Berry phase of phonons and thermal Hall effect in nonmagnetic insulators

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A mechanism for phonon Hall effect (PHE) in non-magnetic insulators under an external magnetic field is theoretically studied. PHE is known in (para)magnetic compounds, where the magnetic moments and spin-orbit interaction play an essential role. In sharp contrast, we here show that a non-zero Berry curvature of acoustic phonons is induced by an external magnetic field due to the correction to the adiabatic Born-Oppenheimer approximation. This results in the finite thermal Hall conductivity $\kappa_H$ in nonmagnetic band insulators. Our estimate of $\kappa_H$ for a simple model gives $\kappa_H \sim 1.0 \times 10^{-5} [\text{W/Km}]$ at $B = 10 [\text{T}]$ and $T = 150 [\text{K}]$.

Introduction — Hall effects are one of the most important subjects in condensed matter physics. It provides the information on the sign and density of the carriers in semiconductors, and the shape of the Fermi surface in metals. Since the discovery of quantum Hall effect [1], the close connection of Hall effects to topological nature of electronic states in solids has become a keen issue. In addition to the quantum Hall effect, the anomalous Hall effect in metallic magnets [2], and spin Hall effect in semiconductors [3] are interpreted as the consequence of the geometric phase of Bloch wavefunctions, i.e., Berry phase in solids [4]. Berry phase can be nonzero even for the neutral particles such as photons [5] and magnons [6–8], and the thermal Hall effects of these particles are observed experimentally in Ref. 9 and Ref. 10, respectively.

Phonon is another neutral particle in solids, and the thermal Hall effect of phonons, phonon Hall effect (PHE), has been studied experimentally [11, 12] and theoretically [13–19]. In most of the theoretical works, the Raman-type interaction is assumed whose Hamiltonian reads

$$H_{\text{Raman}} = \lambda M \cdot (u \times P). \quad (1)$$

where $M$ is the electronic magnetization, $u$ the displacement of nucleus, and $P$ the momentum of nucleus. This coupling $\lambda$ is supposed to originate from the spin-lattice interaction, but the microscopic theory for $\lambda$ is missing in most of the cases.

The charge of the phonon, however, is a subtle issue because the atomic nuclei are positively charged, which is compensated by the electrons. Then the screening effect of electrons should be treated properly to ensure the neutral nature of phonons. The conventional formalism to study the electron-phonon coupled system is the Born-Oppenheimer (BO) approximation [20], which uses the fact that the electron mass $m$ is much lighter than that of atoms $M$. Writing the wave function as the product of electronic and nuclear part, i.e., $\Psi(r, R) = \psi_\text{el}(r, R)\phi_\text{nucl}(R)$ with $r$ and $R$ being the position of electrons and nuclei, respectively, the ratio of the length scales $\ell_\text{el}$ and $\ell_\text{nucl}$ for $\psi_\text{el}(r, R)$ and $\phi_\text{nucl}(R)$ is estimated as

$$\ell_\text{el}/\ell_\text{nucl} \sim (m_\text{nucl}/m_\text{el})^{1/4}. \quad (2)$$

Therefore, the derivative $\nabla_R$ on $\psi_\text{el}(r, R)$ can seemingly be neglected and the Schrödinger equation for $\phi_\text{nucl}(R)$ contains the information of electrons only through the ground state energy $E(R)$ of electrons which depends on the nuclear position $R$ regarded as the static parameter. In this approximation, however, the nucleus feels the external electromagnetic field as the particle with positive charge $Ze$. This drawback can be remedied by introducing the Berry phase into the Hamiltonian of nucleus [20].

$$H_\text{nucl} = \sum_n \frac{(P_n - ZeA_n - a_n(R))^2}{2m_\text{nucl}} + U(R), \quad (3)$$

where $n$ specifies the atom and $R = (R_1, \cdots, R_N)$ represents the coordinates of all the $N$ atoms. Here, $a_n(R)$ is the Berry connection given by

$$a_n(R) = i\hbar \langle \psi_\text{el}(r, R)|\nabla_{R_n}\psi_\text{el}(r, R) \rangle, \quad (4)$$

where $|\psi_\text{el}(R)\rangle$ is the state of electrons with dependence on nuclear coordinates. $U(R)$ is the sum of the electronic ground state energy and the interaction between nuclei.

This $a_n(R)$ cancels the vector potential $A_n$ for the external electromagnetic field in the case of single atom, i.e., the screening of the positive charge of nucleus by electrons is recovered [20]. For the hydrogen molecule, it has been discussed that this screening is perfect for the center-of-mass motion while the magnetic field effect survives for the relative motion of the two atoms [21]. Therefore, the effect of the magnetic field on the phonons in crystal remains an important issue to be studied.

In the present Letter, we study theoretically the Berry phase appearing in the phonon Hamiltonian and the consequent thermal Hall effect in a trivial band insulator. Our model is the spinless fermion model with 1s orbital at each site, and there are no magnetic moments or spin-orbit interaction. Therefore, the effect of the magnetic field is only through the orbital motion of electrons and nuclei. As for the electrons, the Lorentz force is acting to produce the weak orbital diamagnetism but there is no thermal Hall effect because of the energy gap in the low temperature limit. As for the phonons, on the other hand, the acoustic phonons
have gapless dispersions, and hence can be excited thermally even at low temperature.

**Berry curvature and screening** — From the Berry connection given in Eq. (4), we obtain the Berry curvature \( F_{\mu \nu} \) as

\[
F_{\mu \nu} = \partial_\mu a_\nu - \partial_\nu a_\mu - 2\hbar \operatorname{Im} \left( \partial_\mu \psi_\alpha(r, R) | \partial_\nu \psi_\alpha(r, R) \right).
\]  (5)

Here we introduced the symbol \( \mu = (n, \alpha) \) for the \( \alpha \)-component of \( n \)-th nucleus. Therefore, \( F_{\mu \nu} \) is the tensor with \( 3N \times 3N \) components. We also denote it by \( F_{nm}^{\alpha \beta} \) in order to emphasize the nuclear and spacial indices. We note that, as mentioned by Resta [22], \( F_{nm}^{\alpha \beta} \) is antisymmetric for the exchange of \( \mu \) and \( \nu \), but not for \( \alpha \) and \( \beta \), i.e., the condition

\[
F_{nm}^{\alpha \beta} = -F_{nm}^{\beta \alpha} = F_{nm}^{\alpha \beta}
\]  (6)

is not always true.

The EoM of nuclei is obtained from Eq. (3):

\[
\dot{R}_n^\alpha = -\partial_{n\alpha} U + e^{\alpha \beta \gamma} V_n^\beta Z e B^\gamma - \sum_m V_m^\gamma F_{nm}^{\alpha \gamma}.
\]

When Eq. (6) holds, one can define a vector \( b_{nm}^{\alpha \beta} := 1/2 \epsilon^{\alpha \beta \gamma} F_{nm}^{\gamma \beta} \), by which the last term turns into \( \sum_m \epsilon^{\alpha \beta \gamma} V_m^\beta b_{nm}^\gamma \). This means that \( b_{nm} \) works as an effective magnetic field in the system and induces effective Lorentz force.

In a Hydrogen-like atom under magnetic field, the Berry curvature contribution cancels the external magnetic field [20]. The key point is the \( U(1) \) phase attached to the wave function due to the magnetic field. The atomic orbital \( \varphi(r-R) \) acquires an extra phase under the magnetic field:

\[
\varphi(r-R) \rightarrow \varphi'(r-R) = \varphi(r-R) e^{iA(R) \cdot r}.
\]  (7)

Here, we have fixed the gauge and used the symmetric gauge. Although the manner of attaching the phase is a subtle problem, it is known that, as for the symmetric gauge, Eq. (7) yields physically correct results up to \( B \)-linear order. In calculating the curvature, the derivative with respect to the nuclear coordinates is modified by this additional phase, which extracts the effect from the magnetic field.

