A current-induced phonon Hall effect

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Since the first experimental observation of the phonon Hall effect (PHE) was discovered in 2005, its physical origin and theoretical explanation have been extensively investigated. While spin-orbit interactions are believed to play an important role under external magnetic fields, and nonmagnetic effects are also possible. Here, we propose a mechanism of PHE which is induced by electric current in a nonequilibrium system through electron-phonon interactions. The influence of the drift electrons to the phonon degrees of freedom, as a correction to the Born-Oppenheimer approximation, is represented by an antisymmetric matrix which has the same form as in a typical phonon Hall model. We demonstrate the idea with a graphene-like hexagonal lattice having a finite phonon Hall conductivity under a driven electric current.

I. INTRODUCTION

The Hall effects, which have been widely studied in electronic systems, are also observed and explained in recent years in phononic systems. The thermal current could also be bent by a magnetic field through Raman-type spin-phonon interactions. As with the integer quantum Hall effect, the phonon Hall effect can be related to the topological nature of the phonon bands. More generally, parallel to the Hall effect in electron transport, it was proposed that, as long as there is a gauge potential playing a similar role as the vector potential in a magnetic field, there will be PHE. This net vector potential could come from the inner electron structure of an atomic system itself combined with an external magnetic field, which has been observed in very recent experiments, or other more complicated interactions like magnon-phonon interactions. All of the present PHEs, either experimental or theoretical, need external or internal magnetic field to induce the observable phonon Hall conductivity.

In 2010, Liu et al. applied an electric current to a molecular junction and found that the current could break the junction due to a nonconservative force, originated from a Berry phase. This inspires us to think about what could happen if we apply an electric current to a lattice system. Having a current means we have broken the time-reversal symmetry, which in some sense has the same effect as an applied magnetic field. For the Hall conductivity calculation, we follow the modern method of Qin et al., which takes into account the so-called energy magnetization contribution, while those of earlier results of Wang and Zhang based on Green-Kubo formula did not realize such a correction. We compute the phonon Hall conductivity and obtain an approximately linear dependence with the drift velocity.

The paper is organized as follows. In section II, we introduce a general theory for the PHE and the principle of our current-induced PHE. In section III, we demonstrate how we construct our lattice model. In section IV, we show our numerical results and discuss their significance. In section V, we draw a brief conclusion of our work. We also give an Appendix section which contains some key details.

II. MECHANISM OF PHONON HALL EFFECT

A. Phonon Hall effect under non-zero vector potential

What is the most general form of a Hamiltonian for phonons that can result in a Hall effect? Let us consider a very general system described by $2N$ Hermitian variables $y_i$, $i = 1, 2, \cdots, 2N$, for a system of $N$ degrees of freedom. In column vector notation, we denote this by $y$. We assume that the Hamiltonian takes a quadratic form of $H = \frac{1}{2}y^T H y$, here we assume $H$ is real and symmetric, $T$ is the matrix transpose. The operators $y_i$ are completely characterized by their commutation relations, $[y_i, y_j] = i\hbar J_{ij}$. We assume that $J_{ij}$ is a c-number. Since $y$ is Hermitian, we can show that the matrix $J$ is real and antisymmetric. The Heisenberg equation of motion is simply

$$\frac{dy}{dt} = JHy.$$  \hspace{1cm} (1)

Two common choices of $y$ appear in the literature, that of Zhang uses conjugate pairs of displacement coordinates $u$ and momenta $p$, while Qin et al. use the displacements $u$ and velocities $v = du/dt = p - Au$. Here in this paper, we follow Qin’s convention. Then the matrix $J$ takes the following form:

$$J = \begin{pmatrix} 0 & I \\ -I & -2A \end{pmatrix}, \quad \text{with} \quad y = \begin{pmatrix} u \\ v \end{pmatrix},$$  \hspace{1cm} (2)

here the matrix $A$ is antisymmetric.

