Quantum theory of nonlinear thermal response

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The linear behavior of thermal transport has been widely explored, both theoretically and experimentally. On the other hand, the nonlinear thermal response has not been fully discussed. In light of the thermal vector potential theory [Tatara, Phys. Rev. Lett. 114, 196601 (2015)], we develop a general formulation to calculate the linear and nonlinear dynamic thermal responses. In the DC limit, we recover the well-known Mott relation and the Wiedemann-Franz (WF) law at the linear order response, which link the thermoelectric conductivity η , thermal conductivity κ , and electric conductivity σ together. To be specific, the linear Mott relation describes the linear η is proportional to the first derivative of σ with respect to Fermi energy (for brevity we call the first derivative, the others are similar); and the linear WF law shows the linear κ is proportional to the zero derivative (i.e., the σ itself). We found there are higher-order Mott relations and WF laws which follow an order-dependent relation. At the second order, the Mott relation indicates that the second order σ is proportional to the zero derivative of the second order η ; but the second WF law shows that the second σ is proportional to the first derivative of κ . At the third order, the derivative order increases once. Although we only did explicit calculations up to the third-order response, we can deduce that the *n*th-order electric conductivity is proportional to the (n-2)th derivative of the *n*th-order thermoelectric conductivity for the nonlinear Mott relation; and the *n*th-order electric conductivity is proportional to the (n-1)th derivative of the *n*th-order thermal conductivity for the nonlinear WF law. Since the second-order Hall effect has been studied in experiment, our theory may be tested by measuring the second-order Mott and WF as well. Our theory is presented explicitly for fermions, and it can also be applied to bosons. As an example, we calculate the second-order thermal conductivity of magnons in a strained collinear antiferromagnet on a honeycomb, in which the linear response disappears.

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I. INTRODUCTION

The interaction of temperature gradient with matter encompasses a wide range of phenomena, including the conversion of heat and electricity or spins, which is essential for the engineering of thermoelectric and other energy-conversion applications. Significant efforts have been devoted to understanding the thermal response in various materials, but most of them are devoted to linear order. In analogy with the anomalous Hall effect, Berry curvature plays a significant role in thermoelectric transport, known as the anomalous Nernst effect (ANE) [1-4]. Owing to the Onsager's reciprocal relations, the Hall conductivity or Nernst coefficient have to be vanishing in a time-reversal invariant system [5-7]. However, with increasing interests on nonlinear properties of topological materials, the nonlinear responses could appear in the presence of time-reversal symmetry but with broken inversion symmetry. Recently, the nonlinear anomalous Nernst effect has been predicted in transition-metal dichalcogenides [8–10]. These nonlinear thermal responses appear with distinctive behaviors and have become promising tools for understanding novel materials with low crystalline symmetry in experiments.

Most transport theories of thermally driven lattice systems are mostly phenomenological and numerical. This is because temperature gradients are macroscopic quantities after statistical averaging, and thus it is impossible to integrate into the Hamiltonian in a straightforward way. However, Luttinger provided a solution in 1964 [11]. To describe the effect of temperature gradient, he introduced a fictitious scalar field Ψ , which is called the "gravitational" potential, that couples to energy density $h(\mathbf{r})$. The Luttinger's Hamiltonian is

$$H_L = \int d^3 r \, h(\boldsymbol{r}) \Psi(\boldsymbol{r}). \tag{1}$$

The Hamiltonian of the system is then given as $H^{\Psi} = \int d^3r h^{\Psi}(\mathbf{r})$, with the modified energy density $h^{\Psi}(\mathbf{r}) = [1 + \Psi(\mathbf{r})]h(\mathbf{r})$. By the constriction of Einstein relation, the potential satisfies $\nabla \Psi = \nabla T/T$. In this way the dynamical response of the system to the varying field Ψ would be equivalent to the response to a temperature gradient assuming that the latter is slowly varying. Hence, the thermal transport coefficient can be directly calculated by linear response theory

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with Kubo formula. In the following we call this original proposal thermal scalar potential (TSP) method.

In the half century since the proposal of the original idea, Luttinger's method has found several applications in the calculation of the linear thermoelectric response. Nonetheless, a general nonlinear thermoelectric response theory is still lacking. Another point is that the external field may cause the electron to excite to another band or to move to a nearby kpoint on the same band. Hence, it needs a unified treatment of the two drift effects due to an external field in crystalline systems. This problem is handled in nonlinear optical response calculations, both in length gauge [12–16] and velocity gauge [17,18]. Motivated by these developments, we devote to developing a quantum theory for thermal response including generally the linear and nonlinear responses.

However, it is proved that a direct application of the coupling Hamiltonian (1) often leads to unphysical divergent results as $T \rightarrow 0$. It is shown that the divergence can be eliminated by introducing the vector potential representation [19]. By imposing the continuity equation for energy density ε and energy current density j_{ε} , the Luttinger Hamiltonian (1) can be transformed into vector potential form

$$H_L = \int d^3 r \, \boldsymbol{j}_{\varepsilon}(\boldsymbol{r}, t) \cdot \boldsymbol{A}_T(t), \qquad (2)$$

in which j_{ε} is the energy current density and A_T is the thermal vector potential, which satisfies

$$\partial_t A_T(\mathbf{r}, t) = \nabla \Psi(\mathbf{r}, t) = \frac{\nabla T(t)}{T}.$$
 (3)

The Hamiltonian (2) is equivalent to Luttinger's Hamiltonian. The derivation of Eq. (2) in Ref. [19] is under the assumption that the temperature gradient is static. In order to make it universally significant, we adopt a time-dependent temperature gradient, and the vector potential Hamiltonian (2) is still valid. For a comparison, we call the introduction of the vector potential representation as thermal vector potential (TVP) method.

For the case of electromagnetic vector potential A, the charge conservation is guaranteed by the U(1) gauge invariance. However, for TVP A_T , there is no such a gauge symmetry. In velocity gauge, the minimal coupling free-electron Hamiltonian including the thermal vector potential is given by [19]

$$\hat{H}_{A_T} = \frac{\hbar^2}{2m} \sum_{k} (k - \varepsilon_k A_T)^2 \hat{c}_k^{\dagger} \hat{c}_k.$$
(4)

For a general multiband Hamiltonian, the minimal coupling Hamiltonian is generalized to

$$\hat{H}_{A_T} = \hat{H}_0(k - \hat{H}_0 A_T).$$
(5)

The many-body crystalline Hamiltonian reads as

$$\hat{H}_0 = \sum_{p,k} \varepsilon_{pk} \hat{c}^{\dagger}_{pk} \hat{c}_{pk}, \qquad (6)$$

where the latin index *p* is the band index.

In this work, we explicitly derive the *dynamical* thermalthermal and thermoelectirc response coefficients by developing a theory based on TVP, and consider their DC limit. The frequency dependence of thermal-thermal response is receiving more and more attention in recent years, as a crucial issue especially for the thermal design of microprocessors in which the clock frequencies work in GHz. It is crucial to

which the clock frequencies work in GHz. It is crucial to cool the Joule heat in such system [20]. Shastry [21,22] and others [23,24] explored the linear dynamical thermal conductivity and thermoelectric response mediated by electrons and phonons via the TVP method, while the nonlinear counterpart has been given less attention, which should play an important role when the linear part disappears due to symmetry. We apply a canonical perturbation theory, both in velocity gauge and length gauge, to deal with the thermal nonlinear response with quantum effect fully considered. In this method the nonlinear thermal response fundamentally involves interband processes which are difficult to model semiclassically.

The paper is organized as follows: In Sec. II we introduce the perturbation expansion Hamiltonian in velocity gauge and derive the nonlinear thermal response, including nonlinear Nernst conductivity and nonlinear thermal conductivity. In Sec. III we present the formula given by length gauge and compare the semiclassical results in static limit. As an example of application, we present a calculation of nonlinear magnon Hall effect in a collinear antiferromagnetic system in Sec. IV. The last section is dedicated to a summary of our results.

II. PERTURBATION EXPANSION: DIAGRAMMATIC APPROACH

In analogy with the relation between electric field and electromagnetic vector potential, we can define the corresponding "thermal field" (E_T) to thermal vector potential A_T as

$$\boldsymbol{E}_T = -\frac{\partial \boldsymbol{A}_T}{\partial t} = -\frac{\boldsymbol{\nabla}T(t)}{T},\tag{7}$$

and their Fourier transformation

$$\boldsymbol{E}_T(\omega) = i\omega \boldsymbol{A}_T(\omega). \tag{8}$$

The spatial variation of the temperature gradient is assumed to be much larger than the material, so that the thermal field has no spatial dependence. The particle current is expanded in powers of the thermal field

$$\langle \hat{J}_{N}^{\alpha} \rangle (\omega) = \int d\omega_{1} L_{12}^{\alpha\beta}(\omega;\omega_{1}) E_{T}^{\beta} \delta_{\omega_{1},\omega} + \int d\omega_{1} d\omega_{2} L_{12}^{\alpha\beta\gamma}(\omega;\omega_{1},\omega_{2}) E_{T}^{\beta} E_{T}^{\gamma} \delta_{\omega_{1}+\omega_{2},\omega} + \cdots .$$

$$(9)$$

The greek indices $\mu, \alpha, \beta, \dots \in \{x, y, z\}$ are the space indices, and $L_{12}^{\mu\alpha_1\dots\alpha_n}(\omega; \omega_1\dots\omega_n)$ is defined as the *n*th-order thermoelectric conductivity tensor. The frequency before the semicolon in the response thermoelectric conductivity tensor $L_{12}^{\mu\alpha_1\dots\alpha_n}(\omega; \omega_1\dots\omega_n)$ represents the frequency of the output response, and the frequencies after the semicolon represent the frequencies of the input forces.

Before expanding the minimal coupling Hamiltonian (5) in Taylor series, one should deal with the *k*-space derivatives carefully. The important fact is that the Hamiltonian operator is differentiated first and then its matrix elements are calculated. Owing to this covariance *k* derivative of operator $\hat{O}(k)$

is [18,25]

$$\hat{\boldsymbol{D}}_{\boldsymbol{k}}[\hat{\mathcal{O}}(\boldsymbol{k})]_{pq} \equiv [\boldsymbol{\nabla}_{\boldsymbol{k}}\hat{\mathcal{O}}(\boldsymbol{k})]_{pq} = \boldsymbol{\nabla}_{\boldsymbol{k}}\mathcal{O}(\boldsymbol{k})_{pq} - i[\boldsymbol{\mathcal{A}}_{\boldsymbol{k}},\hat{\mathcal{O}}(\boldsymbol{k})]_{pq}.$$
(10)

Here the covariant derivative operator is defined by \hat{D}^{μ} . In Eq. (10) \mathcal{A}_{k} is the Berry connection, and its component in α direction is $\mathcal{A}^{\alpha}_{pq}(\mathbf{k}) = i \langle u_{pk} | \frac{\partial}{\partial k^{\alpha}} | u_{qk} \rangle$.