On the other hand, the situation is quite different if the system contains two or more nuclei. In Hydrogen molecule, for instance, cancellation of the external magnetic field and the Berry curvature is perfect for the translational motion, but not for the relative motion of the two nuclei [21]. In general cases, the screening of the magnetic field is guaranteed only for the translational motion, described by

\[
\sum_{nm} F_{nm}^{\alpha \beta} = -N \epsilon^{\alpha \beta \gamma} e B^\gamma.
\]  (8)

**Effective Hamiltonian for the band insulator** — As a theoretical model, we here study the Berry curvature of phonons in a two-dimensional square lattice with \( N \) nuclei and the same number of spinless electrons. Each electron is tightly bound to each atom, and then the wave function for the non-interacting electrons is given by the Slater determinant of the 1s wave functions of all the \( N \) atoms. We denote the single-particle state of the \( i \)-th electron at the \( n \)-th nucleus by \( \phi_{in} = \varphi_i(r_i, R_n) \), given in Eq. (7). The many-body wavefunction is proportional to the determinant of \( \Phi(r, R) \), an \( N \times N \) matrix whose \((i, n)\)-component is given by \( \phi_{in} \).

The key factor which characterizes the Berry curvature of electron-phonon coupled systems is the overlap integral between the orbitals of \( n \)-th and \( m \)-th atoms, which we denote by \( S_{nm} \). The overlap integral is affected by the additional phase factor of the atomic orbital under the magnetic field. The modified overlap integral, \( S'_{nm} := \int d^3 r_i \phi_{in}^* \phi_{im} \), is given by \( S'_{nm} = S_{nm} e^{i\theta_{nm}} + O(B^2) \), where \( \theta_{nm} := \frac{\pi}{\hbar} A(R_n) \cdot R_m \). For brevity, we here define two matrices, \( S \) and \( S' \), whose \((n, m)\) components are \( S_{nm} \) and \( S'_{nm} \), respectively.

The normalized wave function of this system is given by

\[
\psi_{el}(r, R) = (N! \det S')^{-\frac{1}{2}} \det \Phi(r, R).  \tag{9}
\]

The general formula of \( F_{\mu \nu} \) of lattice systems is obtained by substituting \( \psi_{el}(r, R) \) into Eq. (5), which is reduced to simpler formulae in concrete models, the details of which are given in the Supplemental Materials [30]. Here, we assume that the overlap integral between the nearest-neighbor nuclei is dominant, which is valid when the lattice constant is sufficiently large. Under this assumption, \( F_{nm} \) for the square lattice is obtained up to the linear order in \( B \) [30]:

\[
a_n^\alpha = -\frac{e}{\det S} \left[ A_n^\alpha \tilde{S}_{nm} + \sum_{l \neq n} A_l^\alpha \tilde{S}_{nl} S_{nl} \right], \tag{10a}
\]

\[
F_{nm}^{\alpha \beta} = -\frac{\tilde{S}_{nm}^{\alpha \beta}}{\det S} e^{\alpha \beta \gamma} e B^\gamma - \sum_l \frac{\tilde{S}_{nl}^{\alpha \beta}}{\det S} \left[ e(A_n^\beta - A_l^\beta) \partial_{n\alpha} S_{nl} \right. \\
\left. + e(A_l^\alpha - A_n^\alpha) \partial_{n\beta} S_{nl} \right] + e(A_n^\alpha - A_m^\alpha) \partial_{m\beta} S_{nm}, \tag{10b}
\]

\[
F_{nm}^{\alpha \beta} = -\frac{\tilde{S}_{nm}^{\alpha \beta}}{\det S} e^{\alpha \beta \gamma} e B^\gamma S_{nm} + \sum_l \frac{\tilde{S}_{nl}^{\alpha \beta}}{\det S} \left[ e(A_n^\alpha - A_m^\alpha) \partial_{m\beta} S_{nm} \right. \\
\left. \left. + e(A_n^\alpha - A_m^\alpha) \partial_{m\beta} S_{nm} \right] - e(A_n^\alpha - A_m^\alpha) \partial_{m\beta} S_{nm} \right]. \tag{10c}
\]

Here, \( \tilde{S}_{nm} \) is the \((n, m)\)-component of the cofactor matrix of \( S \), and we abbreviated \( A_n^\alpha (R_n) \) to \( A_n^\alpha \). Equations (10b) and (10c) imply that the curvature is mainly dependent on the overlap integral and its derivative. The obtained expression of \( F_{nm}^{\alpha \beta} \) is antisymmetric for the exchange of \( \alpha \) and \( \beta \), and hence we can define a vector \( b_{nm}^{\alpha \beta} := 1/2 \epsilon^{\alpha \beta \gamma} F_{nm}^{\gamma \beta} \) the curvature felt by nucleus \( n \) and
FIG. 1. Molecular Berry curvature of the nearest-neighboring nuclei, \( F_{nm} \) (or, equivalently, \( b_{nm} \)), is plotted with respect to the lattice constant. The unit of the vertical and horizontal axis is taken as \( Z e B \) and the Bohr radius \( a_B \), respectively. The number of sites is \( N = 20 \times 20 \).

caused by nucleus \( m \). \( b_{nm} \) is parallel to \( B \), and the magnetic screening effect,

\[
\sum_m b_{nm} = -Z e B, \tag{11}
\]
is guaranteed, as in Eq. (8).

The effective Hamiltonian for the phonons are obtained by considering a small deviation \( u_n \) of the nuclei from its ground state position \( R_n^0 \): \( R_n = u_n + R_n^0 \). As for the interaction among nuclei, only quadratic terms of \( u_n \)'s are taken into account. The Berry curvature at the equilibrium atomic positions, i.e., \( F_{nm}^\alpha \bigg|_{R=R^0} \), is included in the Hamiltonian by the minimal coupling, as in Eq. (3). Hereafter, we omit \( ^0 \) and always take this substitution without notice. Figure 1 shows the numerical evaluation of \( F_{nm}^\alpha \) for the nearest-neighbor pair \((n,m)\). The Berry connection can be expressed by using \( b_{nm} \) up to the linear order of \( u_n \):

\[
\alpha_n = \sum_m \frac{1}{2} b_{nm} \times R_m
= \sum_m \frac{1}{2} b_{nm} \times u_m + (\text{const.}), \tag{12}
\]

where the constant term can be removed by gauge transformation. Combining the contributions from the external magnetic field and the Berry curvature, the effective vector potential becomes

\[
\alpha_n' := \frac{Ze}{c} A(R_n) + \alpha_n
= \frac{1}{2} \sum_m b_{nm} \times (u_m - u_n). \tag{13}
\]

In the second line, we used the identity Eq. (11).

The Hamiltonian of the lattice vibration is modified in the existence of \( \alpha_n' \): the resultant Hamiltonian for our model is given by

\[
H_{\text{nucl}} = \sum_n \left[ \frac{\langle F_n - \alpha_n' \rangle^2}{2 m_{\text{nucl}}} + \frac{1}{2} \sum_m u_n^T D_{nm} u_m \right] \tag{14a}
= \sum_k \left[ \frac{1}{2 m_{\text{nucl}}} \Pi_k^{\alpha\dagger} \Pi_k^{\beta} + \frac{1}{2} D_{k}^{\alpha\beta} u_k^\alpha u_k^\beta \right], \tag{14b}
\]

where \( \Pi_k := F_k - \alpha_k \) is the momentum under a magnetic field. It is noted that the commutation relationship of \( u_k \) and \( \Pi_k \) is different from that of usual canonical operators: \( [u_k^\alpha, u_q^\beta] = 0, [u_k^\alpha, \Pi_q^\beta] = i\hbar, \) and \( [\Pi_k^\alpha, \Pi_q^\beta] = i\hbar G_k^{\alpha\beta} \), where \( G_k^{\alpha\beta} := \partial_{\alpha a_k} a_k^\beta - \partial_{\beta a_k} a_k^\alpha \). We can see that the effective vector potential plays a role of the Raman interaction. Compared with the original Raman interaction, \( \alpha_n' \) does not include \( k \)-independent constant terms but second-order derivative, so that it vanishes in the \( k \to 0 \) limit. This is consistent with Eq. (45) of Ref. 19.

