 0)$ and $(a/2, a\sqrt{3}/2)$ with $a = 1 \text{ Å}$.

To obtain the explicit formula for the dynamic matrix, we first define a rotation operator in two dimensions as

$$U(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}.$$ \hspace{1cm} (48)$$

The three kinds of spring-constant matrices between two atoms are $K_{01} = K_x$ (between atoms 1 and 2 in figure 1), $K_{02} = U(\pi/3) K_x U(-\pi/3)$ (between atoms 2 and 3), and $K_{03} = U(-\pi/3) K_x U(\pi/3)$ (between atoms 3 and 1), which are $2 \times 2$ matrices. Then we can obtain the on-site spring-constant matrix and the six spring-constant matrices between the unit cell and its nearest neighbors as

$$K_0 = \begin{pmatrix} 2(K_{01} + K_{02}) & -K_{01} & -K_{02} \\ -K_{01} & 2(K_{01} + K_{03}) & -K_{02} \\ -K_{02} & -K_{02} & 2(K_{02} + K_{03}) \end{pmatrix},$$ \hspace{1cm} (49)$$

where $K_0$ is the $6 \times 6$ identity matrix. Finally we can obtain the $6 \times 6$ dynamic matrix $D(k)$ as

$$D(k) = -A^2 + K_0 + K_1 e^{i k_1} + K_2 e^{i (k_1 + \theta)} e^{-ik_2}$$ \hspace{1cm} (50)$$

$$+ K_3 e^{i (k_1 + \theta)} e^{-ik_2} + K_4 e^{i \theta} e^{-ik_2}$$ \hspace{1cm} (51)$$

where $A^2 = -h^2 \cdot I_6$: here $I_6$ is the $6 \times 6$ identity matrix.
3.2. The PHE and the associated phase transition

After we get the expression for the dynamic matrix, we can calculate the eigenvalues and eigenvectors of the effective Hamiltonian. Inserting the eigenvalues, eigenvectors and the $D$ matrix into the formula (43), we are able to compute the phonon Hall conductivity. As is well known, in the quantum Hall effect for electrons, the Hall conductivity is just the Chern number in units of $e^2/h$ ($h$ is the Planck constant); thus with the varying of magnetic field, the abrupt change of Chern numbers directly induces the obvious discontinuity of the Hall conductivity. However, for the PHE there is an extra weight of $(\omega_0 + \omega_0')^2$ in equation (43) which cannot be moved out of the summation. As a consequence, the change of phonon Hall conductivity is smoothed at the critical magnetic field. However, in the study on the PHE in the honeycomb lattice system [26], from the first derivative of phonon Hall conductivity with respect to the magnetic field $h$, at the critical point $h_c$, we can still observe the divergence (singularity) of $d\kappa_{xy}/dh$, where the phase transition occurs corresponding to the sudden change of the Chern numbers. Can such a mechanism be applied for the kagome lattice system? In the following, we give a detailed discussion of it.

Inserting the dynamic matrix equation (48) into the effective Hamiltonian equation (9), we calculate the eigenvalues and eigenvectors of the system, and also get the dispersion relation of the system. Because each unit cell has three atoms, and we only consider the two-dimensional motion, we get six phonon branches with positive frequencies. The branches with negative frequencies have similar behavior because of $\omega_k = -\omega_k$. We show the contour map of the dispersion relation in figure 2. We can see that the dispersion relations have a six-fold symmetry. For different bands, they are different. With a changing magnetic field, the dispersion relations vary. The point $\Gamma (k = (0, 0))$ is a six-fold symmetric center; the point $K (k = (\frac{4\pi}{3}, 0))$ is a three-fold symmetric center; and the middle point of the line between two six-fold symmetric centers, $X (k = (\pi, \frac{2\sqrt{3}\pi}{3}))$ is a two-fold symmetric center.

