Quantum Kinetic Theory of Nonlinear Nernst Effect

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For a long period of time, we have been seeking how Berry curvature influences the transport properties in materials breaking time-reversal symmetry. In time-reversal symmetric material, there will be no thermoelectric current induced by Berry curvature in linear regime. However, the nonlinear Hall current can be shown in non-magnetic and non-centrosymmetric materials, where Berry curvature dipole plays an important role. Most studies are developed from semi-classical Boltzmann equation. Here we show the quantum kinetic theory for nonlinear Nernst effect and introduce a new type of Berry curvature dipole: thermoelectric Berry curvature dipole. This new Berry curvature dipole will also induce the thermoelectric transport in nonlinear regime even in time-reversal invariant crystals. We will also apply our theory to topological crystalline insulator with tilted Dirac cone.

I. INTRODUCTION

Onsager reciprocity relation indicates that for anomalous Hall effect in linear response regime, selected material is required to break time-reversal symmetry since the Berry curvature is odd in momentum space.[1] Therefore, the integral of Berry curvature over momentum will vanish with Fermi distribution of electrons in equilibrium. This is given by \( \Omega_{\alpha}(-k) = \Omega_{\alpha}(k) \). The Kramer pairs of \( k \) and \( -k \) are both occupied. However, according to recent research, nonlinear Hall conductivity can be still remained in time-reversal symmetric crystals. What we need is only inversion-symmetry breaking. In this case, the energy gap emerges at each Dirac node or Weyl node. More importantly, it has been found out the Berry curvature dipole is responsible for nonlinear Hall response in quantum transport by both experimental and theoretical study.[2][3][4] Indeed, there are two types of materials creating non-trivial Berry curvature dipole. The first kind is topological crystalline insulator SnTe, which will undergo a ferroelectric distortion at low temperature[5], time-reversal symmetric Weyl semimetals in the TaAs material class[2] and Rashba material BiTeI[6] They all have strong spin-orbit coupling contributing to their tilted Dirac cone. These tilted Dirac cones will not change their Berry curvature but crucial to non-vanishing dipole term. The second type is two-dimensional Dirac material without spin-orbit coupling. Their inversion symmetry breaking attributes to external field and substrate. Even more importantly, the appearance of a finite dipole can only be captured taking explicitly into account the terms accounting for the warping of the Fermi surface[7]. This new phenomena has been already studied in quantum nonlinear Hall effect[2] and thermal Hall effect[1] with semi-classical Boltzmann equation. Inspired by the two studies, I expect to explore more on nonlinear Nernst effect. Without conventional Boltzmann equation and semi-classical approximation, I begin with generalization of the quantum kinetic theory which is more fundamental to us. With the theory in temperature field, I will investigate the nonlinear response theory in thermoelectric transport.

In this work I study the quantum kinetic theory of non-linear Nernst effect (NNE) in thermoelectrical transport. I will derive expression and equation of the density matrix from the basic quantum Liouville equation. I develop theory of the nonlinear electronic transport induced by temperature gradient in the presence of disorder. I will also introduce the new type of dipole: thermoelectric Berry curvature dipole instead of dipole before[2]. This new thermoelectric Berry curvature dipole will play an important role in thermoelectric transport. This theory is also crucial to experimental physicists since they can measure the electric current in presence of temperature gradient. I here provide a theoretical prediction of the relationship between thermoelectric conductivity and chemical potential.

This paper is organized as follows. In the second section, I will briefly introduce not only quantum kinetic equation for Bloch electrons in the presence of disorder, temperature gradient but also the solution of density matrix to the equation. In the third part, I give the general expression of the density matrix by solving the quantum kinetic equation and derive the second-order response. It will also be explained that why thermoelectric Berry curvature dipole is constructed and how it influences the transport. To show the adaptability and reliability of my generalized theory, I apply the quantum kinetic theory in the presence of electric field and compare my results with that in the research before. I take disorder effect into account by applying the scattering theory as well. I prove the terms related to Berry curvature and Berry curvature dipole have no effects on the conductivity. In the fourth section, I employ the theory before to a specific model: topological crystalline insulator, which presents the nontrivial thermoelectric Berry curvature dipole. I will show how its thermoelectric Berry curvature dipole and thermoelectric conductivity change with chemical potential of the valley numerically. Last but not the least, I will discuss the quantum kinetic theory in more general case: non-static solution and its application to derivation of optical conductivity. This is still unfamiliar to most of the researchers since all the previous research on quantum kinetic theory only focus on the case in DC limit. Our ambition is to discover the optical current and optical conductivity in any frequency. I will also check the theory with results in semi-classical approximation.

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II. QUANTUM KINETIC THEORY

Without external field, the Hamiltonian of the system is:
\[ H = H_0 + U \], where \( U \) represents disorder potential. The free Hamiltonian satisfies:
\[ H_0(m, k) = \epsilon^m_k |m, k\rangle \]  
(1)

Here \( m \) represents band index and \( \epsilon^m_k \) are dispersion relationship of \( m \)-th band. In the presence of disorder, the quantum Liouville equation after integrating the disorder’s coordinates is our beginning point [11]

\[ \frac{\partial \rho}{\partial t} + i \hbar [H_0, \langle \rho \rangle] + K(\langle \rho \rangle) = 0 \]  
(2)

where \( \langle \rho \rangle \) is density matrix after integrating all the disorder[11, 12]:
\[ \langle \rho \rangle = \frac{1}{V} \int dR_1...dR_n \rho(r, R_1, ..., R_n). \]
\( R_1, ..., R_n \) are coordinates of disorder. For further step, the well-known Luttinger proposal[13][14] is introduced. To describe the thermal transport in material, I similarly add scalar potential \( \psi \) which satisfies \( \nabla \psi = \nabla T/T \). Therefore, the thermal field and the thermal driving term take the forms:

\[ E_T = -\frac{\partial H_T}{\partial t} = -\frac{\nabla T}{T} \]  
(3)

\[ D_T(\langle \rho \rangle) = \frac{1}{2\hbar} \frac{\nabla T}{T} \frac{D(\{H_0, \langle \rho \rangle\})}{Dk} \]  
(4)