**Thermal Hall effect** — The effective vector potential \( \alpha_n' \) induces the thermal Hall effect of phonons. In this section, we derive the analytic expression for the thermal Hall conductance, \( \kappa_H \), and numerically estimate it.

The definition of energy current in lattice systems, which we denote \( J_E \), was given by Hardy [23] as an operator satisfying local energy conservation law. In addition to the usual Kubo formula, we have to take into account the contribution from the energy magnetization, \( M_E \), defined by \( J_E = \nabla \times M_E \) [24]. The complete formula for the thermal Hall conductance is given by

\[
\kappa_H^V = \kappa_H^{\text{Kubo}} + \frac{2 M_E}{T V}. \tag{15}
\]

The detailed calculation was given by Qin et al. [19]. General formula for the thermal Hall conductance of bosonic particles are:

\[
\kappa_H^V = -\frac{(\pi k_B)^2 T}{3h} \left[ Z_{ph} - \frac{1}{T} \int_0^\infty d\epsilon \sigma_{xy}(\epsilon) \frac{dn_B(\epsilon)}{d\epsilon} \right], \tag{15}
\]

where

\[
Z_{ph} := \sum_{i \in \text{particle bands}} \frac{1}{V} \sum_{k \in \BZ} \Omega_{ki}^z, \tag{16}
\]

\[
\sigma_{xy}(\epsilon) := -\frac{1}{V \hbar} \sum_{k \omega_{ki} \leq \epsilon} \Omega_{ki}^z. \tag{17}
\]

Here, \( \omega_{ki} \) is the frequency of the phonon of \( i \)-th mode and \( n_B(\epsilon) = 1/(e^{\beta \epsilon} + 1) \) is the Bose distribution. The Berry curvature of phonons is defined as following [16, 19]: we define two matrices \( \mathcal{A}_k \) and \( \mathcal{B}_k \) by \( \mathcal{A}_k = \begin{bmatrix} O & i\hbar \\ -i\hbar & O \end{bmatrix} \) and \( \mathcal{B}_k = \begin{bmatrix} D_k & O \\ O & 1/M \end{bmatrix} \). Here, \( \mathcal{A}_k \) is the commutation relationship of \( \xi = \begin{bmatrix} u_k \\ \Pi_k \end{bmatrix} \), and \( \mathcal{B}_k \) is the bilinear form of the
Hamiltonian in \( \xi \)-basis. From the EoM, the eigenenergy is obtained by diagonalizing \( \tilde{H}_k := A_k B_k \). We denote the eigenvectors of \( \tilde{H}_k \) by \( |v_i\rangle \). Then the Berry connection and curvature are defined by

\[
\alpha^\xi_k := - \text{Im} \langle v_i | B_k \partial_{\xi_k} | v_i \rangle, \quad (18a)
\]

\[
\Omega_k^\xi := \partial_{\xi_k} \alpha^\xi_k - \partial_{\kappa_i} \alpha^\xi_{k_i}. \quad (18b)
\]

The second term in Eq. (15) consists of a summation of Berry curvature over the Brillouin zone and over all the particle bands, \( Z_{ph} \). In the previous study, \( Z_{ph} \) is supposed to vanish in most cases [19]. For the case of magnonic systems, the summation of Chern number over particle bands is exactly zero [25]. This can be explained by the fact that the BdG Hamiltonian of the system is adiabatically connected to a trivial matrix, whose Berry curvature is zero. A parallel discussion leads to the conclusion that \( Z_{ph} = 0 \) holds exactly in our model [30], if we perturb the system to introduce the gap at \( k = 0 \) so that the Chern number is well-defined.

On the estimation of \( \kappa_H \), it is convenient to introduce the continuum approximation. The dynamical matrix and the vector potential of the general Hamiltonian of phonons with Raman-type interaction are given by \( D_{\alpha\beta} = \mu_1 k^2 \delta_{\alpha\beta} + \mu_2 k \cdot k \delta_{\alpha\beta} \) and \( a^\alpha_k = \gamma_1 \partial_{\alpha} \partial_{\beta} \epsilon^{\sigma\rho\sigma} M^\sigma u^\rho + \gamma_2 \nabla^2 \epsilon^{\alpha\gamma} M^\beta u^\gamma \) in Eq. (14b), where \( \gamma_1 \) and \( \gamma_2 \) are coupling constants [19]. The corresponding geometric curvature is \( G_{\alpha\beta} = \frac{1}{\mu_1} \epsilon^{\alpha\beta\gamma} (\gamma_1 k^2 \cdot \epsilon^{\gamma\alpha} - (\gamma_1 + 2 \gamma_2) k^2 \epsilon^{\gamma\alpha}) \). As long as the temperature is sufficiently low, i.e., the condition \( k_B T \ll \hbar \omega_{D,i} \) is satisfied for each band \( i \) (\( \omega_{D,i} := c_i \pi/k_B \) is the Debye frequency of \( i \)-th band), the contribution from small \( k \) is dominant since the derivative of the Bose distribution function, \( d n_B(\epsilon)/d\epsilon \), decreases drastically as \( h \omega_{k_B} \) becomes higher. Therefore, at sufficiently low temperature, \( \kappa_H \) is well estimated by assuming that the continuum approximation is valid over the whole Brillouin zone. Under these conditions, the thermal Hall conductance in two dimension can be calculated by

\[
\kappa_{H}^{2D} = - \frac{(\pi k_B)^2 T}{3}\frac{Z_{ph}}{h} + \frac{\Gamma^{2D} k_B T^2}{m_{nucl} h^2 c_T} \int_0^\infty dx \frac{x^3 e^x}{(e^x - 1)^2}. \quad (19)
\]

\( \Gamma^{2D} \) is a constant dependent on the ratio of sound speed of the longitudinal and transverse modes, \( \delta := c_L/c_T \), which is given by

\[
\Gamma^{2D} = 2 \pi (2 \gamma_2 - \gamma_1) M^2 \frac{(\delta - 1)^2}{\delta (\delta + 1)}. \quad (20)
\]

Now, we apply the discussion above to our model. In nonmagnetic insulators, the geometric curvature, \( b_{nm} \), plays the role of the magnetization \( M \), and it takes finite value only for nearest-neighbor nuclei. We here denote \( b_{nm} \) of nearest-neighbor nuclei by \( b \). The sum over \( m \) in Eq. (13) is reduced to the sum over nearest-neighbor nuclei, i.e., \( m \) is an integer which satisfies \( R_m^0 = R_n^0 \pm n \delta \).

\[ e_x, R_n^0 \pm e_y \] where \( e_x \) (\( e_y \)) is the lattice vector for \( x \) (\( y \))-direction. Assuming \( u_n \) is a slowly-varying parameter of \( R_n \), we expand it by the gradient as \( u_n^0 \pm a \partial_x u_n^0 + \frac{a^2}{2} \partial_x^2 u_n^0 \). Then the vector potential (13) becomes

\[
a'(R) = a^2 b \times \nabla^2 u(R). \quad (21)
\]

Therefore the coupling constants are replaced as \( \gamma_1 \to 0 \) and \( \gamma_2 M \to a^2 b^2 \).

The dependence on \( T \) of \( \kappa_{H}^{2D} \) is shown in Figure 2 by using typical parameters. Here, the thermal Hall conductance in two-dimensions is translated into one in three-dimensions by assuming that the thickness of the layer is almost the same as the lattice constant, i.e., the plotted value is \( \tilde{\kappa}_H := \kappa_{H}^{2D}/a \). Experimentally, the thermal Hall conductance in magnetic materials is \( \kappa_H \simeq 10^{-5}[\text{W/Km}] \) at \( T \simeq 5[\text{K}] \) [11, 12]. Compared to this, \( \kappa_H \) of our model is much smaller at the same temperature. However, it is detectable enough at higher temperatures. For the experimental realization, Eq. (19) implies that materials with larger overlap integral and smaller transverse sound speed are expected to show larger thermal Hall conductance even without magnetization.