The effect of the Berry phase was long known in coupled electron-nuclear systems, but usually, this extra term is neglected in a Born-Oppenheimer approximation.
When this term is taken back, the Hamiltonian of the nuclei or phonons in a solid is given by Mead and Truhlar [11]:

\[ \hat{H} = \sum_{ij} \frac{-i\hbar \nabla_{ij} - A(R)_{ij}}{2M_j}^2 + U(R), \] (3)

where \( R_{ij} \) is the nucleus position vector of atom \( j \) with mass \( M_j \) in the unit cell \( l \), \( U(R) \) is the potential on the nucleus. Here the vector potential \( A \) comes from the electron Berry phases but can also be the effect of other interactions such Raman-type spin-phonon interaction, external magnetic fields [2], or spin-orbit interaction within electronic structure [3]. In a periodic lattice system with a harmonic approximation, we can transform the system into the reciprocal space, and use a combined coordinate \( \psi \) and velocity variable \( \dot{\psi} \) into the reciprocal space, and use a combined coordinate

Next by assuming \( y_q = \psi_q e^{-i\omega t} \), the corresponding eigensystem of the equation of motion will be

\[ i\dot{J}(q)H(q)\psi_q = H_{eff}\psi_q = \omega\psi_q. \] (5)

Since the effective Hamiltonian is non-Hermitian, the left eigenvector is not related to the right eigenvector by the Hermitian conjugate. We can choose the left eigenvector as \( \psi_q = \psi_q^\dagger H(q) \). The normalization condition is then \( \psi_q^\dagger H(q)\psi_q \equiv \psi_q\psi_q = 1 \). This eigenequation is general to any possible source of the non-zero vector potential. For example, we can choose \( y_q = (u_q,v_q)^T \) where \( v_q = u_q, u_{ij} = \sqrt{M_j/N} \sum x_{ij}e^{-iqR_{ij}} \) with \( R_{ij}^0 \) being the real space lattice vector, \( x_{ij} \) being the deviation from equilibrium positions of atom \( j \) in cell \( l \). \( N \) is the total number of unit cells. We write \( u_q \) without the index \( j \) as a column vector consisting of the degrees in a unit cell. Once we have obtained the eigenvalues and associated eigenvectors of the effective Hamiltonian, we can calculate its Berry curvature and phonon Hall conductivity using the formulas given by Qin et al. [3],

\[ \Omega_{qi} = -\text{Im} \left[ \frac{\partial \psi_{q1}}{\partial q} \times \frac{\partial \psi_{q1}}{\partial q} \right], \] (6)

and [12]

\[ \kappa_{xy} = -\frac{1}{2T} \int_{-\infty}^{\infty} d\epsilon \sigma_{xy}(\epsilon) \frac{dn(\epsilon)}{d\epsilon}, \] (7)

where

\[ \sigma_{xy}(\epsilon) = \frac{1}{Vh} \sum_{\hbar\omega_{q1} \leq \epsilon} \Omega_{q1}^z, \] (8)

where \( n(\epsilon) = 1/(e^{\epsilon/(k_BT)} - 1) \) is the Bose function at temperature \( T \), and \( k_B \) the Boltzmann constant. In the above summation over mode \( q_i \), all modes with both positive and negative frequencies, are included. Since we are dealing with a two-dimensional sheet, the volume \( V \) is an ill-defined concept. We use \( V = L^2a \), the area times the thickness, choosing a somewhat arbitrarily to match the units of \( W/(\text{mK}) \) of the usual three-dimensional thermal conductivity. When estimating the phonon Hall conductivity \( \kappa_{xy} \), we assume the thickness of the sample is the same as the bond length \( a = 1.42 \text{ Å} \) of a graphene lattice.