Figure 2. The contour map of the dispersion relations for the positive frequency bands. For all the insets, the horizontal and vertical axes correspond to the wavevectors $k_x$ and $k_y$, respectively. The upper six insets are the dispersion relations for the bands 1–6 (from left to right) at $h = 0$, respectively, and $h = 10$ rad ps$^{-1}$ for the lower ones.

Figure 3. The phonon Hall conductivity versus magnetic field at different temperatures. The inset is the zoomed-in curve of the phonon Hall conductivity at weak magnetic field. The sample size $N_L = 400$.

In the following discussion, we will see the possible bands touching at these symmetric centers.

Using the formula (43), we calculate the phonon Hall conductivity of the kagome lattice systems; the results are shown in figure 3. Similarly to what was shown in [26], we find nontrivial behavior of the phonon Hall conductivity as a function of the magnetic field. When $h$ is small, $\kappa_{xy}$ is proportional to $h$, which is shown in the inset of figure 3, while the dependence becomes nonlinear when $h$ is large. As $h$ is further increased, the magnitude of $\kappa_{xy}$ increases before it reaches a maximum magnitude at a certain value of $h$. Then the magnitude of $\kappa_{xy}$ decreases and goes to zero at very large $h$. The on-site term $\tilde{A}^2$ in the Hamiltonian (1) increases with $h$ quadratically so as to blockade the phonon transport, which competes with the spin–phonon interaction. Because of the coefficient of $f(\omega_k)$ in the summation of formula (43), the sign of the Hall conductivity will change with temperature, which
is clearly shown in the inset of figure 3. While the phonon Hall conductivity at weak magnetic field is always positive for the honeycomb lattice, the sign reversal of the phonon Hall conductivity with temperature for the kagome lattices is novel and interesting, which could be verified by future experimental measurements.

We plot the curves of the Chern numbers of bands 2 and 3 as a function of the magnetic field in figure 4. The phonon Hall conductivity at $T = 50$ K is also shown for comparison. To calculate the integer Chern numbers, a large number of $k$-sampling points $N$ is needed. However, there is always a zero eigenvalue at the $\Gamma$ point of the dispersion relation, which corresponds to a singularity of the Berry curvature. Therefore, we cannot sum up the Berry curvature very near this point to obtain the Chern number of this band, unless we add a negligible on-site potential $\frac{1}{2}uV_{\text{on-site}}u$ to the original Hamiltonian [26], which will not change the topology of the space of the eigenvectors. In figure 4, we set $V_{\text{on-site}} = 10^{-3}K_L$. The Chern numbers of bands 2 and 3 have three jumps with the increase of the magnetic field, although the phonon Hall conductivity is continuous. For the other bands, the Chern numbers stay constant: $C^1 = C^4 = -1$, $C^5 = 0$, and $C^6 = 1$. For the electronic Hall effect, we know that it is quantized because the Hall conductivity is directly proportional to the quantized Chern numbers. Here we also find the quantized effect of the Chern numbers for the honeycomb lattice system, for the kagome lattice system there are three, corresponding to the Chern numbers of bands 2 and 3, respectively (right scale). The solid line corresponds to the phonon Hall conductivity at $T = 50$ K (left scale); the dashed and dotted lines correspond to the Chern numbers of bands 2 and 3, respectively (right scale). The inset shows the second derivative with respect to the magnetic field $d^2\kappa_{xy}/dh^2$ (vertical axis) versus the magnetic field $h$ (horizontal axis) at $T = 50$ K.

The touching and splitting of the phonon bands near the critical magnetic field induces the abrupt change of the Chern numbers of the phonon band [26]. In [26], for the PHE in the honeycomb lattices, we know that bands 2 and 3 are going to touch each other at the $\Gamma$ point if the magnetic field increases to $h_z$; at the critical magnetic field, the degeneracy occurs and the two bands possess a cone shape; above the critical point $h_c$, the two bands split up. Therefore, the difference Chern numbers have some sudden jumps. From the discussion in [26], the discontinuity of the Chern numbers corresponds to phase transitions and would relate to the divergence of the derivative of the phonon Hall conductivity.