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[30] See supplemental material at [url will be inserted by publisher] for the derivation of the Berry curvature for general lattice systems (Section I) and an argument for $Z_{ph} = 0$ (Section II), which includes Refs. 26–29.
Supplemental Materials: Berry phase of phonons and thermal Hall effect in nonmagnetic insulators

I. Molecular Berry curvature of lattice systems

We here show how Eqs. (10a), (10b) and (10c) in the main text are derived. Using the wave function given by the Slater determinant of all the atoms, \( \psi(\vec{r}, \vec{R}) = (N! \det S^{-\frac{1}{2}} \det \Phi(\vec{r}, \vec{R})) \), the Berry connection and curvature is calculated as

\[
a_n^\alpha = i\hbar \langle \psi_{\vec{r}} | \partial_{n\alpha} | \psi_{\vec{r}} \rangle = i\hbar \left( N \partial_{n\alpha} N | \Phi|^2 + N^2 | \Phi|^2 | \partial_{n\alpha} | \Phi \right)
\]

(1)

\[
F_{nm, \alpha\beta} = \partial_{n\alpha} a_m^\beta - \partial_{m\beta} a_n^\alpha + 2i \hbar \Im \langle \psi_{\vec{r}} | \partial_{n\alpha} \psi_{\vec{r}} | \partial_{m\beta} \psi_{\vec{r}} \rangle = 2i \hbar \Im \left( \langle \psi_{\vec{r}} \partial_{n\alpha} N | (\partial_{m\beta} N) \int d^3 r | \Phi \rangle^2 
\right.
\]

\[
+ \partial_{n\alpha} N \int d^3 r | \Phi|^2 \partial_{m\beta} | \Phi \rangle
\]

\[
+ \partial_{m\beta} N \int d^3 r | \Phi|^2 \partial_{n\alpha} | \Phi \rangle
\]

\[
+ N^2 \int d^3 r | \Phi|^2 | \partial_{n\alpha} | \Phi \rangle.
\]

(2)

In the following, some formulae are provided so as to simplify the analytic form of Eq. (2). Since we are interested in the dependence on the magnetic field, \( B \), we only extract \( B \)-linear terms.

Some formulae for the calculation of \( F_{\mu\nu} \)

The properties of \( S' \)

The derivative of \( S' \) is given by

\[
\partial_{n\alpha} S'_{nm} = \epsilon^{\mu\nu} \left[ \partial_{n\alpha} S_{nm} - i \epsilon A^\alpha_m S_{nm} \right]
\]

(3a)

\[
\partial_{m\beta} S'_{nm} = \epsilon^{\mu\nu} \left[ \partial_{m\beta} S_{nm} + i \epsilon A^\beta_n S_{nm} \right].
\]

(3b)

We here note that, since \( S_{nm} \) is dependent on the distance between \( n \) and \( m \), \( S'_{nm} = S_{mn} \) and \( \partial_{n\alpha} S_{nm} = -\partial_{m\alpha} S_{nm} \) hold.

Since \( S' \) is Hermitian by definition, \( \det S' \) is real-valued. In addition, since the wave function \( \phi \) is real, the expansion of \( \det S' \) in the imaginary unit \( i \) is equivalent to the expansion in \( B \). Therefore, there is no \( B \)-linear term in \( \det S' \):

\[
\det S' = \det S + O(B^2).
\]

(4)

The determinant of a matrix \( X \) is related with its inverse matrix \( X^{-1} \) and cofactor matrix \( \tilde{X} \) as

\[
X^{-1} = \frac{\tilde{X}}{\det X}.
\]

(5)

From here on, we denote a cofactor matrix by \( \tilde{\cdot} \), and the \((k, l)\) cofactor of the \((n, m)\)-submatrix of \( X \) by \( \tilde{X}_{mn,kl} \), where an \((n, m)\)-submatrix is defined as the \((N - 1) \times (N - 1)\) matrix \( Y^{(n,m)} \), given by

\[
Y^{(n,m)} = 
\begin{bmatrix}
X_{1,1} & \cdots & X_{1,m-1} & X_{1,m+1} & \cdots & X_{1,N} \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
X_{n-1,1} & \cdots & X_{n-1,m-1} & X_{n-1,m+1} & \cdots & X_{n-1,N} \\
X_{n+1,1} & \cdots & X_{n+1,m-1} & X_{n+1,m+1} & \cdots & X_{n+1,N} \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
X_{N,1} & \cdots & X_{N,m-1} & X_{N,m+1} & \cdots & X_{N,N}
\end{bmatrix}
\]

(6)

We note that the correspondence between the indices of \( X \) (\( i \) and \( j \)) and those of \( Y^{(n,m)} \) (\( \tilde{i} \) and \( \tilde{j} \)) is given by one-to-one mappings \( \tau_n : \{1, \cdots, N\} \setminus \{n\} \rightarrow \{1, \cdots, N - 1\} \) and \( \tau_m : \{1, \cdots, N\} \setminus \{m\} \rightarrow \{1, \cdots, N - 1\} \) such that

\[
\tilde{i} = \tau_n(i) = \begin{cases} i & i < n \\ i - 1 & i > n \end{cases},
\]

(7a)

\[
\tilde{j} = \tau_m(j) = \begin{cases} j & j < m \\ j - 1 & j > m \end{cases}.
\]

(7b)

The \((k, l)\)-submatrix of \( Y^{(n,m)} \) is the \((N - 2) \times (N - 2)\) matrix \( Z^{(k,l)} \), given by

\[
Z^{(k,l)} = 
\begin{bmatrix}
Y_{1,1}^{(n,m)} & \cdots & Y_{1,l-1}^{(n,m)} & Y_{1,l+1}^{(n,m)} & \cdots & Y_{1,N-1}^{(n,m)} \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
Y_{k-1,1}^{(n,m)} & \cdots & Y_{k-1,l-1}^{(n,m)} & Y_{k-1,l+1}^{(n,m)} & \cdots & Y_{k-1,N-1}^{(n,m)} \\
Y_{k+1,1}^{(n,m)} & \cdots & Y_{k+1,l-1}^{(n,m)} & Y_{k+1,l+1}^{(n,m)} & \cdots & Y_{k+1,N-1}^{(n,m)} \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
Y_{N-1,1}^{(n,m)} & \cdots & Y_{N-1,l-1}^{(n,m)} & Y_{N-1,l+1}^{(n,m)} & \cdots & Y_{N-1,N-1}^{(n,m)}
\end{bmatrix}
\]

(8)