The covariant derivative is defined as[10]:
\[ \frac{DX}{Dk} = \nabla_k X - i[R_k, X] \]  
(5)

where \( X \) is a matrix and \( R \) is Berry connection: \( R_{ka}^{mn} = i\langle u_k^m | \partial_{x_a} u_k^n \rangle \). Then we can construct the kinetic equation in the presence of disorder and thermal field[8]:

\[ \frac{\partial \rho}{\partial t} + i \hbar [H_0, \langle \rho \rangle] + K(\langle \rho \rangle) = D_T(\langle \rho \rangle) \]  
(6)

Here we give the numerical result of scattering term:

\[ K(\langle \rho \rangle) = \frac{1}{\hbar^3} \int_0^\infty dt'[U, e^{-iH_0t'/\hbar} U e^{iH_0t'/\hbar} e^{-iH_0t/\hbar} \langle \rho \rangle e^{iH_0t/\hbar}] \]  
(7)

This can be decomposed into two parts:[15]

\[ [I(\langle \rho \rangle)]_{kk}^{mn} = \frac{2\pi}{\hbar} \sum_{m',k'} \langle U^{m'm'}_kk' | U^{m'm}_kk \rangle (\delta_{m,m'} - \delta_{m',m}) \delta (\epsilon_k - \epsilon_{k'}) \]  
(8)

\[ [J(\langle \rho \rangle)]_{kk}^{mm'} = \frac{\pi}{\hbar} \sum_{m''} \langle U^{m'm'}_kk' | U^{m'm''}_kk \rangle [(\delta_{m,m''} - \delta_{m''-m}) \delta (\epsilon_k - \epsilon_{m'}) + (\delta_{m'',m} - \delta_{m,m'}) \delta (\epsilon_{m''} - \epsilon_k)] , (m \neq m'') \]  
(9)

Especially, due to energy conservation law, the main contribution is only from band-diagonal part \( \langle n \rangle \). Therefore, the two disorder terms can be rewritten into: \( I(\langle n \rangle) \) and \( J(\langle n \rangle) \). These results can also be found in [12][10].

To solve the equation (6), we should separate the density matrix into two parts: \( \langle \rho \rangle = \langle \rho_0 \rangle + \langle \rho_T \rangle \), where \( \langle \rho_0 \rangle = \sum_m f_0(\epsilon_m) |m\rangle \langle m| \) represents the equilibrium state distribution. In this passage we mainly focus on the nonequilibrium part: \( \langle \rho_T \rangle \) induced by temperature gradient in the density matrix. The solution to this part yields:

\[ \langle n_T \rangle_{kk}^m = \tau_k^m \frac{\nabla T}{T} \cdot v_k^m (\epsilon_k^m - \mu) \frac{\partial f_0(\epsilon_m^m)}{\partial \epsilon_k^m} \]  
(10)

\[ \langle S_T \rangle_{kk}^{mm'} = -i\hbar \frac{D_T(\langle \rho_0 \rangle)_{kk}^{mm'} - [J(\langle n \rangle)]_{kk}^{mm'}}{\epsilon_k^m - \epsilon_k^{m'}} \]  
(11)
of density matrix is no contribution comes from the diagonal part. The integral of diagonal part is proven to be zero because it is an odd function of momentum. In addition, we can see the current is proportional to Berry curvature of bands: $\Omega^m_n = i\epsilon_{abc}(\partial_{k_b} m)\partial_{k_c} m$.

However, this current can only be measured in time-reversal symmetry breaking material. For time-reversal symmetric crystals, (12) will contributes nothing. We have to consider the nonlinear Nernst effect.

III. GENERAL THEORY OF NONLINEAR NERNST EFFECT

According to study by Fu [2], nonlinear Hall conductivity tensor in the second harmonic term is for material preserving the time-reversal symmetry. We will here prove its reasonability with quantum kinetic theory and develop theory into thermoelectric transport.

Let’s focus on quantum Liouville equation first. Instead of the form like (6), we give the general expression for the equation with temperature gradient.

$$(\mathcal{L} - D_T)(\rho)_F = D_T\langle \rho_0 \rangle$$

Here we define an operator $\mathcal{L} = P + K$, where $P(\rho)_F \equiv \frac{1}{2} \mathcal{L}^{-1} D_T N \langle \rho_0 \rangle$.

$$(\mathcal{L} - D_T)(\rho)_F = D_T\langle \rho_0 \rangle$$

For simplicity, we have $\sum_m \int \frac{d^dk}{(2\pi)^d} \epsilon_m^2 f_0 \partial_{k_y} \Omega^+_k$. Actually, when the temperature is low enough, there is only contribution from conductance band. Since we only consider the problem on the Fermi surface and we can set the chemical potential to be positive, the relaxation time can be replaced with $\tau^+_k$. In this case, only the electrons near the Fermi surface on the conduction band give rise to transport. So the thermoelectric Berry curvature can be rewritten into another form.

$$D_y = \frac{1}{2\hbar} \int \frac{d^dk}{(2\pi)^d} \epsilon^2 f_0 \partial_{k_y} \Omega^+_k$$

Here we modify the dipole by removing the relaxation time from it. From the result, we can see the current is proportional to the new Berry curvature dipole. This is different from one in [2] since this is thermoelectric current instead of electric current induced by electric field. Since the kinetic theory is consistent with semi-classical wavepacket dynamics[16], it is crucial to check whether the result in nonlinear Hall effect is the same as that before. In this way, we also introduce the formula of off-diagonal part in the density matrix in nonlinear regime. When the external field is electric field, we have:

$$\frac{1}{\Omega} [H_0, (\rho)_F].$$

This is accurate for $\mathcal{L}^{-1} D_T N \langle \rho_0 \rangle = 0$. So we can give the direct solution of it.

$$\langle \rho \rangle_F = \sum_{N=1}^{\infty} (\mathcal{L}^{-1} D_T)^N \langle \rho_0 \rangle$$

(14) is a nontrivial result for the term of $N = 2$ is the response in nonlinear regime which may be related to Berry curvature dipole. The result before is just the simplest approximation of (13). Indeed, equation (14) is obtained by iteration. In linear response theory, we just consider the $N = 1$ case. Now we turn to the quadratic term.