### B. Current-induced non-zero vector potential

Liu et al. [13] theoretically studied the effect of electric current on a molecular bridge connecting two metallic electrodes. They found a new mechanism, which involves Berry phase, that can lead to a breakdown of the bridge by a “run away” mode. Their discovery inspired us to ask if we introduce electric current into a lattice system, e.g., honeycomb lattice, is there a phonon Hall effect? For convenience, we use the renormalized coordinate \( u_{ij} = \sqrt{M_j}x_{ij} \) to denote the nucleus displacement in real space. Electrons in a metal or a semiconductor carrying electric current can interact with the lattice phonons through the electron-phonon interaction (EPI). In the NEGF formalism, EPI effect is included as a self-energy term in the phonon retarded Green’s function [14],

\[ D(\omega, q) = [\omega^2I - \tilde{K}_q - \Pi(\omega = 0) - \Pi_{q}^N(\omega)]^{-1}, \] (9)

where \( I \) is the identity matrix in \( j \) space, \( \tilde{K}_q \) is the dynamic matrix. \( \Pi(\omega = 0) \) is the second term in the equation below. We subtract it off so that the leading contribution is proportional to the frequency \( \omega \) in the so-called non-adiabatic self-energy due to electrons:

\[
\Pi_{q_{ij}}^N(\omega) = \frac{1}{N} \sum_k \sum_{m,n} g_{mij}(k,q) g_{nij'}(k,q) \times \left[ \frac{f_{mk+q} - f_{nk}}{\varepsilon_{mk+q} - \varepsilon_{nk} - \hbar(\omega + i\eta)} - \frac{f_{mk+q} - f_{nk}}{\varepsilon_{mk+q} - \varepsilon_{nk}} \right],
\] (10)

where \( f \) is the Fermi function, \( g \) is the EPI matrix, \( k \) and \( q \) are wave vectors of electrons and phonons respectively, \( \varepsilon_{nk} \) is the electron dispersion relation, the subscripts \( n \) and \( a \) indicate the electron bands, and the subscripts \( j \) and \( j' \) denote the atomic labels in a unit cell. The summation is over the first Brillouin zone of the electrons. A small positive \( \eta \) attributes the electrons with a finite life time. The self energy can be computed from a first-principle package.

Alternatively, the movement of the ions can also be described semi-classically by an equation of motion taking into account the effect of the electrons. In real space under a Markov approximation, it takes the form [12],

\[ \ddot{u} = -Ku - 2Au, \] (11)
where $K$ is the spring constant matrix in real space corresponding to $\tilde{K}_q$ in reciprocal space, and $A$ can be regarded as the matrix representation of the vector potential induced by EPI which is antisymmetric. Therefore, the phonon Green's function is:

$$D(\omega, q) = [\omega^2 I - \tilde{K}_q + 2i\omega \tilde{A}_q]^{-1}. \quad (12)$$

Comparing the two expressions, if we ignore the higher order terms of $\omega$ in $\Pi^{NA}(\omega)$, and note that $\tilde{A}_q$ is anti-Hermitian (the anti-Hermitian part of $\Pi^{NA}(\omega)$ is the source of dissipative Joule heating, which we will ignore.), we can conclude that:

$$\tilde{A}_q = \lim_{\omega \to 0} \frac{\Pi^{NA}(\omega) + (\Pi^{NA})^\dagger(\omega)}{-4i\omega}.$$ \quad (13)

The Markov approximation adopted here is well justified as the electrons move on a much faster time scale than that of the nuclear degrees of freedom. In terms of the energy scale, an electron has typical energy of order $\text{eV}$, while phonon $h\omega$ is of the order $100\text{meV}$ or less. So keeping the leading $\omega$ dependence only on self-energy is a good approximation. We can trace back to an effective Hamiltonian for phonons with the electrons taken into account through a non-dissipative term as

$$\tilde{H} = \frac{1}{2}(p - Au)^2 + \frac{1}{2}u^T K u, \quad (14)$$

and the corresponding eigenequation is

$$\omega \psi_q = i \begin{pmatrix} 0 & I \\ -I & -2\tilde{A}_q \end{pmatrix} \begin{pmatrix} \tilde{K}_q & 0 \\ 0 & I \end{pmatrix} \psi_q,$$

$$= \begin{pmatrix} 0 \\ -i\tilde{K}_q \end{pmatrix} \psi_q. \quad (15)$$

Here we choose $y_q = (u_q, v_q)^T$, and $v_q = p_q - \tilde{A}(q)u_q$ as before.