Then the two kinds of cofactor matrices are given by
\[ i+j = (-1)^{i+j} \det Y^{(n,m)} = (-1)^{i+j} \begin{vmatrix} X_{1,1} & \cdots & X_{1,j-1} & X_{1,j+1} & \cdots & X_{1,N} \\ \vdots & \ddots & \vdots & \ddots & \cdots & \vdots \\ X_{i-1,1} & \cdots & X_{i-1,j-1} & X_{i-1,j+1} & \cdots & X_{i-1,N} \\ \vdots & \ddots & \vdots & \ddots & \cdots & \vdots \\ X_{i+1,1} & \cdots & X_{i+1,j-1} & X_{i+1,j+1} & \cdots & X_{i+1,N} \\ \vdots & \ddots & \vdots & \ddots & \cdots & \vdots \\ X_{N,1} & \cdots & X_{N,j-1} & X_{N,j+1} & \cdots & X_{N,N} \end{vmatrix}, \] (9)

\[ \tilde{X}_{jk} = (-1)^{k+l} \det Z^{(k,j)} \]

\[ (-1)^{k+l} \begin{vmatrix} Y_{1,1}^{(n,m)} & \cdots & Y_{1,j-1}^{(n,m)} & Y_{1,j+1}^{(n,m)} & \cdots & Y_{1,N}^{(n,m)} \\ \vdots & \ddots & \vdots & \ddots & \cdots & \vdots \\ Y_{k-1,1}^{(n,m)} & \cdots & Y_{k-1,j-1}^{(n,m)} & Y_{k-1,j+1}^{(n,m)} & \cdots & Y_{k-1,N}^{(n,m)} \\ \vdots & \ddots & \vdots & \ddots & \cdots & \vdots \\ Y_{k+1,1}^{(n,m)} & \cdots & Y_{k+1,j-1}^{(n,m)} & Y_{k+1,j+1}^{(n,m)} & \cdots & Y_{k+1,N}^{(n,m)} \\ \vdots & \ddots & \vdots & \ddots & \cdots & \vdots \\ Y_{N-1,1}^{(n,m)} & \cdots & Y_{N-1,j-1}^{(n,m)} & Y_{N-1,j+1}^{(n,m)} & \cdots & Y_{N-1,N}^{(n,m)} \\ \vdots & \ddots & \vdots & \ddots & \cdots & \vdots \\ Y_{N,1}^{(n,m)} & \cdots & Y_{N,j-1}^{(n,m)} & Y_{N,j+1}^{(n,m)} & \cdots & Y_{N,N}^{(n,m)} \end{vmatrix}, \] (10)

In the last line, we used the fact that both acting \( \tau_n \) on \( i \) (or \( \tau_m \) on \( j \)) and the exchange of \( i \) and \( k \) (or \( j \) and \( l \)) yield the same factor \(-1\) and therefore the ingredient of the determinant is always expressed in the order shown above.

In the same way as \( \det S' \), \( B \)-linear terms of \( S_{nm} \) and \( \tilde{S}_{nm;kl} \) are zero.

\[ \mathcal{N} \text{ and } \partial_n \mathcal{N} \]

\[ \mathcal{N} = \frac{1}{\sqrt{N! \det S'}} = \frac{1}{\sqrt{N! \det S}} + \mathcal{O}(B^2) \] (11)

\[ \partial_n \mathcal{N} = -\frac{1}{2 \sqrt{N!} (\det S')^{3/2}} \frac{1}{\det S'} \frac{1}{\det S} + \mathcal{O}(B^2) \]

\[ = -\frac{1}{2 \sqrt{N!} (\det S')^{3/2}} + \mathcal{O}(B^2) \]

\[ = -\frac{1}{2 \sqrt{N!} (\det S')^{1/2}} + \mathcal{O}(B^2) \]

From the 2nd line to the 3rd line of (12), the formula \( \partial \mu \det S = \det S \times \text{tr}[S^{-1} \partial \mu S] \) is used. In the last line, since the derivative \( \partial_{n\alpha} \) only hits the \( n \)-th row and column of \( S \),

\[ \text{tr}[S^{-1} \partial_{n\alpha} S] = \sum_{l(\neq n)} [S_{nl}^{-1} \partial_{n\alpha} S_{ln} + S_{ln}^{-1} \partial_{n\alpha} S_{nl}] \]

\[ = 2 \sum_{l(\neq n)} S_{nl}^{-1} \partial_{n\alpha} S_{nl} \]

\[ = \frac{2}{\det S} \sum_{l(\neq n)} \tilde{S}_{nl} \partial_{n\alpha} S_{ln}, \] (13)

In the 2nd line of (13), \( S_{nl} = S_{ln} \) and \( S_{nl}^{-1} = S_{ln}^{-1} \) are used. Due to \( S_{nn} = 1 \), the summation over \( l \) need not
include $l = n$.

\[
N \partial_{n\alpha} N = - \frac{\text{tr}[S^{-1} \partial_n S]}{2N! \det S} + \mathcal{O}(B^2)
= - \frac{1}{N!(\det S)^2} \sum_{\substack{n \neq n \\ell \neq m}} \tilde{S}_{nl} \partial_{n\alpha} S_{\ell n} + \mathcal{O}(B^2). \tag{14}
\]

\[
\partial_{n\alpha} N \times \partial_{m\beta} N = \frac{1}{N!(\det S)^3} \sum_{\substack{n \neq n \\ell \neq m}} \tilde{S}_{nl} \partial_{n\alpha} S_{\ell n} \left[ \tilde{S}_{m\ell} \partial_{m\beta} S_{\ell m} \right] + \mathcal{O}(B^2) \tag{15}
\]

The Berry connection and curvature of atomic orbitals

\[
\langle \phi_n | \partial_{n\alpha} \phi_n \rangle = \int d^3r_i \phi_{i,n}^* \partial_{n\alpha} \phi_{i,n}
= \int d^3r_i \varphi(r_i - R_n) e^{i \theta_{nn}}
\times \left[ \partial_{n\alpha} \varphi(r_i - R_n) - i e A_\alpha(r_i) \varphi(r_i - R_n) \right] e^{-i \theta_{nn}}
= \int d^3r_i \left[ \varphi(r_i - R_n) \partial_{n\alpha} \varphi(r_i - R_n)
- i e (A_\alpha(r_i - R_n) + A_\alpha(R_n)) \varphi(r_i - R_n)^2 \right]
= - i e A_\alpha(R_n). \tag{17}
\]

In the 3rd line, we used \( \int d^3r_i A_\alpha(r_i - R_n) \varphi(r_i - R_n)^2 = 0 \) due to odd parity of the integrand.

\[
\langle \phi_n | \partial_{n\alpha} \phi_m \rangle = \int d^3r_i \phi_{i,n}^* \partial_{m\beta} \phi_{i,m}
= \partial_{n\alpha} S_{nm}
= e^{i \theta_{mn}} \left[ \partial_{n\alpha} S_{nm} - i A_m^\alpha S_{nm} \right]. \tag{18}
\]

Using these integrals,

\[
\int d^3N r | \Phi|^* \partial_{n\alpha} | \Phi| = \int d^3N r | \Phi|^* \sum_j \tilde{\Phi}_{nj} \partial_{n\alpha} \phi_{jn}
= \sum_j \int [d^3(N-1) r \tilde{\Phi}_{nj}^* \tilde{\Phi}_{nj}] [d^3r_j \phi_{nj}^* \partial_{n\alpha} \phi_{jn}]
= (N - 1)! \sum_j [\tilde{S}_{nn}^i (\phi_n | \partial_{n\alpha} \phi_n) + \sum_{l \neq n} \tilde{S}_{nl} \partial_{n\alpha} S_{ln}^i]
= N! [\tilde{S}_{nn}^i (\phi_n | \partial_{n\alpha} \phi_n) + \sum_{l \neq n} \tilde{S}_{nl} \partial_{n\alpha} S_{ln}]
= N! [ie A_n^\alpha \tilde{S}_{nn} + \sum_{l \neq n} \tilde{S}_{nl} (\partial_{n\alpha} S_{nl} + i e A_l^\alpha S_{nl})]
+ \mathcal{O}(B^2)
= N! [\sum_l ie A_l^\alpha \tilde{S}_{nl} S_{ln} + \sum_{l \neq n} \tilde{S}_{nl} \partial_{n\alpha} S_{ln}] + \mathcal{O}(B^2) \tag{19}
\]