The partition function with thermal field is written as the path integral

$$\mathcal{Z} = \int d[\bar{c}, c] \exp\left(-i \int dt \, K_{A_T}\right),\tag{11}$$

in which $K_{A_T} = H_{A_T} - \mu N = \hat{K}_0(\mathbf{k} - \hat{K}_0 \mathbf{A}_T)$, with $K_0 = \sum_{p,\mathbf{k}} \tilde{\varepsilon}_{p\mathbf{k}} \hat{c}^{\dagger}_{p\mathbf{k}} \hat{c}_{p\mathbf{k}}$, and $\tilde{\varepsilon}_p = \varepsilon_p - \mu$ is the energy measured from the Fermi energy.

Different from the direct expansion of Hamiltonian in series of electromagnetic vector potential in calculating the nonlinear electric conductivity, the Hermiticity should be ensured in expanding \hat{K}_{A_T} in series of thermal vector potential A_T . For example, the first-order perturbation of \hat{K}_{A_T} is

$$\hat{K}_{A_T} \approx \hat{K}_0 - \frac{1}{2} A_T^{\alpha} [\hat{K}_0, \hat{D}^{\alpha} [\hat{K}_0]]_+, \qquad (12)$$

where the sum over space index α is implicit, and $[\ldots]_+$ is the anticommutation operation. To distinguish from the normal bracket, we use $[\ldots]_-$ to denote the commutation operation in the following. The grand-canonical ensemble energy operator K_{A_T} can be expanded by Taylor series in terms of thermal vector potential

$$\hat{K}_{A_{T}} = \hat{K}_{0} + \sum_{n=1}^{\infty} \frac{(-1)^{n}}{n!} \prod_{k=1}^{n} \frac{1}{2} A_{T}^{\alpha_{1}} \left[\hat{K}_{0}, \hat{D}^{\alpha_{1}} \left[\frac{1}{2} A_{T}^{\alpha_{2}} \left[\hat{K}_{0}, \dots, \hat{D}^{\alpha_{2}} \left[\frac{1}{2} A_{T}^{\alpha_{k}} [\hat{K}_{0}, \hat{D}^{\alpha_{k}} [\hat{K}_{0}]]_{+} \right] \right]_{+} \right] \right]_{+} \dots$$
(13)

Equation (10) can be used to write the velocity operator of the unperturbed system as

$$\hat{\boldsymbol{v}} = \hat{\boldsymbol{D}}[\hat{K}_0]. \tag{14}$$

The higher-order *direct* derivatives of the unperturbed Hamiltonian are written as

$$\hat{h}^{\alpha_1\dots\alpha_n} = \hat{D}^{\alpha_1}\dots\hat{D}^{\alpha_n}[\hat{K}_0].$$
(15)

We introduce the superoperator \mathcal{D}^{α} which is defined as the *Hermitian* derivative

$$\hat{\mathcal{D}}^{\alpha}[\hat{\mathcal{O}}] = \frac{1}{2} [\hat{K}_0, \hat{D}^{\alpha}[\hat{\mathcal{O}}]]_+.$$
(16)

It should be noted that the Hermitian derivative superoperators defined in Eq. (16) carry an additional dimension [energy]¹ than that of the direct derivative. Hence, the Hermitian derivative of the unperturbed K_0 is defined as

$$\hat{\mathcal{K}}^{\alpha_1\dots\alpha_n} = \hat{\mathcal{D}}^{\alpha_1}\dots\hat{\mathcal{D}}^{\alpha_n}[\hat{K}_0].$$
(17)

Again, the dimension of *n*th-order Hermitian derivative of the unperturbed Hamiltonian is *n*-power higher than that of the *n*th-order direct derivative of the unperturbed Hamiltonian.

Through Fourier transformation, the expanded K_{A_T} is simplified as

$$\hat{K}_{A_T} = \hat{K}_0 + \sum_{n=1}^{\infty} \frac{1}{n!} \prod_{k=1}^n \int d\omega_k e^{i\omega_k t} \frac{-i}{\hbar\omega_k} E_T^{\alpha_k}(\omega_k) \hat{\mathcal{K}}^{\alpha_1 \dots \alpha_k}.$$
(18)

Very recently, a diagrammatic approach has been developed to calculate the optical conductance in velocity gauge [18,26]. We generalize it in calculating the dynamical thermal response: the propagation of the temperature gradient is defined as a quasiparticle "thermalon." With the aid of TVP concept, the linear and nonlinear thermoelectric responses can be derived and the mutual relation between heat and charge can be studied at nonlinear level revealing deeper physics beyond the linear response.

The local particle current operator is defined as $\hat{J}_N \equiv \hat{v}_T$, here \hat{v}_T is the velocity operator in the perturbed system depending on the thermal field

$$\hat{\upsilon}_{T}^{\alpha}(t) = D^{\alpha}[K_{A_{T}}]$$

$$= \sum_{n=1}^{\infty} \frac{1}{n!} \prod_{k=1}^{n} \int d\omega_{k} e^{i\omega_{k}t} \frac{-i}{\hbar\omega_{k}} E_{T}^{\alpha_{k}}(\omega_{k}) \hat{D}^{\alpha}[\hat{\mathcal{K}}^{\alpha_{1}...\alpha_{k}}].$$
(19)

The local heat current operator is defined as $\hat{J}_Q = \hat{J}_E - \mu \hat{J}_N$, with μ the chemical potential. An exact from of the energy current operator \hat{J}_E can be derived from the conservation equation using Luttinger's Hamiltonian [27]

$$\frac{\partial \hat{h}^{\Psi}(\boldsymbol{r})}{\partial t} = \frac{1}{i\hbar} [\hat{h}^{\Psi}(\boldsymbol{r}), \hat{H}^{\Psi}] = -\nabla \cdot \hat{\boldsymbol{J}}_{E}(\boldsymbol{r}).$$
(20)

Using $H^{\Psi} = H_{A_T}$, the result is (for the derivation in detail see Appendix A)

$$\hat{J}_Q^{\alpha} = \frac{1}{2} \left(\hat{v}_T^{\alpha} \hat{K}_{A_T} + \hat{K}_{A_T} \hat{v}_T^{\alpha} \right) - \frac{i\hbar}{8} \sum_{\gamma} \nabla_{\gamma} \left(\hat{v}_T^{\alpha} \hat{v}_T^{\gamma} - \hat{v}_T^{\alpha} \hat{v}_T^{\gamma} \right).$$
(21)

It has been proved that the last term cancels when calculating the Kubo formula. In this case the heat current operator converts to the usual anticommutator representation $\hat{J}_Q = \frac{1}{2}[\hat{K}_{A_T}, \hat{v}_T]_+$. It is worth noting that the heat current operator defined through the conservation equation is compatible with the definition via the thermodynamics of the entropy flux (see Appendix A). An important issue in thermally driven current transport is the magnetization effect. Owing to the orbital motion of Bloch electrons, the magnetization current should be subtracted from the local current [1,27,28]

$$\boldsymbol{J}_{N(E)}^{\text{tr}} = \boldsymbol{J}_{N(E)} - \boldsymbol{\nabla} \times \boldsymbol{M}_{N(E)}(\boldsymbol{r}), \qquad (22)$$

in which $J_{N(E)}^{tr}$ is the electric (energy) current for transport, $J_{N(E)}$ is the local charge (energy) current, and $M_{N(E)}(r)$ is the particle (energy) magnetization density. The transport heat current is evaluated as

$$\boldsymbol{J}_{Q}^{\mathrm{tr}} = \boldsymbol{J}_{E}^{\mathrm{tr}} - \mu \boldsymbol{J}_{N}^{\mathrm{tr}}.$$
 (23)

Alternatively, the heat magnetization can be introduced through the relation [29–31]

$$\boldsymbol{M}_{\boldsymbol{Q}}(\boldsymbol{r}) \equiv \boldsymbol{M}_{\boldsymbol{E}}(\boldsymbol{r}) - \boldsymbol{\mu}\boldsymbol{M}_{\boldsymbol{N}}(\boldsymbol{r}). \tag{24}$$

The transport heat current is given as

$$\boldsymbol{J}_{\boldsymbol{Q}}^{\rm tr} = \boldsymbol{J}_{\boldsymbol{Q}} - \boldsymbol{\nabla} \times \boldsymbol{M}_{\boldsymbol{Q}}(\boldsymbol{r}), \tag{25}$$

in which the local heat current is given as

$$\boldsymbol{J}_{\boldsymbol{Q}} = \boldsymbol{J}_{\boldsymbol{E}} - \boldsymbol{\mu} \boldsymbol{J}_{\boldsymbol{N}}.$$
 (26)

Combining Eqs. (22), (24), and (26), one can verify that the two definitions of transport heat current, Eqs. (23) and (25), are equivalent:

$$J_{Q}^{tr} = J_{Q} - \nabla \times M_{Q}$$

= $J_{E} - \mu J_{N} - \nabla \times (M_{E} - \mu M_{N})$
= $(J_{E} - \nabla \times M_{E}) - \mu (J_{N} - \nabla \times M_{E})$
= $J_{E}^{tr} - \mu J_{N}^{tr}$. (27)

Similar derivation can be found in [32]. In the rest of this paper, the transport heat current is calculated through Eq. (25). The density matrix is written as

$$\hat{\rho} \approx \hat{\rho}_{\text{leq}} + \hat{\rho}_1, \qquad (28)$$

where $\hat{\rho}_{leq}$ is the local equilibrium density matrix characterized by the local chemical potential $\mu(\mathbf{r})$ and local temperature $T(\mathbf{r})$,

$$\hat{\rho}_{\text{leq}} = \frac{1}{Z} \exp\left[-\int d\boldsymbol{r} \frac{\hat{h}(\boldsymbol{r}) - \mu(\boldsymbol{r})\hat{h}(\boldsymbol{r})}{k_B T(\boldsymbol{r})}\right], \quad (29)$$

and ρ_1 is the linear response correction to the local equilibrium density matrix. Therefore, the local current is contributed by two parts

$$\boldsymbol{J}_{N(Q)} = \boldsymbol{J}_{N(Q)}^{\text{Kubo}} + \boldsymbol{J}_{N(Q)}^{\text{leq}}, \qquad (30)$$

where $J_{N(Q)}^{\text{Kubo}}$ is the direct response current, which is the direct conjugate variable of magnetic vector potential A (which will be noted as A_B in the following for clarity) and TVP A_T . $J_{N(Q)}^{\text{leq}}$ is the local equilibrium current, which comes from the inhomogeneous local chemical potential and temperature field. The local equilibrium current satisfies [29]

$$\boldsymbol{J}_{N}^{\text{leq}} = \boldsymbol{\nabla} \times \boldsymbol{M}_{N}(\boldsymbol{r}) - \boldsymbol{M}_{N}(\boldsymbol{r}) \times \boldsymbol{E}_{T}, \qquad (31)$$

$$\boldsymbol{J}_{\boldsymbol{Q}}^{\text{leq}} = \boldsymbol{\nabla} \times \boldsymbol{M}_{\boldsymbol{Q}}(\boldsymbol{r}) - \boldsymbol{M}_{\boldsymbol{N}}(\boldsymbol{r}) \times \boldsymbol{E} - 2\boldsymbol{M}_{\boldsymbol{Q}}(\boldsymbol{r}) \times \boldsymbol{E}_{\boldsymbol{T}}.$$
 (32)