III. MODEL IMPLEMENTATION ON A GRAPHENE-LIKE LATTICE

A. Hamiltonians and self-energy

Graphene has been widely studied and it has remarkably high electron mobility, therefore we choose a graphene-like lattice to implement our settings. We use a standard spinless tight-binding model for the electrons:

$$\tilde{H}_e = -t \sum_{j\delta} [c_{A,j}^\dagger c_{B,j+\delta} + c_{B,j}^\dagger c_{A,j+\delta}], \quad (16)$$

where $t = 2.8\text{eV}$ is the hopping parameter. $A$ and $B$ indicate the two sublattices, and $j$ runs over the Bravais lattice sites and $\delta$ runs over the displacements of the three nearest neighbors of a given site. Zhang et al. [2] have proposed a simple phonon model for a graphene-like lattice in which the coupling matrix is diagonal when the bond orientation is in the $x$ direction between two atoms,

$$K_x = \begin{pmatrix} K_L & 0 \\ 0 & K_T \end{pmatrix}, \quad (17)$$

where $K_L = 0.144\text{eV}/(\text{aA}^2)$ is the longitudinal spring constant and $K_T = K_L/4$ is the transverse spring constant. Other orientations can be obtained by rotations. The dynamic matrix is given by

$$\tilde{K}_q = \sum_{l'} K_{ll'} e^{i(ql'_0 - ql_0)} q, \quad (18)$$

where $K_{ll'}$ is the submatrix between unit cell $l$ and $l'$ in the full $K$. In this model, we have ignored the $z$ mode and consider only the in-plane motion. The reason is that the motion in the direction perpendicular to the plane couples quadratically to the electron degrees of freedom, and this is a high order effect to the electron-phonon interaction.

For the electron-phonon interaction, we take a Sau-Schrieffer-Heeger-like model, as used in a previous work by Jiang and Wang [16].

$$\hat{H}_\text{epi} = J_1 \sum_{j\delta} [c_{A,j}^\dagger c_{B,j+\delta} + c_{B,j}^\dagger c_{A,j+\delta}] 
\times \left[ (u_{B,j+\delta} - u_{A,j}) \cdot \hat{e}_{j,\delta} \right], \quad (19)$$

where $J_1 = -6.0\text{eV}/\text{A}$ and $\hat{e}_{j,\delta}$ is the direction between two nearest atoms. The reciprocal space $g$ matrix is given by

$$g_{mnj}(k, q) = \sum_{m'n'} S_{mn'}^{\dagger}(k + q) \Xi_{m'n'}^{j}(k, q) S_{n'}(k), \quad (20)$$

where

$$S(k) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -e^{-i\phi(k)} & 1 \end{pmatrix}, \quad (21)$$

with $\phi(k) = f(k)/|f(k)|$, $f(k) = e^{-ik\cdot a} + e^{i(k\cdot a/2 + \sqrt{3}k\cdot a/2)} + e^{i(k\cdot a/2 - \sqrt{3}k\cdot a/2)}$, and $\Xi_{m'n'}^{j}(k, q)$ is the reciprocal coupling matrix corresponding to $\tilde{H}_\text{epi}$. The expression is given in Appendix A.