\[
\int d^3N r \partial_{n\alpha} | \Phi|^* \partial_{n\beta} | \Phi| = \int d^3N r \sum_{ij} \tilde{\Phi}_{ni}^* \tilde{\Phi}_{nj} \int d^3r_i \partial_{n\alpha} \phi_{in} \partial_{n\beta} \phi_{jn}
+ \int d^3N r \sum_{ij} \sum_{l \neq n} [ \int d^3(N-2) r \tilde{\Phi}_{nl}^* \tilde{\Phi}_{nj} \int d^3r_j \phi_{jn}^* \partial_{n\beta} \phi_{jn}^* \int d^3r_i \phi_{in}^* \partial_{n\alpha} \phi_{in}]
= \sum_i (N - 1)! \tilde{S}_{nn}^i \langle \partial_{n\alpha} \phi_n | \partial_{n\beta} \phi_n \rangle
+ \sum_i \sum_{l \neq n} (N - 2)! \tilde{S}_{nn}^i \langle \partial_{n\alpha} \phi_n | \partial_{n\beta} \phi_n \rangle
= N! \tilde{S}_{nn}^i e^{i \alpha \beta} e B^2 / 2
+ \sum_i N! \sum_{l \neq n} \tilde{S}_{nn}^i \langle \partial_{n\alpha} \phi_n | \partial_{n\beta} \phi_n \rangle
= N! \tilde{S}_{nn}^i e^{i \alpha \beta} e B^2 / 2
= N! \sum_{l \neq n} \tilde{S}_{nn}^i \sum e^{i \theta_{nl} - \theta_{in}} \left[ \partial_{n\alpha} S_{nl}^i - ie A_l^\alpha S_{nl}^i \right] + \mathcal{O}(B^2)
= N! \sum_{l \neq n} \tilde{S}_{nn}^i e^{i \alpha \beta} e B^2 / 2
+ N! \sum_{l \neq n} \tilde{S}_{nn}^i \sum e^{i \theta_{nl} - \theta_{in}} \left[ \partial_{n\alpha} S_{nl}^i + ie A_l^\alpha S_{nl}^i \right] + \mathcal{O}(B^2) \tag{20}
\]
For \( n \neq m \),

\[
\int d^3N r \partial_n |\Phi|^* \partial_m |\Phi| = \int d^3N r \sum_{i,j} [\tilde{\Phi}^*_n \partial_n \phi^*_m i] [\tilde{\Phi}^*_m \partial_m \phi^*_n j]
\]

\[
+ \int d^3r_i \partial_n \phi^*_n i \int d^3r_j \phi^*_j m \int d^3r_k \phi^*_k l \int d^3r_k \phi^*_k \partial_m \phi^*_j k \times \int d^3r_i \phi^*_i \partial_n \phi^*_n m \int d^3r_j \phi^*_j \partial_m \phi^*_j j
\]

\[
= (N - 1)! \tilde{S}^*_{mn} (\partial_n \phi^*_m i |\partial_m \phi^*_n m)
\]

\[
+ \sum_{i \neq j} \sum_{l \neq n} \sum_{l' \neq m} (N - 2)! \tilde{S}^*_{mn;l'} (\partial_n \phi^*_m i |\partial_l l') (\partial_l l' |\partial_m \phi^*_n m)
\]

\[
= N! \tilde{S}^*_{mn} ie(\partial_n A^\alpha_n S_m + A^\alpha_m \partial_n S_m - A^\alpha_m \partial_m S_m)
\]

\[
+ N! \sum_{l \neq n,m} \tilde{S}^*_{mn;l} i e A^\alpha_n \partial_m S_m
\]

\[
+ N! \sum_{l \neq n,m} \tilde{S}^*_{mn;l} i e A^\alpha_m \partial_n S_n
\]

\[
= N! [\tilde{S}^*_{mn} ie(\partial_n A^\alpha_n S_m + A^\alpha_m \partial_n S_m - A^\alpha_m \partial_m S_m)
\]

\[
+ \sum_{l \neq n,m} [\tilde{S}^*_{mn;l} i e A^\alpha_n \partial_m S_m - \tilde{S}^*_{mn;l} i e A^\alpha_m \partial_n S_n]
\]

\[
+ \sum_{l, l' \neq n,m} \tilde{S}^*_{mn;l'} i e^{i \theta_{l'} l} [\partial_n S_l - i e A^\alpha_l S_l]
\]

\[
= N! [\tilde{S}^*_{mn} ie(\partial_n A^\alpha_n S_m + A^\alpha_m \partial_n S_m - A^\alpha_m \partial_m S_m)
\]

\[
+ \sum_{l \neq n,m} [\tilde{S}^*_{mn;l} i e A^\alpha_n \partial_m S_m - \tilde{S}^*_{mn;l} i e A^\alpha_m \partial_n S_n]
\]

\[
+ \sum_{l \neq n,m} \tilde{S}^*_{mn;l'} i e^{i \theta_{l'} l} [\partial_n S_l - i e A^\alpha_l S_l]
\]

\[
= -i N! (\det S) S_n \partial_n S_m + O(B^2),
\]

(22)

The 2nd term of (1)

\[
= \frac{1}{N! (\det S)^2} \sum_{l \neq n,m} \tilde{S}^*_n \partial_n S_m + O(B^2)
\]

(23)

The reduced form of \( F_{\mu \nu} \)

\[
= -2 \text{Im} \left[ \frac{1}{(\det S)^2} \sum_{l \neq n} \tilde{S}^*_n \partial_n S_m \sum_{l' \neq m} \tilde{S}^*_{m;l'} \partial_m S_{l'} \right]
\]

\[
+ O(B^2)
\]

(24)

In the 2nd line of (24), the ingredient of the parenthesis is real-valued, so that its imaginary part is equal to zero.

The 2nd line of (2)

\[
= \text{Im} \left[ \frac{2}{(\det S)^2} \sum_{l \neq n,m} \tilde{S}^*_n \partial_n S_m \right]
\]

\[
\times \left[ i e A^\beta_m \tilde{S}_{mn} + \sum_{l \neq m} \tilde{S}_{ml'} (\partial_{m \beta} S_{ml'} + i e A^\beta_l S_{ml'}) \right]
\]

\[
+ O(B^2)
\]

(25)

The 3rd line of (2) can be obtained from (25) by exchanging \( n \alpha \) and \( m \beta \) and taking the complex conjugate:

The 3rd line of (2)

\[
= \frac{2}{(\det S)^2} \sum_{l \neq n,m} \tilde{S}^*_n \partial_n S_m
\]

\[
\times \left[ e A^\alpha_n \tilde{S}_{nn} + \sum_{l' \neq n} \tilde{S}_{nl'} S_{nl'} e A^\alpha_l \right] + O(B^2)
\]

(26)

For \( n = m \),

The 4th line of (2)

\[
= \text{Im} \left[ \frac{2}{|S|^2} \tilde{S}^*_n i e^{i \phi} e^{B^\gamma / 2}
\]

\[
+ \sum_{l \neq n,m} \tilde{S}^*_{nn;l'} i e^{i \theta_{l' n'} l} \partial_n S_{n'l'} \partial_{n \beta} S_{l n'}
\]

\[
- i e A^\alpha_n \tilde{S}_{nl'} \partial_{n \beta} S_{l n'} + i e A^\beta_n \tilde{S}_{nl'} \partial_{n \alpha} S_{l n'} \right]
\]