Similarly, we can calculate the off-diagonal term (without impurity):

$$\langle S_{T^2} \rangle = -i\hbar \frac{\partial_y T}{T} \sum_{n,n'} \frac{\epsilon_m(n_{T^2}) - \epsilon_n(n_{T^2})}{\epsilon_m - \epsilon_n} \langle n|\langle n|\partial_{k_y} n'\rangle \langle n'|$$

(15)

Here $\epsilon_m = \epsilon_m^{(2)} - \mu$. In the following parts, we note $\partial_{k_n} \rightarrow \partial_{y}$.

We can also obtain the general expression of thermoelectric current for the quadratic term. Detailed calculation is displayed in Appendix A.

$$\langle S_{E^2} \rangle = \frac{\epsilon E_y}{2\hbar} \sum_{n,n'} \langle n|E_k n'\rangle \langle n|\langle n|\partial_{k_y} n'\rangle \langle n'|$$

(18)

Since we take the zero-temperature limit, there is only contribution from conductance band. With this approximation, we obtain the same result in [2] by repeating the same procedure in Appendix A.

$$J_x = \frac{1}{2} Tr[(-e)v_x, \langle S_{E^2} \rangle] = -\frac{1}{2\hbar} e^3 E_y^2 \sum_n \tau_k \frac{\partial f_0}{\partial k_y} \Omega^+_k$$

(19)

$$\chi = \frac{1}{2\hbar} e^3 \frac{E_y^2}{(2\pi)^d} \int \frac{d^dk}{f_0} \frac{\partial \Omega^+_k}{\partial k_y}$$

(20)
This also indicates that our theory is consistent with semi-classical approximation. But there are some difference between quantum kinetic theory and semi-classical wave-packet dynamics. Here we only focus on physics in just one valley, we cannot figure out the difference. However, if we deal with the problem with transport which is contributed by electrons with different chirality, quantum kinetic theory will provide us with more comprehension since a part of the current is induced by electrons under the Fermi surface. This will be found in [10].

The results (12) and (16) are derived without considering the impurity scattering. With (11) as well as further consideration, current corresponding to linear term which is induced by disorder is given by:

\[ J_{x_1} = \pi e^2 \frac{\partial_y T}{T} \sum_{m,m'} \langle U_{kk'}^{m,m'} (f_{k,k'}^{m,m'}) \rangle (n_k^m - n_{k'}^{m'}) \delta (\epsilon_k^m - \epsilon_{k'}^{m'}) \Omega_{kz}^m \]

This is shown to be 0 after integral where \( n_k^m = (\tau_{k})_m f_0 (\epsilon_k^m) \).

The off-diagonal matrix elements of quadratic term induced by disorder is given by:

\[ \langle S_{Tz}^{m,m'} \rangle = i \hbar \frac{[J((\hbar T z))]^{m,m'}}{\epsilon_k^m - \epsilon_{k'}^{m'}} \]  

So the current can be shown as:

\[ J_{x_2} = \pi e^2 (\frac{\partial_y T}{T})^2 \sum_{m,m'} \langle U_{kk'}^{m,m'} (f_{k,k'}^{m,m'}) \rangle \delta (\epsilon_k^m - \epsilon_{k'}^{m'}) \Omega_{kz}^m \]

Where \( N_{k}^{m} = (\tau_{k})_{m}^2 f_0 (\epsilon_k^m) \).

This current can also be proven to be 0 after integral, which tells that impurity scattering does not contribute in thermoelectric transport. More details are illustrated in Appendix B.

We have to pay attention that these will not necessarily be the case since sometimes off-diagonal part will contribute indeed. Here we only consider the impurity-scattering terms related to Berry curvature and Berry curvature dipole. They will have no effects on transport. Besides, all above is about results in DC limit. We have also developed one in the AC limit which will be discussed in the discussion section. Since then, we have developed quantum kinetic theory of nonlinear Nernst effect in thermoelectric transport. For further step, we are intended to apply our results to a specific system: topological crystalline insulator.

IV. APPLICATION

We firstly consider the Dirac semimetal materials(DSM). In many realistic DSM, Dirac cones are more or less distorted. The tilted Dirac cone can be realized in a number of types of materials. To be specific, we focus on topological crystalline insulators such as SnTe. Experiments tell us there are tilted Dirac cones on (001) surface of it. Therefore, we can calculate the thermoelectric conductance induced by thermoelectric Berry curvature dipole.

Firstly, the low-energy model of the (001) surface is given by

\[ H = \xi w_y k_y \sigma_0 + v_x k_x \sigma_x + \xi v_y k_y \sigma_y + \frac{\Delta}{2} \sigma_z \]  

The energy bands will take the form: \( \epsilon_{k}^x = w_y k_y \pm \sqrt{(v_x k_x)^2 + (v_y k_y)^2 + (\frac{\Delta}{2})^2} \). Here \( w_y \) is the tilted parameter, \( \Delta \) is energy gap, \( v_x, v_y \) represent fermi velocity in different direction. Here \( \xi = \pm 1 \) represents the freedom of valley, which conserves time reversal(TR) symmetry of the system. Due to the ferroelectric distortion, the Dirac cone are turned into gapped one. Meanwhile, form of energy bands is stable since if we take influence of disorder into account, this form is still invariant. To properly account for such a dynamically generated kinetic term, we add a term \( \lambda \omega \sigma_x \) in free fermion action. Since that, we can correct the corresponding dispersion[17]:

\[ ||E - tv_y k_y - \lambda E \sigma_x - v_x k_x \sigma_x - v_y k_y \sigma_y|| = 0 \]

Here we use the convention: \( tv_y = \xi w_y \). After solving the equation, we have the effective band,

\[ E_{\pm} = t_{eff} v_y \pm \sqrt{(v_{eff} k_x)^2 + (v_{eff} k_y)^2} \]

where

\[ t_{eff} = \frac{t + \lambda}{1 + t\lambda} \]  

\[ v_{eff} = \frac{1 + t\lambda}{1 - \lambda^2} v_y \]  

\[ v_{eff}^x = \frac{1}{\sqrt{1 - \lambda^2}} v_x \]

This method has been used by Sikkenk and Fritz to study the disorder effect in 3D tilted Weyl semimetal(WSM)[18]. With renormalization group(RG), this term is determined to be marginal one which can not be ignored simply. However, this perturbation does nothing to the form of energy band since we can turn coefficients into effective one compared with (24).