In this work, we focus on the EPI for $k$ points near the Dirac points of the electrons and $q$ near the $\Gamma$ point of the phonons, for we find that they are dominant in determining the final phonon Hall conductivity. It seems that we have prepared all the ingredients to calculate $\tilde{A}_q$. However, there is a problem that when we apply an electric current to this graphene-like two-dimensional surface, assuming the drift velocity $v_1$ of current is along the $x$ direction, it is in a nonequilibrium state, therefore we cannot just substitute the Fermi function into the formula. To solve this problem, we use a single-mode relaxation approximation [17] so that:

$$f = f^0 - \frac{\partial f^0}{\partial \phi} \Phi \approx f^0 (\varepsilon - \Phi), \quad (22)$$
where \( f^0 = [e^{(e-\mu)/k_BT} + 1]^{-1} \) with \( \mu \) being the chemical potential of electron, and \( \Phi = \Phi_{nk} \) is mode dependent:

\[
\Phi_{nk} = -eE_\tau \frac{\partial \varepsilon_{nk}}{\partial k_x},
\]

(23)

where \( E \) is the applied electric field, \( \tau_{nk} \) is the relaxation time which is only related to the magnitude of the wave vector. In practice, since we don’t know the relaxation time, we combine it with the electric field and replace them with the drift velocity \( v_1 \), for graphene-like lattice \([18]\):

\[
\Phi_{nk} = v_1 \text{Re} \left[ \varepsilon^* \frac{\partial \varepsilon}{\partial k_x} \right]/(hv_F^2),
\]

(24)

where \( v_F = 3a/(2h) \) is the Fermi velocity, \( a = 1.42 \) Å is the distance between atoms, and \( z = -i f(k) \). By requiring this correction to the Fermi function, the self-energy can be numerically calculated, and thereafter, the \( \tilde{A}_q \) matrix.

B. The Berry curvature - is it unique?

As we have discussed in the previous section, the choice of \( y_q \) is not unique – at least three different choices exist in the literature. Zhang et al. choose \( y_q = (u_q, p_q) \), Qin et al. choose \( y_q = (u_q, v_q) \), Liu et al. choose \( y_q = (K_q^{-1} u_q, v_q) \) \([2, 3, 19]\). The difference between Zhang’s and Qin’s choice is like the difference between Lagrangian mechanics and Hamiltonian mechanics, therefore they are more or less equivalent. The special choice of Liu results in a Hermitian effective Hamiltonian, which implies immediately the eigenfrequencies are all real. When the vector potential term can be separated from the usual potential energy term as in our case, these three bases are related by similarity transformations explicitly. However, this kind of variable transformations is not gauge invariant. Therefore, generally, if \( \tilde{A}_q \) is not a constant matrix, they will result in different Berry curvatures. The question then arises as which one should be used to compute the phonon Hall conductivity? To illustrate and confirm that there is indeed a difference, we choose a smooth \( \tilde{A}_q = (A + i|A|)(b \cdot q + c) \) matrix, where \( \Lambda \) is a constant \( 4 \times 4 \) antisymmetric matrix, \( b \) is a constant vector parameter, and \( c \) is another constant parameter. In principle, these three bases should result in different Berry curvatures, but in practice, the differences are small, especially between Zhang’s and Qin’s choices, therefore we choose such a highly anisotropic case. We plot the corresponding Berry curvatures of the three bases along a high-symmetry path of the graphene-like lattice in Fig. 1. We see that there are sharp peaks at the \( \Gamma \) point. However, the signs of the peaks are opposite for Liu et al. definition to that of Zhang and Qin et al. Away from the \( \Gamma \) point, the values tend to be close among the three. In conclusion, since only Qin et al. derived the correct formula for the phonon Hall conductivity with their definition of the Berry curvature, the other two choices are not correct in this sense, at least as far as the phonon Hall conductivity is concerned.

![Berry curvature under different bases](image)

**FIG. 1.** The Berry curvatures along the high-symmetry path under three different bases. Although they do not differ so much from each other, they are indeed different. The parameter set is chosen to be: \( b \cdot q = (1000 \text{ Å, } 1 \text{ Å}) \cdot q, c = 0.1 \text{ rad/ps, and } |A| \) is a constant matrix with all elements being 1.0 rad/ps except diagonal elements being 0.