The expressions for the local equilibrium current (31) and (32) convert to the bulk magnetization current when considering a finite system [27]. Noting that for transport current, the magnetization current should be subtracted [see Eq. (22)]. For electric-electric response, the local equilibrium current exactly cancels the magnetization current, and the transport is uniquely determined by Kubo formula. However, for electric-thermal, thermoelectric, and thermal-thermal responses, the terms proportional to external fields do not cancel the magnetization, which leave as the correction to Kubo formula. Hence, the transport currents become

$$\boldsymbol{J}_{N}^{\rm tr} = \boldsymbol{J}_{N}^{\rm Kubo} - \boldsymbol{M}_{N}(\boldsymbol{r}) \times \boldsymbol{E}_{T}, \qquad (33)$$

$$\boldsymbol{J}_{\boldsymbol{Q}}^{\mathrm{tr}} = \boldsymbol{J}_{\boldsymbol{Q}}^{\mathrm{Kubo}} - \boldsymbol{M}_{N}(\boldsymbol{r}) \times \boldsymbol{E} - 2\boldsymbol{M}_{\boldsymbol{Q}}(\boldsymbol{r}) \times \boldsymbol{E}_{T}.$$
 (34)

The expectation values of Kubo response currents $J_{c(h)}^{\text{Kubo}}$ are

$$\boldsymbol{J}_{N(\mathcal{Q})}^{\text{Kubo}} = \frac{1}{\mathcal{Z}} \frac{\delta \mathcal{Z}[\boldsymbol{A}_{B(T)}]}{\delta \boldsymbol{A}_{B(T)}},$$
(35)

with the path-integral form

where $d[\bar{c}, c]$ denotes the functional measure with \bar{c}, c the Grassmann variables constructing the Hamiltonian.

The zero-field expectation values of the particle magnetization and heat magnetization are

$$\boldsymbol{M}_{N(Q)} = -\lim_{\boldsymbol{B}_{B(T)} \to 0} \frac{\delta \Omega[\boldsymbol{B}_{B(T)}]}{\delta \boldsymbol{B}_{B(T)}},$$
(37)

where $\Omega = F - TS$ is the grand thermodynamic potential, the Landau free energy can be written as $F = -\frac{1}{\beta} \log(\mathcal{Z})$. It is convenient to introduce the auxiliary particle (heat) magnetization

$$\tilde{\boldsymbol{M}}_{N(Q)} = -\lim_{\boldsymbol{B}_{B(T)} \to 0} \frac{\delta F[\boldsymbol{B}_{B(T)}]}{\delta \boldsymbol{B}_{B(T)}}$$
(38)

which can be alternatively written in a TVP form by taking the long-wavelength limit [29,31,33]

$$\tilde{M}_{N(Q)} = \lim_{l \to 0} \nabla_l \times \frac{\delta F[A_{B(T)}]}{\delta A_{B(T),l}}.$$
(39)

 \tilde{M}_N and \tilde{M}_N in path-integral formalism are written as

$$\langle \tilde{\boldsymbol{M}}_{N}(t) \rangle = \frac{\beta}{2i} \nabla_{l} \times \frac{1}{\mathcal{Z}} \int d[\bar{c}, c] K_{A_{T}, -l}(t) \boldsymbol{\mathcal{D}}[K_{0, l}] \\ \times \exp\left[-i \int dt' K_{A_{T}}(t')\right], \qquad (40)$$
$$\langle \tilde{\boldsymbol{\mathcal{M}}}_{Q}(t) \rangle = \frac{\beta}{2i} \nabla_{l} \times \frac{1}{\mathcal{Z}} \int d[\bar{c}, c] K_{A_{T}, -l}(t) \boldsymbol{\mathcal{D}}[K_{0, l}]$$

$$\times \exp\left[-i\int dt' K_{A_T}(t')\right].$$
 (41)

By use of the Maxwell relation $\partial S/\partial B = \partial M/\partial T$, the particle (heat) magnetization satisfies [29,31,33]

$$\frac{\partial(\beta M_N)}{\partial \beta} = \tilde{M}_N,\tag{42}$$

$$\frac{\partial(\beta M_Q - \beta \delta M_Q)}{\partial \beta} = \tilde{M}_Q.$$
(43)

With the notation $J_{1(2)} \equiv J_{c(h)}$, $E_1 \equiv E$, $E_2 \equiv E_T$, and $M_{1(2)} \equiv M_{N(Q)}$, we introduce the set of transport equations

at nth order

$$\begin{bmatrix} J_1^{(n),\alpha}(\omega) \\ J_2^{(n),\alpha}(\omega) \end{bmatrix} = \begin{bmatrix} L_{11}^{\text{tr},(n)} & L_{12}^{\text{tr},(n)} \\ L_{21}^{\text{tr},(n)} & L_{22}^{\text{tr},(n)} \end{bmatrix} \begin{bmatrix} \prod_{k=1}^n E_1^{\alpha_k}(\omega_k) \\ \prod_{k=1}^n E_2^{\alpha_k}(\omega_k) \end{bmatrix},$$
(44)

with the response functions

$$L_{ij}^{\text{tr},(n)} = \left[\prod_{k=1}^{n} \int d\omega_k\right] \left[L_{ij}^{\text{Kubo},\alpha\alpha_1\dots\alpha_n}(\omega;\omega_1\dots\omega_n) - \epsilon^{\alpha\alpha_1\gamma}C_{ij}M_{ij}^{\gamma\alpha_2\dots\alpha_n}(\omega;\omega_1\dots\omega_n)\right]\delta_{\omega,\omega_1+\dots+\omega_n},\tag{45}$$

where $C_{11} = 0$, $C_{12} = C_{21} = 1/\beta$, $C_{22} = 2/\beta$ and $\epsilon^{\alpha\beta\gamma}$ is the Levi-Civita symbol. The Kubo responses L_{ij}^{Kubo} are given by

$$L_{ij}^{\text{Kubo},\alpha\alpha_1\dots\alpha_n}(\omega;\omega_1\dots\omega_k) = \int \frac{dt}{2\pi} e^{i\omega t} \prod_{k=1}^n \int \frac{dt_k}{2\pi} e^{i\omega_k t_k} \frac{\delta}{\delta E_j^{\alpha_k}(\omega_k)} \langle \hat{J}_i^{\alpha}(t) \rangle \Big|_{E_j^{\alpha_k}(\omega_k)=0},$$
(46)

and we define the magnetization response M_{ii} :

$$M_{ij}^{\gamma\alpha_2...\alpha_n}(\omega;\omega_1...\omega_k) = \int \frac{dt}{2\pi} e^{i\omega t} \prod_{k=1}^n \int \frac{dt_k}{2\pi} e^{i\omega_k t_k} \frac{\delta}{\delta E_j^{\alpha_k}(\omega_k)} \left\langle \hat{M}_i^{\gamma}(t) E_j^{\alpha_1}(t) \right\rangle \bigg|_{E_j^{\alpha_k}(\omega_k)=0}.$$
(47)

Based on the form of Eqs. (36) and (40), the Kubo contribution of the charge current is dually expanded in powers of TVP, given that the velocity operator and the exponent depend on TVP, while the magnetization is singly expanded. Hence, the *n*th-order response is computed by drawing all connected diagrams. One should pay attention to drawing the diagrams that the outgoing vertex which corresponds to the expansion of v and incoming vertex which corresponds to the expansion of action should be distinguished.

Thus, the *n*th-order thermoelectric response is calculated using the following rules:

(1) For the Kubo contribution L_{12}^{Kubo} , draw all the connected diagrams including *n* incoming thermalon lines connected by incoming vertexes (symbolled as •) and an outgoing photon line connected by one outgoing vertex (symbolled as \circ). All the inner lines are composed of electron propagators.

For the magnetization M_{12} , a subtle point is that two types of incoming vertices should be distinguished. One of which (symbolled as \blacksquare) connects a thermalon line with the momentum l, the other is the one identical to that of L_{12}^{Kubo} . The outgoing vertex (symbolled as \odot) connects only one photon line with the momentum -l.

(2) Integrate over the internal frequencies. The electron propagator is the free-fermion Green's function $G_p(\omega) = 1/(\omega - \varepsilon_p + \mu)$. The propagation of thermalon is treated classically, with the propagator being unity. For the Kubo term L_{12}^{Kubo} , the value of incoming vertex connecting *n* thermalon is $\prod_{k=1}^{n} (\frac{i}{\hbar\omega_k}) \mathcal{K}_{pq}^{\alpha_1...\alpha_n}$, and the value of outgoing vertex connecting *n* thermalon is $\prod_{k=1}^{n} (\frac{i}{\hbar\omega_k}) D^{\alpha_1} [\mathcal{K}]_{pq}^{\alpha_2...\alpha_n}$.

For the magnetization M_{12} , the *l*-dependent incoming vertex is $\frac{1}{2} [\prod_{k=1}^{n} (\frac{i}{\hbar\omega_k}) \mathcal{K}_{pq,k}^{\alpha_1...\alpha_n} + \prod_{k=1}^{n} (\frac{i}{\hbar\omega_k}) \mathcal{K}_{pq,k+l}^{\alpha_1...\alpha_n}]$. The outgoing vertex is $\frac{1}{2} (h_{pq,k}^{\alpha} + h_{pq,k+l}^{\alpha})$. Then calculate the curl with respect to *l* in the long-wavelength limit $l \to 0$, and integrate the auxiliary magnetization with respect to β by use of the relations (42) and (43) to obtain the magnetization.

(3) Multiply the symmetry factor by permuting α_k and ω_k . The values of the vertices for the Kubo contribution are listed in Table I and that for the magnetization are listed in Table II.

A. Linear thermoelectric response

The linear thermoelectric response is given by $L_{12}^{\text{Kubo},\alpha\beta}(\omega;\omega_1) - \epsilon^{\alpha\beta\gamma}M_N^{\gamma}|_{E_T=0}$. Following these rules, $L_{12}^{\text{Kubo},\alpha\beta}(\omega;\omega_1)$ is found to be

$$L_{12}^{\text{Kubo},\alpha\beta}(\omega;\omega_1) = \frac{i}{\hbar\omega_1} \sum_{p,q} \int_{k} \int d\omega' \{\mathcal{K}^{\beta}_{pq} G_q(\omega'+\omega) \times h^{\alpha}_{pq} G_p(\omega') + D^{\alpha} [\mathcal{K}^{\beta}]_{pp} G_p(\omega')\}.$$
(48)

The integration is over the first Brillouin zone (FBZ), with $\int_{k} = \int_{\text{FBZ}} d^{3}k/(2\pi)^{3}$. The corresponding diagrams are shown in Fig. 1. This expansion closely resembles that of [18] but has several differences due to the structure of the minimal coupling thermally perturbed Hamiltonian (4). The first-order Hermitian derivative is expanded as

$$\hat{\mathcal{K}}^{\alpha} = \frac{1}{2}(\hat{K}_0\hat{h}^{\alpha} + \hat{h}^{\alpha}\hat{K}_0) \tag{49}$$

TABLE I. Values of vertices for the Kubo contribution of electric-electric, thermal-electric, electric-thermal, and thermal-thermal responses.