We begin with the topological band and Berry curvature. Although we introduce the tilted parameter, the corresponding eigenvectors are still invariant:

\[ |\pm, k\rangle = \frac{1}{\sqrt{2}} \left( \begin{pmatrix} 1 \\ \pm e^{i\theta} \end{pmatrix} \right) \]

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The angle $\theta$ is defined by $e^{i\theta} = \frac{v_x k_x + iv_y k_y}{k_\perp}$, where $k_\perp = \sqrt{v_x^2 k_x^2 + v_y^2 k_y^2}$. In this way, we also have the Berry curvature which is the same one in 2D WSM.

$$\Omega_{k,z}^\pm = i\epsilon_{zhc} \langle \partial_b \pm |\partial_c \pm \rangle = \mp \frac{\xi \Delta v_x v_y}{4\epsilon_k}$$ (31)

Where $\epsilon_k = \sqrt{(v_x k_x)^2 + (v_y k_y)^2 + (\frac{\Delta}{\epsilon_k})^2}$. In general case, this will contribute nothing to transport after sum of $\xi$. However, we will obtain the nonlinear Hall conductivity by taking the nonlinear Hall effect into account. After calculating the relaxation time, we will give the form of conductivity. Due to the same contribution from the different valleys, we just calculate one and multiply it by 2. Before approaching the final result, we just make some basic assumptions: firstly, we also consider the case with low-enough temperature. Further, we assume that warping of the Fermi surface can be ignored when calculating the relaxation time.

In this way, The form of the Berry curvature dipole and conductivity are taken as:

$$D_y = \frac{1}{2\hbar} \int \frac{d^2k}{(2\pi)^2} L^2 \langle \partial_b^+ \rangle_{\Omega_{k,z}^+}$$ (32)

$$\chi = \frac{4\hbar e v_x v_y}{n_{imp} U_0^2 \mu (1 + \frac{3\mu^2}{\Delta^2})} D_y$$ (33)

More details will be displayed in Appendix C. With dipole $\partial_y \Omega_{k,z}^\pm = \pm \frac{3\epsilon_{zhc} \Delta k_x}{\epsilon_k}$, we can also see that the integral will vanish if the Dirac cone is not tilted. Although the untitled Dirac cone gives finite Berry curvature, the Berry curvature dipole comes to zero since $\partial_y \Omega_{k,z}$ is odd function under Fermi surface. The parameter set is $v_x \approx v_y \approx 2.6328 eV \cdot A$, $\Delta = 20 meV$, $w_\mu = 0.026328 eV \cdot A$.

V. DISCUSSION

In summary, we begin with the quantum Liouville equation and its solution in the presence of disorder and temperature gradient. Further, we develop quantum kinetic theory of nonlinear Nernst effect with general solution to density matrix. We prove the persistence of Nernst coefficient in nonlinear regime with calculation. It also establishes a new concept of thermoelectric Berry curvature dipole dominant in the quadratic term and electric current in TR-invariant systems. The Berry curvature giving rise to linear response does not contribute to electric current without breaking time-reversal symmetry. Meanwhile, we have also proved that the main impurity scattering contributes nothing to thermoelectric transport. Finally, we apply our theory to SnTe, a topological crystalline insulator with time-reversal symmetry which has been intensively studied by recent experiments, and give numerical result of the thermoelectric Berry curvature dipole and thermoelectric conductivity. However, this theory also remains us some problems: if the external field is intensive, could we also expand the formula (13) as (14)? When the external field is in the DC limit, how could we solve the kinetic equation (6)? Since we only care about second-order response, we can solve equation (13) iteratively. In this way, $\langle p_T^r \rangle = L^{-1} D_T \langle p_{T_0} \rangle$, $\langle p_T^2 \rangle = L^{-1} D_T \langle p_T^r \rangle = (L^{-1} D_T)^2 \langle p_0 \rangle$, $\langle p_T^n \rangle = L^{-1} D_T \langle p_{T_{n-1}} \rangle = (L^{-1} D_T)^n \langle p_0 \rangle$. In this way, we can derive any-order response iteratively. We can always derive the nonlinear response with (14) however intensive the external field is. In the AC limit, when the external field is replaced with an oscillating one $E(t) = E_0 e^{i\omega t}$, we are still unfamiliar with the solution of the density matrix. We can solve the kinetic equation by replacing the operator $L$ with: $\mathcal{M} = L - i\omega = P + K - i\omega$ for we only consider the distribution in frequency space instead of time space. Then we can similarly derive the unsteady-state kinetic equation as:

$$\langle p \rangle_F(\omega) = \sum_{N=1}^{\infty} (\mathcal{M}^{-1} D_T)^N \langle p_0 \rangle$$. However, what does the unsteady-state stand for? To further consider this problem, we firstly write down the corresponding conductivity $\sigma_{\mu\nu}(\omega) = Tr([-e]^{\mu}(\rho) e^{\nu} \langle \omega \rangle) / |E_0'\rangle$. This indicates conductivity when the external is oscillating one. In other words, this
conductivity corresponds to optical conductivity in the experiments.

To clarify our quantum kinetic theory can be developed into one in AC limit, we shall calculate the second-order response in oscillating external electric field and check it with one in semi-classical approximation. We firstly ignore the scattering term to focus on the effects of semi-classical approximation. We firstly ignore the scattering in oscillating external electric field and check it with one in AC limit, we shall calculate the second-order response in AC limit and that in DC limit: \( \langle n \rangle_k^m(\omega) = \frac{\langle n \rangle_k^m}{1 + i\omega\tau_{k_F}} \). Hence we come to the conclusion that by replacing the diagonal part in (18) with generalized one, we can get the nonlinear optical conductivity. (we also assume \( \mu > 0 \) which indicates \( m = + \))

\[
\chi = \frac{e^3 \tau_{k_F}^+}{2(1 + i\omega\tau_{k_F}^-)} \int \frac{d^2 k}{(2\pi)^2} f_0 \frac{\partial \Omega_k n}{\partial k_y}
\]

This is consistent with the result in [2].