(27)
For \(n \neq m\),
(The 4th line of (2))
\[
\text{Im} \frac{-2}{|S|} \left[ S_{mn} e^{i \frac{1}{2} e^{\alpha \beta \gamma} B^\gamma S_{nm}} + A^\alpha_m \partial_n S_{nm} - A^\alpha_n \partial_m S_{nm} \right] + \sum_{l \neq n, m} \left[ \tilde{S}_{mn;nl} e^{i \frac{1}{2} e^{\alpha \beta \gamma} B^\gamma S_{lm}} - \tilde{S}_{mn;lm} e^{i \frac{1}{2} e^{\alpha \beta \gamma} B^\gamma S_{lm}} \right]
\]
\[
+ \sum_{l, l', l'' \neq n, m} \tilde{S}_{mn;ll'} \times \left[ \delta(e^{i \phi_{lm} - e^{i \phi_{l'}}) \partial_n S_{ll'} \partial_m S_{lm} + i e^{i \frac{1}{2} e^{\alpha \beta \gamma} B^\gamma S_{lm}} \partial_n S_{lm} \right]
\]

\[
\text{Special case: square lattice}
\]
We now derive the explicit form of \(a^\alpha_n\) and \(F_{nm}^\alpha\) of the square lattice under uniform magnetic field in \(z\)-direction.
Here, we assume that the overlap integral of the nearest-neighbor atoms is dominant. Moreover, due to the translational and rotational symmetry, \(S_{nm}\) takes the same value for all the nearest-neighbor pair \((n, m)\), and \(\partial_{\alpha N} = 0\). Then, from Eqs. (22) and (23),
\[
a^\alpha_n = -\frac{e B}{2 \det S} [\sum_{e = \pm x, y} Y_n e^{i \phi}_{n+e} \tilde{S}_{n,n+e} + e^{i \phi}_{n,n+e} \tilde{S}_{n,n+e}]
\]
\[
a^\alpha_n = -\frac{e B}{2 \det S} [\sum_{e = \pm x, y} X_n e^{i \phi}_{n+e} \tilde{S}_{n,n+e} + e^{i \phi}_{n,n+e} \tilde{S}_{n,n+e}]
\]
\[
a^\alpha_n = 0
\]
where \(n = n \pm (x, y)\) indicates the neighboring cite of \(n\) in the \((x, y)\)-direction. These are also unifiedly written as
\[
a^\alpha_n = -\frac{e B}{2 \det S} [A^\alpha_n \tilde{S}_{n,n} + A^\alpha_n \tilde{S}_{n,n}]
\]

\[
F_{nm}^{\alpha \beta} = -\frac{\tilde{S}_{nm} e^{\alpha \beta \gamma} B^\gamma}{\det S} \left[ e (A^\alpha_m - A^\alpha_n) \partial_n S_{nl} + e (A^\alpha_n - A^\alpha_m) \partial_m S_{nm} \right]
\]
\[
F_{nm}^{\alpha \beta} = -\frac{\tilde{S}_{nm} e^{\alpha \beta \gamma} B^\gamma}{\det S} \left[ e (A^\alpha_m - A^\alpha_n) \partial_n S_{nl} + e (A^\alpha_n - A^\alpha_m) \partial_m S_{nm} \right] - e (A^\alpha_n - A^\alpha_m) \partial_m S_{nm}
\]

The obtained formula is symmetric for the exchange of \(n\) and \(m\), and also ensures the screening effect, \(\sum_m F_{nm}^{\alpha \beta} = -Ze B\) for any \(n\).

\[\text{II. BAND STRUCTURE OF PHONONS}\]
In this section, we show that \(Z_{ph} = 0\) holds in our system. The argument is essentially the same as the one in Ref. 1, where \(Z_{ph} = 0\) was proven for magnons. We generalized it to phonons by using the unified perspective of the Berry curvature of bosonic systems.

\[\text{Consistency of the two definitions}\]
Here, we will review the general argument given in Ref. 2. We consider the system with some degrees of freedom \(\{x_i\}\) or \(\{b_i, b_i^\dagger\}\). Concretely, \(i\) stands for the spatial index, polarization degrees of freedom, etc. Note that \(x_i\) may include both the coordinate \(q_i\) and the momentum \(p_i\).
We assume that the Hamiltonian of the system is given as follows:
\[
H = \begin{cases} \frac{1}{2} \sum_{i,j} B_{ij} x_i x_j & (\text{real case}) \\ \sum_{i,j} B_{ij} b_i b_j & (\text{complex case}) \end{cases}
\]
where \(B\) is a real symmetric matrix in real case, and is a hermitian matrix in complex case. We also assume that \(B\) is positive semi-definite from the stability condition. Furthermore, we need an information of the commutation relation of \(\{x_i\}\)s and \(\{b_i, b_i^\dagger\}\). We assume
\[
[x_i, x_j] = A_{ij}, \quad [b_i, b_j] = A_{ij}, \quad A_{ij} := (i \Omega^{-1})_{ij}
\]
\(A\) is a pure imaginary anti-symmetric matrix in real case, and is a hermitian matrix in complex case. We further assume that \(A_{ij}\) does not depend on \(\{x_i\}\)s, and not singular (i.e., has a full rank). The case where \(\Omega_{ij}\) is singular corresponds to the system with constraints [4], and we will not consider such a case here. Then the EoM is given as
\[
i \dot{x}_i = (AB)_{ij} x_j, \quad i \dot{b}_i = (AB)_{ij} b_j
\]
If the system possesses the translational symmetry, we can Fourier transform Eq. (34) to obtain \(i \dot{\xi}_n^\alpha = (A_k B_k)^{\alpha \beta} \xi_n^\beta, \quad i \dot{b}_n^\alpha = (A_k B_k)^{\alpha \beta} b_n^\beta\), where \(A_k, B_k\) are hermitian matrices which, in the real case, additionally satisfy \(A_k = -A_{-k}\) and \(B_k = B_{-k}\) from the (anti-)symmetry.

The “non-hermitian Hamiltonian” given in Ref. 3 corresponds to \(A_k B_k\). Concretely, in \(\{q_{x,k}, q_{y,k}, \Pi_{x,k}, \Pi_{y,k}\}\) basis,
\[
A_k = \begin{pmatrix} 0 & I_2 \\ -I_2 & 0 \end{pmatrix}, \quad B_k = \begin{pmatrix} D_k & 0 \\ 0 & I_2 \end{pmatrix},
\]
\[
A_k B_k = \begin{pmatrix} 0 & I_2 \\ -i D_k & 0 \end{pmatrix}, \quad I_2 \text{ represents 2 by 2 unit matrix. The corresponding quantity in Ref. 1 is, in } \{\beta_k, \beta_{-k}\} \text{ basis,}
\]
\[
A_k = \sigma_3, \quad B_k = H_k = \begin{pmatrix} a_k & b_k \\ b_{-k} & a_{-k} \end{pmatrix},
\]
\[
A_k B_k = \sigma_3 H_k.
\]
Diagonalization of $A_k B_k$ amounts to solving the full problem, since it leads to the diagonal EoM.

Here, we will show that the definition of Berry curvature given in Ref. 3 is equivalent in the general setting given above, and the only difference resides in the form of $A_k$. Here we will write $A_k B_k$ as $\tilde{H}_k$, following Ref. 3. Then, if $B_k$ is positive definite, we can consider the following similarity transformation:

$$\tilde{H}_k \rightarrow B_k^{1/2} \tilde{H}_k B_k^{-1/2} = B_k^{1/2} A_k B_k^{1/2},$$ \hspace{1cm} (37)

which is hermitian, so $\tilde{H}_k$ can be diagonalized. Therefore for positive definite $B_k$, $\tilde{H}_k$ is quasi-hermitian. From $\tilde{H}_k = B_k \tilde{H}_k B_k^{-1}$, it is also pseudo-hermitian. However, if there is a zero eigenvalue of $B_k$, then we cannot construct $B_k^{-1/2}$, so the above argument fails. This failure of the diagonalization is known in the literature as the defective point or non-hermitian degeneracy [5]. The characteristic feature of a defective point is the square root dispersion near the degeneracy, and at $k = 0$ in the phonon system, it leads to the linear spectrum $\omega_k = c \sqrt{k^2}$ even though the dynamical matrix is quadratic in $k^\alpha$.