	Incoming vertex •	Outgoing vertex \circ
$ \begin{array}{c} L_{11}^{\mathrm{Kubo}} \\ L_{12}^{\mathrm{Kubo}} \\ L_{21}^{\mathrm{Kubo}} \\ L_{21}^{\mathrm{Kubo}} \end{array} $	$ \begin{array}{l} \prod_{k=1}^{n}(\frac{ie}{\hbar\omega_{k}})h_{pq}^{\alpha_{1}\ldots\alpha_{n}} \\ \prod_{k=1}^{n}(\frac{i}{\hbar\omega_{k}})\mathcal{K}_{pq}^{\alpha_{1}\ldots\alpha_{n}} \\ \prod_{k=1}^{n}(\frac{ie}{\hbar\omega_{k}})h_{pq}^{\alpha_{1}\ldots\alpha_{n}} \\ \prod_{k=1}^{n}(\frac{i}{\hbar\omega_{k}})\mathcal{K}_{pq}^{\alpha_{1}\ldots\alpha_{n}} \end{array} $	$e \prod_{k=1}^{n} (\frac{i}{\hbar\omega_k}) h_{pq}^{\mu\alpha_1\alpha_n} \\ e \prod_{k=1}^{n} (\frac{i}{\hbar\omega_k}) D^{\mu} [\mathcal{K}]_{pq}^{\alpha_1\alpha_n} \\ \prod_{k=1}^{n} \sum_{a=0}^{n} (\frac{i}{\hbar\omega_k}) \frac{1}{2} [\mathcal{K}^{\alpha_1\alpha_a}, e^{n-a} h^{\mu\alpha_a\alpha_{n-a}}]_{pq} \\ \prod_{k=1}^{n} \sum_{a=0}^{n} (\frac{i}{\hbar\omega_k}) \frac{1}{2} [\mathcal{K}^{\alpha_1\alpha_a}, \mathcal{K}^{\mu\alpha_a\alpha_{n-a}}]_{pq}$

	Incoming vertex	Outgoing vertex \odot	
<i>M</i> ₁₁	$\frac{1}{2}\left[\prod_{k=1}^{n}\left(\frac{i}{\hbar\omega_{k}}\right)h_{pq,k}^{\alpha_{1}\alpha_{n}}+\prod_{k=1}^{n}\left(\frac{i}{\hbar\omega_{k}}\right)h_{pq,k+l}^{\alpha_{1}\alpha_{n}}\right]$	$\frac{1}{2}(h^{lpha}_{pq,k}+h^{lpha}_{pq,k+l})$	
M_{12}	$\frac{1}{2}\left[\prod_{k=1}^{n}\left(\frac{i}{\hbar\omega_{k}}\right)\right]_{pa,k}^{\alpha_{1}\alpha_{n}}+\prod_{k=1}^{n}\left(\frac{i}{\hbar\omega_{k}}\right)\mathcal{K}_{pa,k+l}^{\alpha_{1}\alpha_{n}}$	$\frac{1}{4}[(\tilde{\varepsilon}_{p,k}+\tilde{\varepsilon}_{q,k})h^{\alpha}_{pq,k}+(\tilde{\varepsilon}_{p,k+l}+\tilde{\varepsilon}_{q,k+l})h^{\alpha}_{pq,k+l}]$	
M_{21}	$\frac{1}{2}\left[\prod_{k=1}^{n} \left(\frac{i}{\hbar\omega_{k}}\right) h_{pa,k}^{\alpha_{1}\dots\alpha_{n}} + \prod_{k=1}^{n} \left(\frac{i}{\hbar\omega_{k}}\right) h_{pa,k+l}^{\alpha_{1}\dots\alpha_{n}}\right]$	$\frac{1}{2}(h_{pa,k}^{\alpha}+h_{pa,k+l}^{\alpha})$	
M_{22}	$\frac{1}{2}\left[\prod_{k=1}^{n}\left(\frac{i}{\hbar\omega_{k}}\right)\mathcal{K}_{pq,k}^{\alpha_{1}\ldots\alpha_{n}}+\prod_{k=1}^{n}\left(\frac{i}{\hbar\omega_{k}}\right)\mathcal{K}_{pq,k+l}^{\alpha_{1}\ldots\alpha_{n}}\right]$	$\frac{1}{4}[(\tilde{\varepsilon}_{p,k}+\tilde{\varepsilon}_{q,k})h^{\alpha}_{pq,k}+(\tilde{\varepsilon}_{p,k+l}+\tilde{\varepsilon}_{q,k+l})h^{\alpha}_{pq,k+l}]$	

TABLE II. Values of the momentum-dependent vertices for the particle and heat magnetization.

and

D

$${}^{\alpha}[\hat{K}^{\beta}] = \frac{1}{2} D^{\alpha}[\hat{K}_{0}D^{\beta}[\hat{K}_{0}] + D^{\beta}[\hat{K}_{0}]\hat{K}_{0}]$$

= $\frac{1}{2}(\hat{h}^{\alpha}\hat{h}^{\beta} + \hat{K}_{0}\hat{h}^{\alpha\beta} + \hat{h}^{\alpha\beta}\hat{K}_{0} + \hat{h}^{\beta}\hat{h}^{\alpha}).$ (50)

Noting that the \hat{K}_0 is a diagonal matrix, the Nernst coefficient becomes $[\alpha^{\alpha\beta}(\omega;\omega_1)]$ reduces to $\alpha^{\alpha\beta}(\omega)$ due to the conservation of energy]

$$L_{12}^{\text{Kubo,}\alpha\beta}(\omega) = \frac{i}{\hbar\omega_{1}} \sum_{p,q} \int_{k} \int d\omega' \bigg\{ \frac{1}{2} \big[\tilde{\varepsilon}_{p} h_{pq}^{\alpha} G_{q}(\omega'+\omega) \times h_{qp}^{\alpha} G_{p}(\omega') + h_{pq}^{\beta} G_{q}(\omega'+\omega) \tilde{\varepsilon}_{q} h_{qp}^{\alpha} G_{p}(\omega') \big] \\ + \bigg(\tilde{\varepsilon}_{p} h_{pp}^{\alpha\beta} + \frac{1}{2} h_{pq}^{\alpha} h_{qp}^{\beta} + \frac{1}{2} h_{pq}^{\beta} h_{qp}^{\alpha} \bigg) G_{p}(\omega') \bigg\}.$$
(51)

The $\tilde{\varepsilon}$ should be read as $\varepsilon - \mu$ for simplicity. According to Eq. (10), the second-order covariant derivative of \hat{K}_0 is

$$h_{pq}^{\alpha\beta} = D^{\alpha}[h^{\beta}]_{pq} = \partial^{\beta}h_{pq}^{\alpha} - i[\mathcal{A}^{\beta}, h^{\alpha}]_{pq}.$$
 (52)

Together with the relation $\mathcal{A}_{pq}^{\alpha} = v_{pq}^{\alpha}/i\varepsilon_{pq}(p \neq q)$ (originating from the relation $v_{pq}^{\alpha} = \partial^{\alpha}\varepsilon_{p}\delta_{pq} - i[\mathcal{A}^{\alpha}, H_{0}]_{pq}$), the linear



FIG. 1. Diagrammatic representation of $L_{12}^{\text{Kubo},\alpha\beta}$ and \tilde{M}_{12}^{γ} . The dashed line connects to a current operator, and the wavy lines are thermalons describing the couplings to thermal field. The momentum of the electron propagators in $L_{12}^{\text{Kubo},\alpha\beta}$ is suppressed.

thermoelectric response is given by

$$\begin{split} L_{12}^{\text{Kubo},\alpha\beta}(\omega) &= \frac{i}{\hbar\omega_1} \sum_{p,q} \int_{k} \bigg[\tilde{\varepsilon}_p \partial^{\beta} f_p v_p^{\alpha} + \frac{1}{2} (\tilde{\varepsilon}_p + \tilde{\varepsilon}_q) v_{pq}^{\beta} \\ &\times v_{qp}^{\alpha} \frac{f_{pq}}{\omega + \varepsilon_{pq}} - \tilde{\varepsilon}_p \bigg(\frac{v_{pq}^{\beta} v_{qp}^{\alpha}}{\varepsilon_{pq}} - \frac{v_{pq}^{\alpha} v_{qp}^{\beta}}{\varepsilon_{qp}} \bigg) f_p \\ &+ \frac{1}{2} \big(v_{pq}^{\beta} v_{qp}^{\alpha} + v_{pq}^{\alpha} v_{qp}^{\beta} \big) f_p \bigg], \end{split}$$

where $f_{pq} = f_p - f_q$ and $\varepsilon_{pq} = \varepsilon_p - \varepsilon_q$, and the sum over band indices is only performed over the indices appearing in each term. After some simple algebra, we obtain

$$L_{12}^{\text{Kubo,}\alpha\beta}(\omega) = \frac{i}{\hbar\omega_1} \sum_{p,q} \int_k \left[\tilde{\varepsilon}_p \partial^\beta f_p v_p^\alpha + \frac{1}{2} (\tilde{\varepsilon}_p + \tilde{\varepsilon}_q) \times v_{pq}^\beta v_{qp}^\alpha \left(\frac{f_{pq}}{\omega + \varepsilon_{pq}} - \frac{f_{pq}}{\varepsilon_{pq}} \right) \right],$$
(53)

where the identity $v_{pq}^{\alpha} = h_{pq}^{\alpha}$ is used. The first term corresponds to the intraband contribution with normal derivative, playing the role of the Drude weight in the dynamical thermoelectric response, and the later terms are the interband contributions and as we demonstrate below, they manifest themselves as the Berry curvature in the static state limit.