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Appendix A: Derivation of (16,17)

Firstly, let’s focus on the derivation of off-diagonal part of linear response \( \langle S_T \rangle \). According to (14), the lowest order should be:

\[
\langle \rho_T \rangle = \mathcal{L}^{-1} D_T (\langle \rho_0 \rangle)
\]

Therefore, the matrix elements should be:

\[
\langle n_T \rangle_k^m = \tau_k^m [D_T (\langle \rho_0 \rangle)]_{mm}^m
\]

\[
\langle S_T \rangle_k^{nn'} = -i\hbar \frac{D_T (\langle \rho_0 \rangle)|_{nn'}^m - J (\langle n_T \rangle)|_{nn'}^m}{\epsilon_n - \epsilon_{n'}}
\]

To be specific, the off-diagonal one can take another form:

\[
\langle S_T \rangle = \sum_{nn'} \frac{\partial_T \epsilon_{n'} f_{0n'} - \epsilon_n f_{0n}}{\epsilon_n - \epsilon_{n'}} |n\rangle \langle n| \partial_T n' \rangle \langle n'|
\]

Similarly, compared with (A3), we can also derive both the off-diagonal part and the diagonal part of the quadratic term.

\[
\langle S_{T^2} \rangle_k^{nn'} = -i\hbar \frac{D_T (\langle n_T \rangle)|_{nn'}^m - J (\langle n_T^2 \rangle)|_{nn'}^m}{\epsilon_n - \epsilon_{n'}}
\]

\[
\langle n_{T^2} \rangle_k^m = \tau_k^m D_T (\langle n_T \rangle)_k^m = \tau_k^m \frac{1}{2\hbar} \partial_T \frac{D (\{H_0, \langle n_T \rangle\})}{Dk_y}
\]

These are the nonlinear responses in the presence of temperature gradient. Here I remain further discussion on influence caused by impurity scattering in Appendix B. We here just care about the part induced by temperature gradient. In this way, the off-diagonal term of (A5) can be obtained as

\[
\langle S_{T^2} \rangle_k^{nn'} = -i\frac{\partial_T}{T} \sum_{nn'} \frac{\epsilon_{n'} (n_T)^{n'}_k - \epsilon_n (n_T)^n_k}{\epsilon_n - \epsilon_{n'}} |n\rangle \langle n| \partial_T n' \rangle \langle n'|
\]

So the electric current induced by thermal flow takes the form:
\[ J_x^{(2)} = \frac{1}{2} Tr[\{-e\}^{\{v_x, \langle S_{T^2} \rangle\}^m}] \]  

(A8)

This formula contains two parts: \( \langle m|v_x\langle S_{T^2}\rangle|m \rangle \) and \( \langle m|\langle S_{T^2}\rangle v_x|m \rangle \). Let’s calculate the two parts separately. Since \( \sum_m |\partial_y m\rangle \langle m| + |m\rangle \langle \partial_y m | = \partial_y (\sum_m |m\rangle \langle m|) = \partial_y I = 0 \), we can write down another form of the intrinsic velocity operator.

\[
v_x = \sum_{m'} (\epsilon_{m'} - \epsilon_n)|\partial_y m'\rangle \langle m'| + |m'\rangle \langle \partial_y m' | = \sum_{m'} (\epsilon_{m'} - \epsilon_n)|\partial_y m'\rangle \langle m'| + |m'\rangle \langle \partial_y m' |
\]  

(A9)

\[
\langle m|(-e)v_x\langle S_{T^2}\rangle|m \rangle = ie \frac{\partial_y T}{T} \sum_{m'n'\partial_y} \frac{\epsilon_{m'}(n_{T^2})_{n'}^m - \epsilon_n(n_{T^2})_n^m}{\epsilon_n - \epsilon_{n'}} (\epsilon_{m'} - \epsilon_n) \langle n|\partial_y m \rangle \langle m|\partial_x n \rangle \delta_{m'n} \delta_{n'm}
\]

\[
= ie \frac{\partial_y T}{T} \sum_{n} [\epsilon_{n'}(n_{T^2})_{n'}^m - \epsilon_n(n_{T^2})_n^m] \langle n|\partial_x m \rangle \langle m|\partial_y n \rangle
\]

\[
= -ie \frac{\partial_y T}{T} [\epsilon_{m}(n_{T^2})_{m}^m \langle \partial_x m|\partial_y m \rangle - \sum_n \epsilon_n(n_{T^2})_n^m \langle \partial_x m|\partial_y n \rangle]  
\]

(A10)

\[
\langle m|(-e)\langle S_{T^2}\rangle v_x|m \rangle = ie \frac{\partial_y T}{T} \sum_{m'n'\partial_y} \frac{\epsilon_{m'}(n_{T^2})_{n'}^m - \epsilon_n(n_{T^2})_n^m}{\epsilon_n - \epsilon_{n'}} (\epsilon_{m'} - \epsilon_n) \langle n|\partial_y m' \rangle \langle m'|\partial_x n' \rangle \delta_{m'n} \delta_{n'm}
\]

\[
= ie \frac{\partial_y T}{T} [\epsilon_{m}(n_{T^2})_{m}^m \langle \partial_y m'|\partial_x m \rangle - \sum_n \epsilon_n(n_{T^2})_n^m \langle \partial_y m'|\partial_x n \rangle]  
\]

(A11)

The first term of (A10,A11) can be pointed out as Berry curvature:

\[
-ie \frac{\partial_y T}{T} \sum_m [\epsilon_{m}(n_{T^2})_{m}^m \langle \partial_x m|\partial_y m \rangle - \epsilon_m(n_{T^2})_{m}^m \langle \partial_y m|\partial_x m \rangle] = -\frac{\partial_y T}{T} \sum_m \epsilon_m(n_{T^2})_{m}^m \Omega_{k,z}^m  
\]

(A12)

Due to the sum of index \( m \), the second term of (A10,A11) can be combined together.

\[
\]

(A13)

Correspondingly, the current can be figured out:
\[ J_{x}^{(2)} = -e(\frac{\partial y}{T})^{2} \sum_{m} \int \frac{d^{d}k}{(2\pi)^{d}} c_{m}^{\dagger} \frac{\partial f_{0}(\epsilon_{k}^{m})}{\partial k_{z}} \Omega_{k_z}^{m} \]  

(A14)

where \( \Omega_{k_z}^{m} = i(\partial_{x}m|\partial_{y}m) - (\partial_{y}m|\partial_{x}m) \) represents Berry curvature.