![Dispersion relation](image)

**FIG. 2.** The dispersion relation of positive branches along high-symmetry path \( \Gamma - M - K - \Gamma \) with \( v_1 = 1.0 \times 10^4 \text{ m/s, } T = 300 \text{ K, } \mu = 0.1 \text{ eV} \). A small onsite potential \( V_{\text{ onsite}} = 1.0 \times 10^{-3} K_L \) and a nearly 0 magnetic field measured by effective parameter \( h = 1.0 \times 10^{-9} \text{ rad/ps} \) are employed to perturb the system. The inset shows one of the anti-crossing points.

IV. NUMERICAL RESULTS AND DISCUSSION

In order to have a well-defined topological structure, we need to perturb our system to open tiny gaps at \( \Gamma \) and \( K \) points, as the Berry curvature becomes ill-defined.
when the bands are degenerate. This goal is achieved by adding a small onsite potential term to the phonon dy-
namic matrix and a nearly zero magnetic field which goes into the Hamiltonian through Raman-type spin-phonon interaction \( \mathcal{A} \). The effect of the magnetic field is de-
scribed by a constant antisymmetric matrix \( \mathcal{A}_A \):\[
\mathcal{A}_A = \begin{pmatrix} B_a & 0 \\ 0 & B_b \end{pmatrix}, B_b = \begin{pmatrix} 0 & h \\ -h & 0 \end{pmatrix},
\]
where \( h \) is an effective parameter representing magnetic field with unit \( \text{rad/ps} \). Add this matrix to our previous \( \mathcal{A} \) will introduce magnetic field into our system. We note that as a function of a constant magnetic field \( h \), the Berry curvatures and the Chern numbers are odd functions of \( h \) and experience a discontinuity at \( h = 0 \), thus ill-defined at \( h = 0 \). Our results presented below thus should be considered as the limit when \( h \to 0^+ \) and \( V_{\text{ onsite}} \to 0^+ \). This is physical since we can always apply a small magnetic field and put the system on a substrate, thereby acquiring an onsite interaction.

Figure 2 shows the positive part of the dispersion re-
lation of our current-induced system, from which we can see that the two acoustic branches are very close to the pure phonon system without the drift current, while the two optical branches get modified drastically. This behavior is easy to understand if we review the EPI form of our model. The strength of EPI in our model is propor-
tional to the relative displacement of atoms, therefore the optical modes, in which atoms move relatively, are equipped with stronger EPI than acoustic ones. It des-
ers notice that there are several anti-crossing points in the dispersion relations. These points will possess much larger Berry curvature, therefore they are dominant in determining the topological properties of the system. Points in acoustic branches near \( \Gamma \) point and anti-crossing points near \( K \) points also have large Berry curvatures. However, these pairs of Berry curvatures should cancel each other for they are similar to pure phonon system where there are no PHE.

Figure 3a demonstrates the relationship between \( \kappa_{xy} \) and the drift velocity \( v_1 \), from which we find that there is a range of \( v_1 \) in which there is almost no PHE. This is expected as extremely small drift velocity should not induce observable PHE, but the details are difficult to explore numerically. When \( v_1 \) crosses this range, about \( 80 \text{ m/s} \), \( \kappa_{xy} \) is roughly linear dependent on \( v_1 \) for our picked velocity sequence. When \( v_1 \) is gradually close to the Fermi velocity of this graphene-like lattice sys-
tem, our theory and approximation on EPI will gradually break down. The Chern numbers of positive branches are \( C^1 = 1, C^2 = C^3 = 0, C^4 = -1 \), where larger indices are associated with higher frequencies. In our range of the drift velocity, there is no jump among Chern numbers, which seems kind of trivial. Figure 3b shows tempera-
ture dependence of \( \kappa_{xy} \). When the temperature is very small, PHE tends to disappear, and in our temperature range, \( \kappa_{xy} \) seems to have a third-degree polynomial relation-
ship with temperature.