Now we give the derivation of M_{12}^{γ} . Referring to Eq. (40), we first derive \tilde{M}_{12}^{γ} as

$$\tilde{M}_{12}^{\gamma} = \frac{i}{4\hbar} \sum_{p,q} \int_{k} \int d\omega' \frac{\partial}{i\partial l^{\beta}} \Big[(\tilde{\varepsilon}_{p,k} + \tilde{\varepsilon}_{q,k+l}) \\ \times G_{p,k}(\omega' + \omega) \big(h_{pq,k}^{\alpha} + h_{pq,k+l}^{\alpha} \big) G_{q,k+l}(\omega) \Big].$$
(54)

Performing the frequency integral, it becomes

$$\tilde{M}_{12}^{\gamma} = \frac{i}{4\hbar} \sum_{p,q} \int_{k} \int d\omega' \frac{\partial}{i\partial l^{\beta}} \bigg[(\tilde{\varepsilon}_{p,k} + \tilde{\varepsilon}_{q,k+l}) \\ \times (v_{pq,k}^{\alpha} + v_{pq,k+l}^{\alpha}) \frac{f_{p,k} - f_{q,k+l}}{\omega - (\varepsilon_{p,k} - \varepsilon_{q,k+l})} \bigg].$$
(55)

We first consider the interband contribution for $p \neq q$. In the long-wavelength limit $l \rightarrow 0$, we have

$$\tilde{M}_{12}^{\gamma,\text{inter}} = \frac{i}{\hbar} \sum_{p \neq q} \int_{k} \frac{1}{2} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q}) \frac{v_{pq}^{\alpha} v_{qp}^{\beta}}{(\omega - \varepsilon_{pq}) \varepsilon_{pq}} f_{pq}.$$
 (56)

The intraband contribution $\tilde{M}_{12}^{\gamma,\text{intra}}$ at $l \to 0$ when p = q is given by

$$\tilde{M}_{12}^{\gamma,\text{intra}} = \frac{i}{2\hbar} \sum_{p,q} \int_{k} \left[-\tilde{\varepsilon}_{p} \frac{\left(v_{pq}^{\alpha} v_{qp}^{\beta} - v_{pq}^{\beta} v_{qp}^{\alpha} \right)}{(\omega - \varepsilon_{pq})\varepsilon_{pq}} \frac{\partial f_{p}}{\partial \varepsilon_{p}} \right].$$
(57)

Therefore, we have

$$\tilde{M}_{12}^{\gamma} = \frac{i}{2\hbar} \sum_{p,q} \int_{k} \left[(\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q}) \frac{v_{pq}^{\alpha} v_{qp}^{\beta}}{(\omega - \varepsilon_{pq}) \varepsilon_{pq}} f_{pq} - \tilde{\varepsilon}_{p} \frac{(v_{pq}^{\alpha} v_{qp}^{\beta} - v_{pq}^{\beta} v_{qp}^{\alpha})}{(\omega - \varepsilon_{pq}) \varepsilon_{pq}} \frac{\partial f_{p}}{\partial \varepsilon_{p}} \right].$$
(58)

Integrating Eq. (58) with respect to β from Eq. (42), we obtain (see Appendix C for detail)

$$M_{12}^{\gamma} = \frac{i}{\hbar} \sum_{p,q} \int_{k} \left\{ \frac{\left(v_{pq}^{\alpha} v_{qp}^{\beta} - v_{pq}^{\beta} v_{qp}^{\alpha} \right)}{(\omega - \varepsilon_{pq})\varepsilon_{pq}} \times \left[\frac{1}{2} (\tilde{\varepsilon}_{p} - \tilde{\varepsilon}_{q}) f_{p} + \frac{1}{\beta} \ln(1 + e^{-\beta \varepsilon_{p}}) \right] \right\}.$$
 (59)

In the DC limit, it becomes

$$M_{12}^{\gamma} = \sum_{p} \int_{k} \left[m_{1,p}^{\gamma} f_{p} + \frac{1}{\beta \hbar} \Omega_{p}^{\gamma} \ln(1 + e^{-\beta \tilde{\varepsilon}_{p}}) \right]. \quad (60)$$

The first term manifests itself as the particle magnetic moment, which is given as [1,34]

$$m_p^{\gamma} = -\frac{1}{\hbar} \epsilon^{\alpha\beta\gamma} \operatorname{Im} \langle \partial^{\alpha} u_p | (\hat{H}_0 - \varepsilon_p) | \partial^{\beta} u_p \rangle.$$
 (61)

In Refs. [1,34], the derivation of Eq. (61) starts from a wave-packet hypothesis, however, its final expression does not depend on the actual shape and size of the wave packet and only depends on the Bloch functions. Therefore, the orbital moment is an intrinsic property of the band. Alternatively, integrating by part, the magnetization (60) can be given as

$$M_{12}^{\gamma} = \sum_{p} \int_{k} \left[m_{p}^{\gamma} f_{p} - \frac{1}{e^{2}} \int d\varepsilon \, \sigma_{p}^{\gamma}(\varepsilon) f_{p} \right], \quad (62)$$

where $\sigma_p^{\gamma}(\varepsilon) = \frac{e^2}{\hbar} \int [d\mathbf{k}] \Theta(\varepsilon - \varepsilon_k) \Omega_p^{\gamma}(\mathbf{k})$ is the *p*-band contribution to the zero-temperature Hall conductivity with Fermi energy ε . Combining Eqs. (53) and (59), we finally obtain the dynamical linear thermoelectric response

$$L_{12}^{\mathrm{tr},\alpha\beta} = \frac{i}{\hbar} \sum_{p,q} \int_{k} \left[\frac{1}{\omega} \tilde{\varepsilon}_{p} v_{p}^{\beta} v_{p}^{\alpha} \frac{\partial f_{p}}{\partial \varepsilon_{p}} - \frac{\left(v_{pq}^{\alpha} v_{qp}^{\beta} - v_{pq}^{\beta} v_{qp}^{\alpha} \right)}{(\omega - \varepsilon_{pq}) \varepsilon_{pq}} \times [\tilde{\varepsilon}_{p} f_{p} + k_{B} T \ln(1 + e^{-\beta \tilde{\varepsilon}_{p}})] \right].$$
(63)

In the DC limit, $\sum_{q} (v_{pq}^{\beta} v_{qp}^{\alpha} - v_{pq}^{\alpha} v_{qp}^{\beta}) / \varepsilon_{qp}^{2}$ is recognized as the Berry curvature. Hence, we have

$$L_{\text{DC},12}^{\text{tr},\alpha\beta}(\omega) = \frac{1}{\hbar} \sum_{p} \int_{k} \left\{ i \frac{1}{\omega} \tilde{\varepsilon}_{p} v_{p}^{\beta} v_{p}^{\alpha} \frac{\partial f_{p}}{\partial \varepsilon_{p}} + \epsilon^{\alpha\beta\gamma} \Omega_{p}^{\gamma} \right. \\ \left. \times [\tilde{\varepsilon}_{p} f_{p} + k_{B} T \ln(1 + e^{-\beta\tilde{\varepsilon}_{p}})] \right\}.$$
(64)

The first term corresponds to the Drude weight of energy current transport, which diverges in the DC limit. This is because the considered system is a clean one. In real materials the electrons are scattered and have finite lifetime, where the electrons are not accelerated everlastingly. The second term is the topological contribution, which is represented by the Berry curvature. It is seen that the fictitious divergence is eliminated in the TVP method.

The thermoelectric conductivity η is related to the thermoelectric response by $\eta^{\alpha\alpha_1...\alpha_n} = L_{12}^{\text{tr},\alpha\alpha_1...\alpha_n}/T^n$. The linear anomalous Nernst conductivity is given by $\eta^{\alpha\beta} = L_{12}^{\text{tr},\alpha\beta}/T$. By introducing the entropy density $S_p = -f_p \ln f_p - (1 - f_p) \ln(1 - f_p)$ of *p*-band electrons and neglecting the Drude term, the anomalous Nernst conductivity can be written as

$$\eta^{\alpha\beta}(\omega) = \frac{ek_B}{\hbar} \varepsilon^{\alpha\beta\gamma} \sum_p \int_k \Omega_p^{\gamma} S_p.$$
(65)

Referring to Eq. (65), the expression of anomalous Nernst conductivity is consistent with the formula derived by wave-packet theory in Ref. [1].

B. Linear thermal-thermal response

The rules of dynamical thermal conductivity are similar to those of thermoelectric response, but with different vertex functions. The value of outgoing vertex connecting *n* photon is $\prod_{k=1}^{n} (\frac{i}{h\omega_k}) \frac{1}{2} [h^{\alpha_1...\alpha_p}, h^{\alpha_\mu\alpha_p...\alpha_{n-p}}]_{pq}$, and for incoming vertex it is $\prod_{k=1}^{n} (\frac{i}{h\omega_k}) \mathcal{K}_{pq}^{\alpha_1...\alpha_n}$. Hence, the linear thermal-thermal response is given by

$$L_{22}^{\text{Kubo,}\alpha\beta}(\omega) = \frac{i}{\hbar\omega_{1}} \sum_{p,q} \int_{k} \int d\omega' \mathcal{K}_{pq}^{\beta} G_{q}(\omega'+\omega) \mathcal{K}_{qp}^{\alpha} G_{p}(\omega') + \frac{e}{\hbar\omega_{1}} \sum_{p} \int_{k} \int d\omega' \left(\mathcal{K}_{pp}^{\alpha\beta} + \frac{1}{2} [\mathcal{K}^{\beta}, h^{\alpha}]_{pp} \right) G_{p}(\omega'),$$
(66)

where the expansion of the second-order Hermitian derivative $\mathcal{K}^{\mu\alpha}$ is involved (see Appendix B). Integrating the Matsubara frequencies, it yields

$$L_{22}^{\text{Kubo,}\alpha\beta}(\omega) = \frac{i}{\hbar\omega_{1}} \sum_{p,q} \int_{k} \left[\tilde{\varepsilon}_{p}^{2} \partial^{\beta} f_{p} v_{p}^{\alpha} + \frac{1}{4} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q})^{2} \right. \\ \left. \times v_{pq}^{\beta} v_{qp}^{\alpha} \frac{f_{pq}}{\omega - \varepsilon_{pq}} + \frac{1}{2} \tilde{\varepsilon}_{p} (h_{pq}^{\alpha} h_{qp}^{\beta} + h_{pq}^{\beta} h_{qp}^{\alpha}) f_{p} \right. \\ \left. + \frac{1}{4} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q}) (h_{pq}^{\alpha} h_{qp}^{\beta} + h_{pq}^{\beta} h_{qp}^{\alpha}) f_{p} \right. \\ \left. - \tilde{\varepsilon}_{p}^{2} \left(\frac{h_{pq}^{\beta} h_{qp}^{\alpha}}{\varepsilon_{pq}} - \frac{h_{pq}^{\alpha} h_{qp}^{\beta}}{\varepsilon_{qp}} \right) f_{pq} \right],$$
(67)

which can be written in a compact form

$$L_{22}^{\text{Kubo},\alpha\beta}(\omega) = \frac{i}{\hbar\omega} \sum_{p,q} \int_{k} \left\{ \tilde{\varepsilon}_{p}^{2} v_{p}^{\alpha} \partial^{\beta} f_{p} + \frac{1}{4} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q})^{2} \times v_{pq}^{\beta} v_{qp}^{\alpha} f_{pq} \left(\frac{1}{\omega - \varepsilon_{pq}} + \frac{1}{\varepsilon_{pq}} \right) \right\}.$$
(68)

$$\tilde{M}_{22}^{\gamma} = \frac{i}{4\hbar} \sum_{p,q} \int_{k} \int d\omega' \frac{\partial}{i\partial l^{\beta}} \Big[(\tilde{\varepsilon}_{p,k} + \tilde{\varepsilon}_{q,k+l}) G_{p,k}(\omega' + \omega) \\ \times \big(\mathcal{K}_{pq,k}^{\alpha} + \mathcal{K}_{pq,k+l}^{\alpha} \big) G_{q,k+l}(\omega) \Big].$$
(69)