However, in the zero-temperature limit, only conductance band contributes to conductivity. In this way, we have the form of thermoelectric conductivity related to dipole with (A14):

\[ \chi = e\tau_{k_{z}}^{+} \int \frac{d^{d}k}{(2\pi)^{d}} c_{m}^{\dagger} f_{0}(\epsilon_{k}^{m}) \partial_{y} \Omega_{k_z}^{m} = e\tau_{k_{z}}^{+} D_{y} \]  

(A15)

Here \( D_{y} = \int \frac{d^{d}k}{(2\pi)^{d}} c_{m}^{\dagger} f_{0}(\epsilon_{k}^{m}) \partial_{y} \Omega_{k_z}^{m} \) represents the new type of Berry curvature dipole. We can see that the conductivity is proportional to the new dipole in thermoelectric transport. We ignore other terms for time-reversal symmetry.

Appendix B: Derivation of (20,22)

At the beginning, let’s focus on the impurity scattering of the linear term.

\[ J_{x}^{(1)} = \frac{1}{2} Tr[(-e)v_{x}, \{S_{T}^{'}\}] \]  

(B1)

\[ \langle S_{T}^{'} \rangle = i\hbar \sum_{n'n} \frac{[J((n_{T}))]|n'n'|}{\epsilon_{n} - \epsilon_{n'}} \langle m||\partial_{x}m'\rangle \langle m'|\partial_{x}m'||\rangle \langle n'|m \rangle \]  

(B2)

With intrinsic velocity(A9), you can also obtain the current density(B1). To begin with, let’s firstly consider the related two terms: \( \langle m|v_{x}\langle S_{T}^{'}\rangle|m \rangle \) and \( \langle m|\langle S_{T}^{'}\rangle v_{x}|m \rangle \):

\[ \langle m|v_{x}\langle S_{T}^{'}\rangle|m \rangle = i \sum_{m'n'n'} (\epsilon_{m'} - \epsilon_{n'}) \frac{[J((n_{T}))]|n'n'|}{\epsilon_{n} - \epsilon_{n'}} \langle m||\partial_{x}m'\rangle \langle m'|\partial_{x}m'||\rangle + \langle m'\rangle \langle \partial_{x}m'||\rangle \langle n'|\rangle \langle m \rangle \]

\[ = i \sum_{n} [J((n_{T}))]|nm| \langle m|\partial_{x}n \rangle \]  

(B3)

\[ \langle m|\langle S_{T}^{'}\rangle v_{x}|m \rangle = i \sum_{m'n'n'} (\epsilon_{m'} - \epsilon_{n}) \frac{[J((n_{T}))]|n'n'|}{\epsilon_{n} - \epsilon_{n'}} \langle m||\partial_{x}m'\rangle \langle m'|\partial_{x}m'||\rangle + \langle m'\rangle \langle \partial_{x}m'||\rangle \langle n'|\rangle \langle m \rangle \]

\[ = -i \sum_{n} [J((n_{T}))]|nm| \langle \partial_{x}n|m \rangle \]  

(B4)

With (B3,B4) we can directly figure out the form of .

\[ J_{x}^{(1)} = e \sum_{n,m} \int \frac{d^{d}k}{(2\pi)^{d}} [J((n_{T}))]|nm| Im(\langle m|\partial_{x}n \rangle) \]  

(B5)

If we take the zero-temperature approximation, the non-equilibrium distribution induced by temperature gradient will just take place on the conductance band. So this will contribute nothing after sum of band index. However, if we take the band-diagonal part into account, we can find the term related to Berry curvature. We assume the Born approximation: \( \langle U(r)U'(r') \rangle = n_{imp}U_{0}^{2} \delta(r - r') \)\(^{(19)}\) Then we have:

\[ \langle U_{kk'}^{nm}U_{kk'}^{m'n} \rangle = n_{imp}U_{0}^{2} \langle u_{k}^{m}|u_{k'}^{n} \rangle \langle u_{k'}^{m'}|u_{k}^{n} \rangle \]  

(B6)

In most cases, this is not a trivial result since we may have strong SOC in the material. We can not simply come to the general case. However, we can still make some approximation. Firstly, the temperature is low enough that we can still replace the
relaxation time with one on the Fermi surface which is noted by $\tau^m_{k'}$. Further, even though the Fermi surface is partly distorted, we still assume the diagonal part $\langle n_T^m \rangle_k$ and $\langle n_T^{m'} \rangle_k$ are approximately considered as functions of $\epsilon^m_k$.

\[
J_{x1}^i = -i\pi e \sum_{m,m'} \langle U_{kk'}^{mm'} U_{kk'}^{mm'} \rangle \langle (n_T^m)_k - (n_T^{m'})_k \rangle \delta(\epsilon^m_k - \epsilon^{m'}_{k'}) \langle (m|\partial_x m') - (\partial_x m'|m) \rangle
\]

\[
= -i\pi e \sum_{m} \langle U_{kk'}^{mm} U_{kk'}^{mm} \rangle \langle (n_T^m)_k - (n_T^{m'})_k \rangle \delta(\epsilon^m_k - \epsilon^{m'}_{k'}) \langle (m|\partial_x m) - (\partial_x m|m) \rangle
\]

\[
\rightarrow \pi e \frac{\partial_y T}{T} \sum_{m} \tau^m_{k'} (\epsilon^m_k - \epsilon^{m'}_{k'}) \delta(\epsilon^m_k - \epsilon^{m'}_{k'}) \Omega^m_{k'z}
\]

where $\tau^m_{k'} = (\tau^m_{k'})_k e_m f_0(\epsilon^m_k)$. This is exactly the equation(21), which is only connected to $\epsilon^m_k$. Therefore, this current will vanish after integrating $k'$.