The order of magnitude of our current-induced \( \kappa_{xy} \) is the same as the case with the magnetic field parameter \( h \) being several rad/ps. It is instructive to compare the magnitude of the Hall conductivity to the universal con-
ductance quantum which is \( G_0 = T(\pi k_B)^2/(3h) \), when converted into the same units of conductivity, \( G_0/a \), at \( 300 \text{K} \), we find about \( 2 \text{W/(mK)} \). Our result is about \( 1/10\)-th of the conductance quantum. Since \( \kappa_{xy} \) with our model has the same order of magnitude as a pure magnetic field experimental results \([1]\), it should be observable experimentally in principle. In section II, we said we ignore the Joule heating effect. However, in practice, Joule heating always exists without special flowing di-
rection. Therefore, it will not prevent us from observing PHE. We simply measure the temperature differences in the direction transverse to the current flow twice by \( v_1 \) and \( -v_1 \). The Joule heating effect does not change sign while the Hall effect changes sign. From this, we can deduce the pure Hall contribution.

In summary, we have proposed a new mechanism of PHE induced by electric current. Compared with other PHEs, no significant magnetic field is needed in our sys-
tem. We also find non-trivial topology in our system in the sense that the Chern numbers are not 0. The magni-
tude of our phonon Hall conductivity is comparable with a magnetic field-induced one, therefore it is indeed possible to be observed. The property of our system is that if the drift velocity is too small, there is no observable PHE, and for a suitable range of the drift velocities, the phonon Hall conductivity has a roughly linear dependence rela-
tion on the drift velocity, which is proportional to the applied current.
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Appendix A: Dynamic matrix and EPI tensor elements

Start from basic coupling matrix between two atoms in x direction \( K_x \), we can construct dynamic matrix of our lattice model [2]. In our coordinates, unit cell lattice vectors are \( a_1 = (3a/2, \sqrt{3}a/2) \) and \( a_2 = (3a/2, -\sqrt{3}a/2) \). The explicit coupling matrices among three nearest pair can be obtained by a rotation matrix \( U \) which are \( K_{01} = U(\pi/3)K_xU(-\pi/3), K_{02} = U(-\pi/3)K_xU(\pi/3) \) and \( K_{03} = U(\pi)K_xU(-\pi) \) respectively. Based on these matrices, we can construct five coupling matrices between unit cells.

\[
K_0 = \begin{pmatrix}
K_{01} + K_{02} + K_{03} & -K_{03} \\
-K_{03} & K_{01} + K_{02} + K_{03}
\end{pmatrix},
\]

\[
K_1 = \begin{pmatrix}
0 & 0 \\
-K_{02} & 0
\end{pmatrix},
\]

\[
K_2 = \begin{pmatrix}
0 & 0 \\
-K_{01} & 0
\end{pmatrix},
\]

\[
K_3 = \begin{pmatrix}
0 & -K_{02} \\
0 & 0
\end{pmatrix},
\]

\[
K_4 = \begin{pmatrix}
0 & 0 \\
0 & 0
\end{pmatrix}.
\]

Then the dynamic matrix is

\[
K_{\text{eff}} = K_0 + K_1e^{i(3q_xa/2)}/\sqrt{3}q_ya/2 + K_2e^{-i(3q_xa/2+\sqrt{3}q_ya/2)} + K_3e^{-i(3q_xa/2-\sqrt{3}q_ya/2)} + K_4e^{-i(3q_xa/2+\sqrt{3}q_ya/2)}.
\]