Performing the frequency integral, it becomes

$$\tilde{M}_{22}^{\gamma} = \frac{i}{4\hbar} \sum_{p,q} \int_{k} \int d\omega' \frac{\partial}{i\partial l^{\beta}} \bigg[(\tilde{\varepsilon}_{p,k} + \tilde{\varepsilon}_{q,k+l}) \\ \times \big(\tilde{\varepsilon}_{p,k} v_{pq,k}^{\alpha} + v_{pq,k+l}^{\alpha} \tilde{\varepsilon}_{q,k+l} \big) \frac{f_{p,k} - f_{q,k+l}}{\omega - (\varepsilon_{p,k} - \varepsilon_{q,k+l})} \bigg].$$

$$\tag{70}$$

Following the same steps as in the previous section by collecting both the intraband and interband contributions, we have

$$\tilde{M}_{22}^{\gamma} = -\frac{i}{4\hbar} \sum_{p,q} \int_{k} \left[2(\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q})^{2} \frac{v_{pq}^{\alpha} v_{qp}^{\beta}}{(\omega - \varepsilon_{pq})\varepsilon_{pq}} f_{pq} + (\tilde{\varepsilon}_{p} \varepsilon_{pq}^{2} - 4\tilde{\varepsilon}_{p}^{2} \varepsilon_{pq}) \frac{(v_{pq}^{\alpha} v_{qp}^{\beta} - v_{pq}^{\beta} v_{qp}^{\alpha})}{(\omega - \varepsilon_{pq})\varepsilon_{pq}} \frac{\partial f_{p}}{\partial \varepsilon_{p}} \right].$$
(71)

Integrating Eq. (71) with respect to β [via Eq. (43)] from β to ∞ , we obtain (see Appendix C for details)

$$M_{22}^{\gamma} = -\frac{i}{\hbar} \sum_{p,q} \int_{k} \left\{ \frac{\left(v_{pq}^{\alpha} v_{qp}^{\beta} - v_{pq}^{\beta} v_{qp}^{\alpha} \right)}{(\omega - \varepsilon_{pq})\varepsilon_{pq}} \times \left[\frac{1}{4} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q})^{2} f_{p} + \int_{\tilde{\varepsilon}_{p}}^{\infty} d\lambda \,\lambda^{2} \frac{\partial f_{p}(\lambda)}{\partial\lambda} \right] \right\}.$$
(72)

By use of the identity $\int_{\tilde{\varepsilon}_p}^{\infty} d\lambda \,\lambda^2 \frac{\partial f_p(\lambda)}{\partial \lambda} = -\int_0^{f_p} (\log \frac{1+t}{t})^2 dt = c_2(f_p)$ and taking DC limit, we have

$$M_{22}^{\gamma} = - \frac{1}{\hbar} \sum_{p} \int_{k} \left[w_{p}^{\gamma} f_{p} + c_{2}(f_{p}) \Omega_{p}^{\gamma} \right], \qquad (73)$$

where the weight function is $c_2(f_p) = (f_p - 1) \ln^2(f_p^{-1} - 1) + \ln^2 f_p + 2\text{Li}_2(f_p)$, with $\text{Li}_2(x)$ being the polylogarithm function. We introduce the notation

$$w_p^{\gamma} = \frac{1}{\hbar} \varepsilon^{\alpha\beta\gamma} \sum_p \frac{1}{2} \operatorname{Im} \langle \partial^{\alpha} u_p | (\hat{H}_0 + \varepsilon_p)^2 | \partial^{\beta} u_p \rangle.$$
(74)

Combining Eqs. (72) and (68), we have

$$L_{22}^{\mathrm{tr},\alpha\beta}(\omega) = \frac{i}{\hbar} \sum_{p,q} \int_{k} \left[\frac{1}{\omega} \tilde{\varepsilon}_{p}^{2} \partial^{\beta} f_{p} v_{p}^{\alpha} + \frac{\left(v_{pq}^{\alpha} v_{qp}^{\beta} - v_{pq}^{\beta} v_{qp}^{\alpha} \right)}{(\omega - \varepsilon_{pq}) \varepsilon_{pq}} c_{2}(f_{p}) \right].$$
(75)

In the DC limit, it yields

$$L_{22}^{\mathrm{tr},\alpha\beta}(\omega) = \frac{1}{\hbar} \sum_{p} \int_{k} \left[i \frac{1}{\omega} \tilde{\varepsilon}_{p}^{2} \partial^{\beta} f_{p} v_{p}^{\alpha} - c_{2}(f_{p}) \Omega_{p}^{\gamma} \right].$$
(76)

The first term is the Drude-type term in heat transport, the second term is the Berry curvature contribution.

Now we present a study of correlations between the thermal conductivity and electric conductivity. Including the transverse transport, the Lorentz number should be generalized into a tensor form

$$\frac{\kappa^{\alpha\beta}}{\sigma^{\alpha\beta}} = L^{\alpha\beta}T,\tag{77}$$

where $L^{\alpha\beta}$ is defined as the Lorentz tensor. First, we consider the longitudinal transport. Note that the Drude term in the linear response of κ and σ corresponds to the contribution of intraband elements. When $\alpha = \beta$, the topological term vanishes and only the Drude term survives. Hence, the longitudinal response is fully determined by the Drude term. We write the longitudinal electric conductivity as

$$\sigma_L^{xx}(\omega;\omega_1) = \frac{e^2}{\hbar} \sum_p \int_k \frac{\partial^x f_p v_p^x}{\omega},$$
(78)

which is written as

$$\sigma_L^{xx}(\omega;\omega_1) = \frac{e^2}{\hbar\omega} \sum_p \int d\varepsilon_p \int_{\boldsymbol{k}} \frac{\partial f_p}{\partial \varepsilon_p} \left(\frac{\partial \varepsilon_p}{\partial k^x}\right)^2 \delta(\varepsilon_p - \varepsilon_{p,\boldsymbol{k}}).$$
(79)

The longitudinal thermal conductivity is given by

$$\kappa_{L}^{xx}(\omega;\omega_{1}) = \frac{1}{T\hbar\omega} \sum_{p} \int d\varepsilon_{p} \int_{k} \varepsilon_{p}^{2} \frac{\partial f_{p}}{\partial \varepsilon_{p}} \left(\frac{\partial \varepsilon_{p}}{\partial k^{x}}\right)^{2} \times \delta(\varepsilon_{p} - \varepsilon_{p,k}).$$
(80)

We can make use of the low-temperature expansion

$$\frac{\partial f_p}{\partial \varepsilon_p} = \delta(\varepsilon_p - \mu) + \frac{\pi^2}{6} (k_B T)^2 \frac{\partial^2}{\partial \varepsilon_p^2} \delta(\varepsilon_p - \mu) + \frac{7\pi^4}{360} (k_B T)^4 \frac{\partial^4}{\partial \varepsilon_p^4} \delta(\varepsilon_p - \mu) + \cdots .$$
(81)

Inserting Eq. (81) into (80) and (79), the WF law in longitudinal direction is obtained

$$\frac{\kappa_L^{xx}}{\sigma_L^{xx}} = LT,$$
(82)

with $L = \frac{1}{3} (\frac{k_B \pi}{e})^2 = 2.44 \times 10^{-8} \text{ W } \Omega/\text{K}^2$ is the well-known Lorentz number [35].

For transverse transport, according to the expression (76), the thermal conductivity can be rewritten as

$$\kappa_T^{xy} = -\frac{1}{e^2 T} \int d\epsilon (\epsilon - \mu)^2 \frac{\partial f(\epsilon)}{\partial \epsilon} \sigma^{xy}(\epsilon), \qquad (83)$$

where $\sigma^{xy}(\epsilon) = \frac{-e^2}{\hbar} \sum_p \int_k \theta(\epsilon - \varepsilon_{p,k}) \Omega^{xy}(k)$ is the intrinsic anomalous Hall conductivity at zero temperature with Fermi energy ϵ . Given a similar low-temperature expansion, the WF law for transverse transport is verified [36], with the offdiagonal elements of the Lorentz tensor given by $L^{xy} = L$. We conclude that the linear WF law reads as

$$\kappa^{\alpha\beta} = LT\sigma^{\alpha\beta},\tag{84}$$



FIG. 2. Diagrammatic representation of second-order thermoelectric response, including the second-order Kubo contribution $L_{12}^{\text{Kubo},\alpha\beta\gamma}$ and the local equilibrium contribution $\tilde{M}_{12}^{\gamma\beta}$.

which states that the linear thermal conductivity is proportional to the linear electric conductivity both for the PHYSICAL REVIEW B 106, 035148 (2022)

longitudinal and transverse transport. In this work, we call Eq. (84) as the linear WF law or the first-order WF law.

C. Second-order thermoelectric response

Now we consider the second-order thermoelectric response $L_{12}^{\alpha\beta\gamma}$. At second order it is composed of four types diagrams, as shown in Fig. 2. By using of the Hermitian derivation operator $\mathcal{K}^{\alpha_1...\alpha_k}$ defined in Sec. II, the Kubo contribution to second-order thermoelectric response is given by

$$L_{12}^{\text{Kubo},\alpha\beta\gamma}(\omega;\omega_{1},\omega_{2})$$

$$= -\frac{1}{\hbar^{2}\omega_{1}\omega_{2}}\sum_{p,q,r}\int_{k}\int d\omega' \{ [D^{\alpha}[\mathcal{K}^{\beta\gamma}]]_{pp}G_{p}(\omega')$$

$$+ 2G_{p}(\omega')\mathcal{K}^{\beta}_{pq}G_{q}(\omega'+\omega_{1})D^{\alpha}[\mathcal{K}^{\gamma}]_{qp}$$

$$+ G_{p}(\omega')\mathcal{K}^{\beta\gamma}_{pq}G_{q}(\omega'+\omega_{12})h^{\alpha}_{qp}$$

$$+ G_{p}(\omega')\mathcal{K}^{\beta}_{pq}G_{q}(\omega'+\omega_{1})\mathcal{K}^{\gamma}_{qr}G_{r}(\omega'+\omega_{2})h^{\alpha}_{rp} \}$$

$$+ (\beta \leftrightarrow \gamma, \omega_{1} \leftrightarrow \omega_{2}), \qquad (85)$$

where $(\beta \leftrightarrow \gamma, \omega_1 \leftrightarrow \omega_2)$ denotes symmetrization under simultaneous swap of the indices (β, γ) and the frequencies (ω_1, ω_2) . The energy conservation is constrained by $\omega = \omega_{12} = \omega_1 + \omega_2$. It can be seen from Fig. 2 that for the Kubo contribution, the first diagram describes a process where thermalons interact sequentially. In contrast, the other three diagrams contain vertices of order greater than one, which is described by instantaneous processes with two or three interaction events. Performing the integral over Matsubara frequencies, we obtain

$$L_{12}^{\text{Kubo},\alpha\beta\gamma}(\omega;\omega_{1},\omega_{2}) = -\frac{1}{\hbar^{2}\omega_{1}\omega_{2}}\sum_{p,q,r}\int_{k}\left\{\frac{1}{2}f_{p}[D^{\alpha}[\mathcal{K}^{\beta\gamma}]]_{pp}\frac{f_{pq}}{\omega_{1}-\varepsilon_{pq}}\mathcal{K}^{\beta}_{pq}D^{\alpha}[\mathcal{K}^{\gamma}]_{qp} + \frac{1}{2}\frac{f_{pq}}{\omega_{1}+\omega_{2}-\varepsilon_{pq}}\mathcal{K}^{\beta\gamma}_{pq}h^{\alpha}_{qp} + \mathcal{K}^{\beta}_{pq}\mathcal{K}^{\gamma}_{qr}h^{\alpha}_{rp}\frac{(\omega_{1}-\varepsilon_{rq})f_{pq}+(\omega_{1}-\varepsilon_{qp})f_{rq}}{(\omega_{1}-\varepsilon_{qp})(\omega_{2}-\varepsilon_{rq})(\omega_{1}+\omega_{2}-\varepsilon_{qp})}\right\}.$$
(86)