We can clearly see that the term connected with Berry curvature has no effect on transport in linear regime. However, current from other terms is still unknown to us in general case. Hence, we can only consider other terms in specific models.

Let’s turn to the band-diagonal part of the quadratic term.

\[
\langle n_T^{m'} \rangle_k^m = \frac{\tau^m_{k'}}{\hbar} \frac{\partial_y T}{T} \frac{D(H_0(n_T))}{Dk_y} \bigg|_k = \frac{(\tau^m_{k'})^2}{\hbar} \frac{\partial_y T}{T} \frac{2}{\partial_y} (\epsilon^m_k - \epsilon^{m'}_k) \Omega^m_{k'z}
\]

In this way, the impurity scattering part is derived as:

\[
\langle S_{T2}^{m'} \rangle_k^{mm'} = i\hbar \frac{[J(\langle n_T^{m'} \rangle)]^m_{k'}}{\epsilon^m_k - \epsilon^{m'}_k}
\]

\[
\langle S_{T2}^{m'} \rangle_k^{mm'} = i\pi \sum_{m,m',m''} \sum_{k'} \langle U_{kk'}^{mm'} U_{kk'}^{mm'} \rangle \left( \frac{g(m,m',n')}{\epsilon_m - \epsilon_{n'}} \langle n|\partial_y m \rangle \delta_{m''n'} + \frac{g(n,m',m'')}{\epsilon_n - \epsilon_{m''}} \langle \partial_y m''|n' \rangle \delta_{m'mn} \right)
\]

Here $n_k^{(2)m}$ is not the one in quadratic term. It is given by:

\[
n_k^{(2)m} = \frac{\tau^m_{k'}}{\hbar} \frac{\partial_y T}{T} \frac{2}{\partial_y} \epsilon^m_k \partial_y f_0(\epsilon^m_k)
\]

So we can calculate each matrix element of it. (Here we also use the simplest approximation)

\[
\langle S_{T2}^{m'} \rangle_k^{mm'} = i\pi \sum_{m,m',m''} \sum_{k'} \langle U_{kk'}^{mm'} U_{kk'}^{mm'} \rangle \left[ \frac{g(m,m',n')}{\epsilon_m - \epsilon_{n'}} \langle n|\partial_y m \rangle \delta_{m''n'} + \frac{g(n,m',m'')}{\epsilon_n - \epsilon_{m''}} \langle \partial_y m''|n' \rangle \delta_{m'mn} \right]
\]

With $g(m,m',n') = (n_k^{(2)m} - n_k^{(2)m'}) \delta(\epsilon^m_k - \epsilon^{m'}_{k'}) + (n_k^{(2)m''} - n_k^{(2)m'}) \delta(\epsilon^{m''}_k - \epsilon^{m'}_{k'})$. The intrinsic contribution to velocity operator in the eigenstate basis is

\[
v_x = \sum_{l'} (\epsilon_{l'} - \epsilon_{m''}) [l'|\partial_x l'] + [l'|\partial_x l']]
\]

So the diagonal part is given by

\[
\langle l'|v_x (S_{T2}^{m'})|l \rangle = i\pi \sum_{l'n'n'm,m',m''} \langle U_{kk'}^{mm'} U_{kk'}^{mm'} \rangle \left[ \frac{g(m,m',n')}{\epsilon_m - \epsilon_{n'}} \langle n|\partial_y m \rangle \delta_{m''n'} + \frac{g(n,m',m'')}{\epsilon_n - \epsilon_{m''}} \langle \partial_y m''|n' \rangle \delta_{m'mn} \right]
\]

\[
\times (\epsilon_{l'} - \epsilon_{m''}) [l'||\partial_x l'] + [l'||\partial_x l']]
\]

With tedious calculation, we obtain the only term seemingly connected to Berry curvature dipole.
With (C1), we have the Born approximation in the Bloch space \[19\]:

\[ i\pi \sum_{l,m,m',m''} \langle U_{kk'}^{mm'} U_{kk''}^{m'm''} \rangle g(m, m', m'') \langle \partial_y m'' | l \rangle \langle l | \partial_x m \rangle \] (B16)

The other parts come to zero if sum over all the \( l \). This is the only part seemingly not to be 0. The parts with \( m \neq m'' \) in (B16) are 0 since \( n_{\mathbf{k}'} = 0 \). We can see the conductivity induced by disorder is also proportional to term like Berry curvature. Here we take the parts with \( m = m'' \) into account.

\[ i\pi \sum_{l,m,m'} \langle U_{kk'}^{mm'} U_{kk''}^{m'm''} \rangle g(m, m', m) \langle \partial_y m | l \rangle \langle l | \partial_x m \rangle \] (B17)

In this way, the current related to impurity scattering can be figured out:

\[ J_{x2}^i = \frac{1}{2} Tr[(-e)\{ v_x, \langle S_y^2 \rangle \}] = \pi e \sum_{m,m'} \langle U_{kk'}^{mm'} U_{kk''}^{m'm''} \rangle (N^m_k - N^m_{k'}) \delta (\epsilon^m_k - \epsilon^{m'}_k) \partial_y \Omega_{k,z} \] (B18)

where \( N^m_k = (\tau^m_{k'})^2 \epsilon^m_k f_0(\epsilon^m_k) \), which is only connected with \( \epsilon^m_k \). Therefore, this current will vanish after integrating \( \mathbf{k}' \).

To conclude, we have proved the current density induced by impurity scattering is zero in both linear regime and nonlinear regime. Similar results can be found in [10][8].