So, except for the defective point, $\tilde{H}_k$ can be diagonalized by the matrix $T_k$, which is not necessarily unitary:

$$T_k^{-1} \tilde{H}_k T_k = \begin{bmatrix} \omega_1 & & \\ & \ddots & \\ & & \omega_N \end{bmatrix},$$

$$T_k = (|u_1\rangle \ldots |u_N\rangle),$$ \hspace{1cm} (38)

where $|u_i\rangle$ is the $N$ dimensional column vector, and is the $i$th eigenvector. Then the Berry connection is defined as

$$a^i_\mu = \text{Re} \left( i \langle u_i | B_k \partial_{k_\mu} | u_i \rangle \right),$$ \hspace{1cm} (39)

where we imposed the normalization:

$$\langle u_i | B_k | u_j \rangle = \delta_{ij}, \quad \langle u_i | = \langle |u_i\rangle^\dagger.$$ \hspace{1cm} (40)

We note that, given the right eigenvector of $\tilde{H}_k = A_k B_k$ as $|u_i\rangle$, we can construct the left eigenvector as $B_k^\dagger |u_i\rangle$, since

$$\tilde{H}_k (B_k |u_i\rangle) = B_k A_k B_k |u_i\rangle = \epsilon_i B_k |u_i\rangle,$$ \hspace{1cm} (41)

where we used the hermicity of $A_k$ and $B_k$. So the normalization (40) amounts to choosing the biorthogonal basis.

On the other hand, the definition of Berry connection in Ref. 1 is given as:

$$a^i_\mu = i \text{Tr} \left[ \Gamma_1 \sigma_3 T_k^\mu \sigma_3 (\partial_{k_\mu} T_k) \right],$$ \hspace{1cm} (42)

where $\Gamma_1$ is a matrix taking $+1$ for the $j$th diagonal component and zero otherwise. We note that $T_k$, which is the paraunitary matrix which diagonalizes $H_k$, ($T_k^\dagger H_k T_k = d_k$, where $d_k$ is a diagonal matrix) is the same matrix as $T_k$ in Eq. (38), since

$$T_k^{-1} \tilde{H}_k T_k = T_k^{-1} \sigma_3 H_k T_k = \sigma_3 T_k^\dagger H_k T_k = \sigma_3 d_k,$$ \hspace{1cm} (43)

so it also diagonalizes $\tilde{H}_k$, where we used the paraunitarity of $T_k$. Noting that, from the biorthogonality (40),

$$T_k^{-1} = \left( \begin{array}{c} \langle u_1 | H_k \\ \vdots \\ \langle u_N | H_k \end{array} \right),$$ \hspace{1cm} (44)

then, from Eq. (42),

$$a^i_\mu = i \text{Tr} \left[ \Gamma_1 T_k^{-1} (\partial_{k_\mu} T_k) \right] = i (T_k^{-1} (\partial_{k_\mu} T_k))_{\mu i} = \text{Re} \left( i T^\mu_\mu (\partial_{k_\mu} T_k) \right).$$ \hspace{1cm} (45)

So if we properly identify the matrices $A, B$, these two expressions are consistent. Moreover, we can show that the Berry connection (42) is real by using the fact that $[\Gamma_1, \sigma_3] = 0$:

$$(a^i_\mu)^* = - i \text{Tr} \left[ (\partial_{k_\mu} T_k^\mu) \sigma_3 T_k \sigma_3 \Gamma_1 \right]$$

$$= i \text{Tr} \left[ T_k^\mu \sigma_3 \partial_{k_\mu} T_k \sigma_3 \Gamma_1 \right]$$

$$= i \text{Tr} \left[ \sigma_3 T_k^\mu \sigma_3 \partial_{k_\mu} T_k \right]$$

$$= i \text{Tr} \left[ \Gamma_1 \sigma_3 T_k^\mu \sigma_3 \partial_{k_\mu} T_k \right]$$

$$= a^i_\mu.$$ \hspace{1cm} (46)

In general, the Berry connection is complex and we need to take the real part of it as is done in Eq. (39) and as is pointed out in Ref. 2.

Although the Berry connection in phonon system is completely given as Eq. (39), we can consider the following step-by-step transformation to compare to the definition in the magnon system. First, we diagonalize $A_k$ by the unitary matrix $U_k$:

$$\tilde{H}_k \rightarrow U_k^\dagger A_k B_k U_k = D_k U_k^\dagger B_k U_k := D_k \tilde{B}_k,$$ \hspace{1cm} (46)

where $D_k$ is the diagonal matrix with both positive and negative element, but does not have a zero component from the assumption of nonsingularity. Then we consider the following transformation:

$$D_k \tilde{B}_k \rightarrow (D_k^+)^{-\frac{1}{2}} D_k \tilde{B}_k (D_k^+)\frac{1}{2}$$

$$=((D_k^+)^{-\frac{1}{2}} D_k) ((D_k^+)\frac{1}{2} \tilde{B}_k (D_k^+)\frac{1}{2})$$

$$= : \omega \tilde{B}_k^\prime,$$ \hspace{1cm} (47)

where $\omega$ is the diagonal matrix with $p$ numbers of $+1$ components and $q$ numbers of $-1$ components, and the superscript “$+$” here indicates taking the absolute value of each component. In the case of Eq. (35), $p = q$, so $\omega = \sigma_3$. Therefore, the problem has been reduced to the same structure as Eq. (36). In general, we consider the matrix $T_k \in SU(p, q)$ which diagonalizes $B_k^\prime \rightarrow T_k^\dagger B_k^\prime T_k = D_k^\prime$. Then the Berry connection is given as

$$a^i_\mu = \text{Re} \left( i \text{Tr} \left[ \Gamma_1 (U_k (D_k^+)\frac{1}{2} T_k) T_k^{-1} \partial_{k_\mu} (U_k (D_k^+)\frac{1}{2} T_k) \right] \right)$$

$$= \text{Re} \left( i \text{Tr} \left[ \Gamma_1 \omega (D_k^+)\frac{1}{2} T_k \partial_{k_\mu} (U_k (D_k^+)\frac{1}{2} T_k) \right] \right).$$ \hspace{1cm} (48)

(49)
SUM RULE OF CHERN NUMBER FOR POSITIVE FREQUENCY BANDS

In Ref. 1, the authors showed that the sum of Chern numbers of positive frequency bands is zero. Here we will show that the same result holds for Eq. (35) with positive definite $D_k$. First, we construct the adiabatic path $B_{k,\lambda}$ and $\tilde{H}_{k,\lambda}$ as $B_{k,\lambda} = (1-\lambda)B_k + \lambda I_4$ and $\tilde{H}_{k,\lambda} = A_k B_{k,\lambda}$ ($\lambda \in [0, 1]$). We observe that,

$$\det (\tilde{H}_{k,\lambda}) = \det (A_k) \det (B_{k,\lambda}) = \det (D_{k,\lambda}),$$

(50)

where $D_{k,\lambda} = (1 - \lambda)D_k + \lambda I_2$. So the spectrum of $\tilde{H}_{k,\lambda}$ never crosses zero, since $D_{k,\lambda}$ is positive definite. Therefore, we can deform $\tilde{H}_k$ to $A_k$ without closing the gap between positive and negative energy subspaces.

Then the sum of Chern numbers of positive frequency bands for $\tilde{H}_k$ is the same as that of $A_k$. So the remaining problem is to determine the sum of Chern numbers of $A_k$. Here,

$$A_k = \sigma_2 \otimes I_2 + g(k) \left( \frac{I_2 - \sigma_3}{2} \right) \otimes \sigma_3 = \begin{pmatrix} 0 & iI_2 \\ -iI_2 & g(k) \sigma_2 \end{pmatrix}$$

(51)

By rotating $\sigma_2 \rightarrow \sigma_3$ and interchanging the basis $s_i \leftrightarrow \sigma_i$,

$$A_k = \sigma_2 \otimes I_2 + g(k) \left( \frac{I_2 - \sigma_3}{2} \right) \otimes \sigma_3 = \begin{pmatrix} \sigma_2 + g(k) \left( \frac{I_2 - \sigma_3}{2} \right) & 0 \\ 0 & \sigma_2 - g(k) \left( \frac{I_2 - \sigma_3}{2} \right) \end{pmatrix},$$

(52)

so the system is block diagonalized into two sectors. However, each sector only contains two Pauli matrices $\sigma_2$ and $\sigma_3$, so the Chern number is identically zero for each band. Therefore, we showed that the sum of Chern numbers of positive frequency bands are zero for (35).

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