To keep the shorthand notation, we leave the expansion of the vertices in Appendix B. The magnetization response is given by

$$\tilde{M}_{12}^{\gamma\beta}(\omega;\omega_{1},\omega_{2}) = \frac{i}{4\hbar} \sum_{p,q,r} \int_{k} \int d\omega' \frac{\partial}{i\partial l^{\beta}} \Big[G_{p,k}(\omega') \Big(\mathcal{K}_{pq,k}^{\gamma} + \mathcal{K}_{pq,k+l}^{\gamma} \Big) G_{q,k+l}(\omega' + \omega_{1} + \omega_{2}) \Big(h_{qp,k}^{\alpha} + h_{qp,k+l}^{\alpha} \Big) \\ + G_{p,k}(\omega') (\tilde{\varepsilon}_{p,k} + \tilde{\varepsilon}_{q,k+l}) G_{q,k+l}(\omega' + \omega_{1}) \Big(h_{qr,k}^{\alpha} + h_{qr,k+l}^{\alpha} \Big) G_{r,k}(\omega' + \omega_{1} + \omega_{2}) \mathcal{K}_{rp,k}^{\beta} \Big].$$

$$(87)$$

After the integral over ω' , we derive

$$\tilde{M}_{12}^{\gamma\beta}(\omega;\omega_{1},\omega_{2}) = \frac{i}{4\hbar} \sum_{p,q,r} \int_{\boldsymbol{k}} \frac{\partial}{i\partial l^{\beta}} \bigg[\frac{1}{2} \big(\mathcal{K}_{pq,\boldsymbol{k}}^{\gamma} + \mathcal{K}_{pq,\boldsymbol{k}+l}^{\gamma} \big) \big(h_{qp,\boldsymbol{k}}^{\alpha} + h_{qp,\boldsymbol{k}+l}^{\alpha} \big) \frac{f_{pq}}{\omega_{1} + \omega_{2} - \varepsilon_{pq}} \\ + (\tilde{\varepsilon}_{p,\boldsymbol{k}} + \tilde{\varepsilon}_{q,\boldsymbol{k}+l}) \big(h_{qr,\boldsymbol{k}}^{\alpha} + h_{qr,\boldsymbol{k}+l}^{\alpha} \big) \mathcal{K}_{qr,\boldsymbol{k}}^{\beta} \frac{(\omega_{1} - \varepsilon_{rq})f_{pq} + (\omega_{1} - \varepsilon_{qp})f_{rq}}{(\omega_{1} - \varepsilon_{qp})(\omega_{2} - \varepsilon_{rq})(\omega_{1} + \omega_{2} - \varepsilon_{qp})} \bigg].$$
(88)

Considering that the partial differential in $\tilde{M}_{12}^{\gamma\beta}$ involves many terms, an analytical treatment of $\tilde{M}_{12}^{\gamma\beta}$ is rather tedious. Instead, it is more convenient to treat it numerically.

The same process applies to the second-order electric-thermal response $L_{21}^{\text{tr},\alpha\beta\gamma}$ and thermal-thermal response $L_{22}^{\text{tr},\alpha\beta\gamma}$.

Different methods are proposed to include finite relaxation rates into nonlinear responses [37–39], both in length gauge and velocity gauge. Referring to Eq. (86), which involves the electron transfer processes between two or more bands leading to different relaxation times, it is more accurate to correct the covariant derivative by relaxation rate Γ_{mn} for excited states [40]

$$v_{pq}^{\alpha} = \partial^{\alpha} \varepsilon_{p} \delta_{pq} - i \varepsilon_{pq} \mathcal{A}_{pq}^{\alpha} - \sum_{r} \left(\mathcal{A}_{pr}^{\alpha} \Gamma_{rq} - \Gamma_{pr} \mathcal{A}_{rq}^{\alpha} \right).$$
(89)

In order to make a direct connection to the semiclassical result, the simple replacement $\omega \rightarrow \omega + i\Gamma$ is adopted. Due to the finite lifetime of electrons, the propagator is replaced by $1/(\omega + i\Gamma)$, where Γ is the imaginary part of the self-energy and $\tau = 1/\Gamma$ is the electron relaxation time.

The expansion of the vertices might appear pretty verbose, but crucially it allows us a straightforward identification of the physical processes. By taking $\omega \rightarrow 0$ the static limit response can be directly implemented in numerics. However, a direct conversion to the static-state results is rather laborious. As we show in the following, it is much easier to do this in length gauge.

III. STATIC-STATE RESULTS: LENGTH GAUGE

As discussed in Sec. II, the formalism given in velocity gauge pertains to more apparent physical picture for the resonant structure of interband transition induced by the thermal field. However, in most cases we focus on the analysis of the steady-state response of temperature gradient and it is easier to do it in length gauge. Both approaches yield identical results in the clean limit. The wave functions between the two gauges are related by a time-dependent unitary transformation [38,40,41]. After taking many sum rules the results in velocity gauge are transformed to those of length gauge.

Perturbed by the thermal field, the Hamiltonian in length gauge is given as

$$\hat{H}_{E_T} = \hat{H}_0 + \frac{1}{2}(\hat{H}_0\hat{r} + \hat{r}\hat{H}_0) \cdot E_T.$$
(90)

In terms of the relation $\hat{\mathbf{r}} = i\hat{\mathbf{D}}$ between the covariant derivative and the position operator, H_{E_T} is rewritten as

$$\hat{H}_{E_T} = \hat{H}_0 + i\hat{\mathcal{D}} \cdot \boldsymbol{E}_T, \qquad (91)$$

where the definition $\hat{\mathcal{D}}[\mathcal{O}] = \frac{1}{2}[\hat{H}_0, \hat{D}[\mathcal{O}]]_+$ is used. We adopt the reduced density matrix (RDM) equations-of-motion approach [38] to calculate the nonlinear thermal response in length gauge. The RDM in band space is given by the average of the product of a creation and a destruction operator in Bloch states

$$\rho_{\boldsymbol{k}pq}(t) \equiv \langle c_{\boldsymbol{p}\boldsymbol{k}}^{\dagger}(t)c_{\boldsymbol{q}\boldsymbol{k}}(t)\rangle.$$
(92)

The standard density-matrix formalism is performed by expanding the RDM in powers of the thermal field in calculating the nonlinear thermal response. In analogy with the optical conductivity $\sigma(\omega)$ which describes the response of the transient charge current to a time-dependent electric field E(t), we can define the dynamical Nernst (or thermal Hall) conductivity, as the response of the transient charge (heat) current to a time-dependent temperature gradient field $\nabla T(t)$.

The expectation values of the Kubo contribution of the charge (heat) current are given by

$$J_{N(Q)}^{\text{Kubo},\alpha}(t) = \text{Tr}[\hat{J}_{N(Q)}^{\alpha}\rho(t)], \qquad (93)$$

where $\alpha = x, y, z, \hat{J}_c^{\alpha} \equiv e\hat{v}^{\alpha}$, and $\hat{J}_h^{\alpha} \equiv \frac{1}{2}[\hat{H}_0, \hat{v}^{\alpha}]_+$. For simplicity we suppose that the system is only perturbed by the thermal field. According to Eqs. (60) and (73), the particle magnetization which can be expressed in form of the RDM

$$M_N^{\gamma} = \operatorname{Tr}\left[\int_k m^{\gamma} \rho - \frac{1}{e^2} \int d\varepsilon \,\sigma^{\gamma}(\varepsilon)\rho\right],\tag{94}$$

where the orbital magnetic moment and zero-temperature Hall conductivity are generalized to the matrix form $m_{pq}^{\gamma} = m_p^{\gamma} \delta_{pq}$, $\sigma_{pq}^{\gamma} = \sigma_p^{\gamma} \delta_{pq}$ and similar for the heat magnetization

$$M_{Q}^{\gamma} = \operatorname{Tr}\left[\int_{k} w^{\gamma} \rho - \frac{1}{e^{2}} \int d\varepsilon \,\tilde{\varepsilon} \sigma^{\gamma}(\varepsilon) \rho\right], \qquad (95)$$

with $w_{pq}^{\gamma} = w_p^{\gamma} \delta_{pq}$ and $\tilde{\varepsilon}_{pq} = \tilde{\varepsilon}_p \delta_{pq}$. The equation of motion of the RDM is

$$i\hbar \frac{\partial \rho_{kpq}(t)}{\partial t} = \operatorname{Tr}\left[i\hbar \frac{\partial \rho(t)}{\partial t} c^{\dagger}_{pk} c_{qk}\right]$$
$$= \langle [c^{\dagger}_{pk}(t) c_{qk}(t), H_{E_{T}}(t)]_{-} \rangle.$$
(96)

Substituting the Hamiltonian (90) into (96), and expanding RDM in powers of the external field $\rho = \sum_{n} \rho^{(n)}$, the equation of motion can be solved recursively

$$\left(i\hbar\frac{\partial}{\partial t} - \varepsilon_{kpq}\right)\rho_{kpq}^{(n)}(t) = \boldsymbol{E}_{T}\cdot\hat{\boldsymbol{\mathcal{D}}}[\rho^{(n-1)}(t)]_{kpq}.$$
 (97)

Therefore, the *n*th-order RDM can be expressed via the zeroth-order RDM by iterating Eq. (97), and the zeroth-order RDM is the Fermi-Dirac distribution function times the unit matrix in band space $\rho_{pq}^{(0)} = f_p \delta_{pq}$. To solve the equation, we need to transform it into frequency space. The time derivative in the equations of motion is replaced by a frequency factor that is collected into an energy denominator $d_{kpq}(\omega) = 1/(\omega - \varepsilon_{kpq})$, and the iterative relation is given by

$$\rho_{kpq}^{(n)}(\omega) = i \int \frac{d\omega'}{2\pi} E_T^{\alpha_1}[d(\omega) \circ \hat{\mathcal{D}}^{\alpha_1}[\rho^{(n-1)}(\omega - \omega')]]_{kpq},$$
(98)

where \circ is the Hadamard product $(A \circ B)_{pq} = A_{pq}B_{pq}$. The *n*th-order RDM is

$$\rho^{(n)}(\omega)_{pq} = (i)^n \left[\prod_{i=1}^n \int d\omega_i E_T^{\alpha_i}(\omega_i) \right] [d(\omega) \circ [\mathcal{D}^{\alpha_1}[d(\omega - \omega_1) \dots [\mathcal{D}^{\alpha_k}[d(\omega - \omega_k) \dots \circ [\mathcal{D}^{\alpha_n}[\rho^{(0)}]]]]]] \delta(\omega_{[n]} - \omega), \quad (99)$$

where $\omega_{[n]} \equiv \sum_{i}^{n} \omega_{n}$. The *n*th-order components of the Kubo particle (heat) current are written as

$$J_i^{\text{Kubo},(n),\alpha}(\omega) = \int_k \text{Tr}[\hat{J}_i^{\alpha} \rho^{(n)}(\omega)].$$
(100)