Appendix C: More details of calculation on topological crystalline insulator

After constructing the effective Hamiltonian of strained single-layer graphene, we can calculate the eigenstates \( H | u^\pm_k \rangle = \pm \epsilon_k | u^\pm_k \rangle \) and Berry curvature of the model.

\[ | u^\pm_k \rangle = \frac{1}{\sqrt{2}} \left( \begin{array}{c} \pm \frac{1}{\sqrt{1 + \frac{m}{\epsilon_k}}} \\ \pm \frac{1}{\sqrt{1 + \frac{m}{\epsilon_k}}} \end{array} \right) \] (C1)

where angle \( \theta \) and \( \epsilon_k \) is defined by \( e^{i\theta} = \frac{A_1 + iA_2}{\sqrt{A_1^2 + A_2^2}} \) and \( \epsilon_k = \sqrt{A_1^2 + A_2^2 + m^2} \).

\[ \partial_x | u^\pm_k \rangle = \frac{1}{\sqrt{2}} \left( \begin{array}{c} \frac{1}{\sqrt{1 + \frac{m}{\epsilon_k}}} \frac{\partial \epsilon_k}{\partial k_x} \pm \frac{i}{\sqrt{1 + \frac{m}{\epsilon_k}}} \frac{\partial \epsilon_k}{\partial k_y} \\ \frac{1}{\sqrt{1 + \frac{m}{\epsilon_k}}} \frac{\partial \epsilon_k}{\partial k_x} \mp \frac{i}{\sqrt{1 + \frac{m}{\epsilon_k}}} \frac{\partial \epsilon_k}{\partial k_y} \end{array} \right) \] (C2)

\[ \Omega^\pm_{k,z} = i(\langle \partial_x u^\pm_k | \partial_y u^\pm_k \rangle - \langle \partial_y u^\pm_k | \partial_x u^\pm_k \rangle) = \mp \frac{m}{2\epsilon_k} \left( \frac{\partial A_1}{\partial k_x} \frac{\partial A_2}{\partial k_y} - \frac{\partial A_1}{\partial k_y} \frac{\partial A_2}{\partial k_x} \right) \] (C3)

With the form of \( A_1 = v_x k_z \) and \( A_2 = v_y k_x \), you can obtain (28,29) automatically.

For further step, we focus on the relaxation time.

\[ \frac{1}{\tau_{k}} = \frac{1}{\hbar} \int \frac{dk'_x}{(2\pi)^2} \sum_{m,m'} \langle U_{kk'}^{mm'} U_{kk''}^{m'm''} \rangle \delta (\epsilon^m_k - \epsilon^{m'}_{k'}) \] (C4)

We here take \( m = m' = + \) since not only there is no crossover near each valley but also we just basically assume \( \mu > 0 \) for simplicity. In this way, only electrons from the conduction band contribute. So the relaxation time is:

\[ \frac{1}{\tau^+_{k}} = \frac{1}{\hbar} \int \frac{dk'_x}{(2\pi)^2} \langle U^{++}_{kk'} U^{++}_{kk''} \rangle \delta (\epsilon^+_k - \epsilon^{+}_{k'}) \] (C5)

With (C1), we have the Born approximation in the Bloch space\[19\]:

\[ U^{++}_{kk'} = U \langle u^+_k | u^+_k \rangle = \frac{U_0}{2} \sqrt{(1 + \frac{m}{\epsilon_k})(1 + \frac{m}{\epsilon_{k'}}) + e^{i(\varphi - \theta)} \sqrt{(1 - \frac{m}{\epsilon_k})(1 - \frac{m}{\epsilon_{k'}})}} \] (C6)
By neglecting the warping effect, we obtain the relaxation time:

\[ \frac{1}{\tau_k} = \frac{n_{imp}U_0^2 \mu}{4h\epsilon_x\epsilon_y} (1 + 3\frac{m^2}{\mu^2}) \]  

(C8)

In SnTe, the energy bands are:

\[ E = w_y k_y \pm \sqrt{v_x^2 k_x^2 + v_y^2 k_y^2 + \left(\frac{\Delta}{2}\right)^2}, \]

which can be calculated analytically. Energy surface is given by:

\[ \frac{(k_y + k_0)^2}{s^2_y} + \frac{k_x^2}{s^2_x} = 1 \]  

(C9)

In the formula:

\[ s_y^2 = \left(\frac{v_x^2}{v_y^2 - w_y^2}E^2 - \left(\frac{\Delta}{2}\right)^2\right) / (v_y^2 - w_y^2), \]

\[ s_x^2 = \left(\frac{v_x^2}{v_y^2 - w_y^2}E^2 - \left(\frac{\Delta}{2}\right)^2\right) v_x \]

With \( k_y = -k_0 + s_y \sin \theta \), \( k_x = s_x \cos \theta \),

\[ dk_x dk_y = \left| \frac{\partial}{\partial \theta} \right. \left. \frac{\partial}{\partial \theta} \right| dE d\theta = \left[ \frac{v_x^2}{v_x(v_y^2 - w_y^2)^{3/2}} E - \frac{w_y}{v_x(v_y^2 - w_y^2)^{3/2}} \sqrt{\frac{v_x^2}{v_y^2 - w_y^2}E^2 - \left(\frac{\Delta}{2}\right)^2 \sin \theta} \right] dE d\theta \]  

(C10)

After preparation, let’s focus on the conductivity and Berry curvature dipole. According to (17), we can derive \( D_y \) first.

\[ D_y = \frac{1}{2h} \int \frac{d^2 k}{(2\pi)^2} \epsilon^2_+ f_0(\epsilon^+_{\mathbf k}) \partial_\theta \Omega^+_x \]

\[ = \frac{1}{2h} \int_{E<\mu} \frac{dE d\theta}{(2\pi)^2} \left[ \frac{v_x}{v_x(v_y^2 - w_y^2)^{3/2}} E - \frac{w_y}{v_x(v_y^2 - w_y^2)^{3/2}} \sqrt{\frac{v_x^2}{v_y^2 - w_y^2}E^2 - \left(\frac{\Delta}{2}\right)^2 \sin \theta} \right] (E - \mu)^2 3\Delta v_x v_y^3 (-k_0 + s_y \sin \theta) / 4(E + w_y k_0 - w_y s_y \sin \theta)^5 \]

With calculation tools, we can give the result as Fig.1 in the context. Meanwhile, we can derive the conductivity with the relaxation time.

\[ \chi = e\tau_{k_F}^+ D_y = \frac{4h\epsilon_x \epsilon_y}{n_{imp}U_0^2 \mu (1 + 3\left(\frac{\Delta}{2}\right)^2)} D_y \]

(C11)

We can numerically depict the result as Fig.2 above.

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