To calculate the non-adiabatic self energy \( \Pi_{\text{eff}} \), we need to know EPI tensor in reciprocal space. By transforming \( H_{\text{eff}} \) into reciprocal space, we can extract tensor elements. We use A, B to represent two atoms in a unit cell and \( \{Ax, Ay, Bx, By\} \) to represent four degrees of freedom of EPI in our lattice model. Then the EPI tensor elements are

\[
\Xi_{AB}(k, q) = -J_1e^{ik_xa/2}\cos(\sqrt{3}kya/2) - e^{-ik_xa/2},
\]

\[
\Xi_{AB}(k, q) = J_1\sqrt{3}e^{ik_xa/2}\sin(\sqrt{3}kya/2),
\]

\[
\Xi_{AB}(k, q) = J_1[e^{ik_ya/2}]2\cos(\sqrt{3}(ky + q_y)a/2) - e^{-ik_ya/2},
\]

\[
\Xi_{AB}(k, q) = J_1\sqrt{3}e^{ik_ya/2}\sin(\sqrt{3}(ky + q_y)a/2),
\]

\[
\Xi_{AB}(k, q) = (\Xi_{AB}(k + q, -q))^*, \ j = \{Ax, Ay, Bx, By\}.
\]

Appendix B: Equation of motion containing A matrix

For a general electron-phonon system, there is a generalized Langevin equation describing the atoms’ movement [15]:

\[
\vec{u} = -K\vec{u} - \int^t \Pi_{\text{epi}}(t - t')\vec{u}(t')dt' + \xi.
\]

Here we do not consider the bath contribution and set the noise term \( \xi \) to zero, for our system is infinitely large. We can define \( d\Gamma(t)/dt \equiv \Pi_{\text{epi}}(t) \) and integrate by parts so that the equation of motion becomes:

\[
\vec{u} = -K\vec{u} - \int^t \Gamma(t - t')\vec{u}(t')dt'.
\]

Next we apply a Markov approximation to \( \Gamma(t - t') \) so that \( \Gamma(t-t') \approx 4A(t-t') \delta(t-t') \) (factor 4 is for consistency). The final expression of the equation of motion will be:

\[
\vec{u} = -K\vec{u} - 2A\vec{u},
\]

which is used in section II.

Appendix C: Berry curvature

Usually there are two ways of calculating the Berry curvature, one is the explicit way by inserting the completeness identity into the definition of the Berry curvature. In our system, the explicit formula is

\[
\Omega_i = -\text{Im} \sum_{i' \neq i} \frac{\psi_{i'}^* \partial H_{\text{eff}} \psi_i \psi_{i'} \partial H_{\text{eff}} \psi_i}{(\omega_i - \omega_i')^2}.
\]

However, to calculate the partial derivative of \( H_{\text{eff}} \), we need numerical differentiation which will cost a large amount of computation to be precise enough. Therefore we choose another way, a geometric way by dividing the Brillouin zone into plaquettes each consisting of four points on a square with area \( \Delta S \) and calculating the Berry phase around them [20][21].

\[
\phi = -\text{Im} \ln(\bar{\psi}_1\psi_2\bar{\psi}_3\psi_4)\bar{\psi}_4\psi_1,
\]

Compared with the Hermitian case, we have replaced the Hermitian conjugate of the eigenvector by the left eigenvector. If investigated further, we find that this replacement is not correct for \( \bar{\psi}_1\psi_2 \neq (\bar{\psi}_2\psi_1)^* \). This break of the equality, a fundamental property of the inner product in Hilbert space, will invalidate Stokes’ theorem so that we cannot obtain Berry curvature through Berry phase. To overcome this, we define a new version of inner product:

\[
\langle \bar{\psi}_1\psi_2 \rangle = \frac{(\bar{\psi}_1\psi_2 + (\bar{\psi}_2\psi_1))^*}{2}.
\]
With this definition, property of inner product in Hilbert space and validity of Stokes' theorem are restored. Then the Berry curvature is calculated by:

$$\Omega = \lim_{\Delta S \to 0} -\text{Im} \ln \left( \frac{\langle \bar{\psi}_1 \psi_2 \rangle \langle \bar{\psi}_2 \psi_3 \rangle \langle \bar{\psi}_3 \psi_4 \rangle \langle \bar{\psi}_4 \psi_1 \rangle}{\Delta S} \right). \quad (C4)$$

One can show that the two ways computing the Berry curvature are mathematically equivalent.

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