Figure 5 shows the curves of the derivative of the phonon Hall conductivity $d\kappa_{xy}/dh$ at $T = 50$ K and the Chern numbers of bands 2 and 3 in the vicinity of the magnetic fields. The solid line corresponds to $d\kappa_{xy}/dh$ at $T = 50$ K (left scale); the dashed and dotted lines correspond to the Chern numbers of bands 2 and 3, respectively (right scale). The inset shows the second derivative of the phonon conductivity, which is shown in the inset of figure 5, across which phase transitions occur. For different temperatures, the phase transitions occur at exactly the same critical values. Thus the temperature-independent phase transition does not come from the thermodynamic effect, but is induced by the topology of the phonon band structure, which corresponds to the sudden change of the Chern numbers. While there is one discontinuity of the Chern numbers for the honeycomb lattice system, for the kagome lattice system there are three, corresponding to the divergence of the derivative of the phonon conductivity, which can be seen in figure 5.
between the two bands decreases below and increases above the critical magnetic field, and is zero at the critical point. The eigenfrequency difference is in the denominator of the Berry curvature; thus the variation of the difference around the critical magnetic field dramatically affects the Berry curvature of the corresponding bands. In the kagome lattice systems, we find that the touching and splitting of the phonon bands not only occurs at the \( \Gamma \) point, but also occurs at other points, which is shown in figure 6. At the first critical point \( h_{c1} \), the bands 2 and 3 touch at the point \( K \) (marked by a square with the number 1); at \( h_{c2} \) the two bands touch at \( X \) (marked by a square with the number 2); while only for the third critical point \( h_{c3} \), do bands 2 and 3 degenerate at the point \( \Gamma \) (marked by a square with the number 3). From the contour maps of bands 2 and 3, we clearly see that at the critical magnetic fields \( h_{c1} \), \( h_{c2} \), and \( h_{c3} \), there is a local maximum for the band 2 and a local minimum for the band 3. Thus for all the critical magnetic fields where the Chern numbers have abrupt changes, in the wavevector space we can always find the phonon bands touching and splitting at some symmetric center points.

Therefore, through the study of the PHE in both honeycomb lattices [26] and kagome lattices, we find discontinuous jumps in the Chern numbers, which manifest themselves as singularities of the first derivative of the phonon Hall conductivity with respect to the magnetic field. Such an associated phase transition is connected with the crossing of bands 2 and 3, which corresponds to the touching between an acoustic band and an optical band. However,
we cannot observe a similar associated phase transition in triangular lattices because there are no optical bands where the Chern number of each band remains zero while the phonon Hall conductivity is nonzero because of the nonzero Berry curvatures.

4. Conclusion

We present a new systematic theory of the PHE in the ballistic crystal lattice system, and give an example application of the PHE in the kagome lattice which is a model structure of many real magnetic materials. By the proper second quantization of the Hamiltonian, we obtain the formula for the heat current density, which considers all the phonon bands including both positive and negative frequencies. The heat current density can be divided into two parts; one is diagonal, the other is off-diagonal. The diagonal part corresponds to the normal velocity, and the off-diagonal part corresponds to the anomalous velocity which is induced by the Berry vector potential. Such an anomalous velocity induces the PHE in the crystal lattice. Based on such a heat current density we derive the formula of the phonon Hall conductivity which is in terms of the Berry curvatures. From the application on the kagome lattices, we find that at weak magnetic field, the phonon Hall conductivity changes sign with varying temperatures. It is also found that the mechanism on the PHE for the relation between the phonon Hall conductivity, the Chern numbers and the phonon band structure can be generally applied for kagome lattices. While there is only one discontinuity in the PHE of honeycomb lattices, in kagome lattices there are three singularities induced by the abrupt change of the phonon band topology, which correspond to the touching and splitting at three different symmetric center points in the wavevector space.

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