For the *n*th-order current, the magnetization is expanded up to the (n - 1)th order of thermal field, which is given by

$$M_{N}^{(n),\gamma}(\omega) = \operatorname{Tr}\left[\int_{k} m^{\gamma} \rho^{(n-1)}(\omega) + \frac{1}{e} \int d\varepsilon \,\sigma^{\gamma}(\varepsilon) \rho^{(n-1)}(\omega)\right],$$
(101)

$$M_{Q}^{(n),\gamma}(\omega) = \operatorname{Tr}\left[\int_{k} w^{\gamma} \rho^{(n-1)}(\omega) - \frac{1}{e^{2}} \int d\varepsilon (\varepsilon - \mu) \sigma^{\gamma}(\varepsilon) \rho^{(n-1)}(\omega)\right].$$
(102)

The higher-order derivatives follow from an expansion of the time evolution of the instantaneous eigenstates beyond linear approximation. Recently, a quantum kinetic theory that incorporates with the disorder and the thermal vector potential has been developed [42]. Incorporated with covariant derivatives, the linear thermal transport coefficients are reproduced as well. There are two differences between our approach and that in Ref. [42]. First, the thermal vector potential is generalized to the multiband systems in terms of the Wigner distribution function in Ref. [42], while in our approach the generalization is made by introducing the coupling of the Hermitian derivative and the thermal field in length gauge. Second, the density matrix is disorder averaged by explicitly introducing the disorder potential in the Hamiltonian in Ref. [42], while in our approach the effect of disorder is introduced through the self-energy of the propagator. Considering the presence of magnetic field, the quantum kinetic equation approach in Ref. [42] enables a systematic calculation of magnetothermoelectric and magnetothermal conductivities of systems with momentum-space Berry curvatures. Particularly, in Ref. [42], it is discovered that in Weyl semimetals the Mott relation is satisfied for the chiral-anomaly-induced magnetothermoelectric conductivity, and the WF law is violated for the chiral-anomaly-induced magnetothermal conductivity. In addition, it has been successfully applied to the topological insulators in Ref. [43]. By contrast, as we will show in the following, we aim to investigate the nonlinear thermal transport in the absence of magnetic field and relations among the nonlinear transport coefficients.

A. Linear thermoelectric and thermal-thermal response

First, we rederive the first-order thermoelectric response coefficient, as a pedagogical demonstration of our method. $L_{12}^{\text{Kubo},\alpha\beta}$ is related to the first-order RDM, which is expanded as

$$\rho_{pq}^{(1)} = iE_T^{\beta}(\omega)[d(\omega) \circ \hat{\mathcal{D}}^{\beta}[\rho^{(0)}]_{-}]_{pq}$$
$$= iE_T^{\beta}(\omega) \left[\frac{\tilde{\varepsilon}_p}{\omega} \partial^{\beta} f_p \delta_{pq} - i\frac{\tilde{\varepsilon}_p + \tilde{\varepsilon}_q}{2(\varepsilon_{pq} + \omega)} \mathcal{A}_{pq}^{\beta} f_{pq}\right]. \quad (103)$$

The linear Kubo current is

$$J_N^{\text{Kubo},(1),\alpha}(\omega) = \int_k \text{Tr}[\hat{J}_N^{\alpha} \rho^{(1)}(\omega)], \qquad (104)$$

and the Kubo contribution of transport coefficient is found as (Appendix D)

$$L_{12}^{\text{Kubo,}\alpha\beta}(\omega) = i \sum_{p,q} \int_{k} \left[\frac{\tilde{\varepsilon}_{p}}{\omega} v_{p}^{\alpha} \partial^{\beta} f_{p} - i \frac{\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q}}{2(\varepsilon_{pq} + \omega)} \mathcal{A}_{pq}^{\beta} v_{qp}^{\alpha} f_{pq} \right].$$
(105)

It is equivalent to the expression (53) derived by diagrammatic approach in velocity gauge. Using Eq. (101), the first-order particle magnetization density is written as

$$M_N^{(1),\gamma} = \sum_p \int_k \left[m_p^{\gamma} f_p + k_B T \,\Omega_p^{\gamma} \ln(1 + e^{-\beta \tilde{\varepsilon}_p}) \right].$$
(106)

Considering the DC limit by taking $\omega \rightarrow 0$, we obtain the linear thermoelectric response for transport current by collecting the Kubo contribution (105) and the magnetization correction (106), which is given by

$$L_{\rm DC,12}^{\rm tr,\alpha\beta}(\omega) = L_{12,\rm DC}^{\rm Kubo,\alpha\beta}(\omega) - \epsilon^{\alpha\beta\gamma} M_N^{\gamma}.$$
 (107)

By separating all the terms with the Berry connection, the transport coefficient can be written as

$$L_{\text{DC},12}^{\text{tr},\alpha\beta}(\omega) = L_{D,12}^{\alpha\beta}(\omega) + L_{A,12}^{\alpha\beta}(\omega), \qquad (108)$$

in which the first term is the usual Drude term

$$L_{D,12}^{\alpha\beta}(\omega) = \frac{i}{\hbar} \sum_{p} \int_{k} \frac{1}{\omega} v_{p}^{\alpha} v_{p}^{\beta} \frac{\partial f_{p}}{\partial \varepsilon_{p}}, \qquad (109)$$

and the second term is the anomalous term contributed by the Berry curvature

$$L_{A,12}^{\alpha\beta}(\omega) = \frac{e}{\hbar} \sum_{p} \int_{k} \Omega_{p}^{\gamma} [\tilde{\varepsilon}_{p} f_{p} + k_{B}T \ln(1 + e^{-\beta\tilde{\varepsilon}_{p}})].$$
(110)

Not surprisingly, Eqs. (109) and (110) recover Eq. (64) obtained in length gauge.

In analogy, the linear thermal-thermal response $L_{22}^{\text{tr},\alpha\beta}$ is derived in a similar process. The linear Kubo heat current is

$$J_{\mathcal{Q}}^{\text{Kubo},(1),\alpha}(\omega) = \int_{k} \text{Tr} \big[\hat{J}_{\mathcal{Q}}^{\alpha} \rho^{(1)}(\omega) \big], \qquad (111)$$

and the Kubo contribution to transport coefficient is given by

$$L_{22}^{\text{Kubo},\alpha\beta}(\omega) = i \sum_{p,q} \int_{k} \left[\frac{1}{\omega} \tilde{\varepsilon}_{p}^{2} v_{p}^{\alpha} \partial^{\beta} f_{p} - i \frac{(\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q})^{2}}{4(\varepsilon_{pq} - \omega)} \mathcal{A}_{pq}^{\alpha} v_{qp}^{\mu} f_{pq} \right].$$
(112)

The heat magnetization is

$$M_{Q}^{(1),\gamma} = \int_{k} \operatorname{Tr}\{w^{\gamma}\rho^{(0)} - \Omega^{\gamma}c_{2}[\rho^{(0)}]\}$$

= $\sum_{p} \int_{k} \left[w_{p}^{\gamma}f_{p} - \Omega_{p}^{\gamma}c_{2,p}(f_{p})\right].$ (113)

Combining Eqs. (112) and (113) and taking the DC limit, we obtain the response coefficient for transport thermal current

$$L_{22}^{\mathrm{tr},\alpha\beta}(\omega) = \frac{1}{\hbar} \sum_{p} \int_{k} \left[i \frac{1}{\omega} \tilde{\varepsilon}_{p}^{2} \partial^{\beta} f_{p} v_{p}^{\alpha} - c_{2}(f_{p}) \Omega_{p}^{\gamma} \right], \quad (114)$$

which recovers the expression Eq. (76).

B. Second-order thermoelectric conductivity and Mott relation

The Kubo contribution to the second-order thermoelectric response coefficient is related to the second-order RDM

$$\rho^{(2)} = -\int d\omega_1 \int d\omega_2 E_T^\beta(\omega_1) E_T^\delta(\omega_2) d(\omega)$$
$$\circ \mathcal{D}^\beta[d(\omega - \omega_1) \circ \mathcal{D}^\delta[\rho^{(0)}]] \delta(\omega_{[2]} - \omega). \quad (115)$$

We aim to obtain the expression in the $\omega \rightarrow 0$ limit and then compare with the semiclassical results. The Kubo contribution of the second-order particle current is given by

$$J_N^{\text{Kubo},(2),\alpha}(\omega) = \int_k \text{Tr}[j_N^{\alpha}\rho^{(2)}].$$
 (116)

Substituting Eq. (115) into Eq. (116), and using Eq. (46), the second-order thermoelectric response is expanded as the summation of four integral kernels

$$L_{12}^{\text{Kubo},\alpha\beta\delta} = e \int_{k} [\Pi^{(2),\beta\delta} + \Pi^{(2),\beta} + \Pi^{(2),\delta} + \Pi^{(2)}], \quad (117)$$

where the superscripts α , β , and δ (α , β , $\delta = x$, y, z) of Π denote the k^{α} , k^{β} , and k^{δ} Hermitian derivatives defined in Eq. (16) and the superscript (2) denotes the second order. The expressions for the integral kernels are obtained as (detailed derivation is sketched in Appendix D)

$$\Pi^{(2),\beta\delta} = \sum_{p} v_{p}^{\alpha} \frac{1}{\omega} \frac{1}{\omega - \omega_{1}} \tilde{\varepsilon}_{p} \partial^{\beta} (\tilde{\varepsilon}_{p} \partial^{\delta} f_{p}),$$

$$\Pi^{(2),\beta} = \sum_{p,q} \frac{-i}{2} v_{pq}^{\alpha} \frac{1}{\omega - \varepsilon_{qp}} \tilde{\varepsilon}_{p} \partial^{\beta} \left[\frac{1}{\omega - \omega_{1} - \varepsilon_{qp}} \times (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q}) \mathcal{A}_{qp}^{\delta} f_{pq} \right],$$

$$\Pi^{(2),\delta} = \sum_{p,q} \frac{-i}{2} v_{pq}^{\alpha} \frac{1}{(\omega - \varepsilon_{qp})} \frac{1}{(\omega - \omega_{1})} \mathcal{A}_{qp}^{\beta} \times (\tilde{\varepsilon}_{p} \tilde{\varepsilon}_{q} \partial^{\delta} f_{pq} + \tilde{\varepsilon}_{p}^{2} \partial^{\delta} f_{p} - \tilde{\varepsilon}_{q}^{2} \partial^{\delta} f_{q}),$$

$$\Pi^{(2)} = -\sum_{p,q,r} \frac{1}{4} v_{pq}^{\alpha} \frac{1}{\omega - \varepsilon_{qp}} (\tilde{\varepsilon}_{q} + \tilde{\varepsilon}_{r}) \mathcal{A}_{qr}^{\beta} \frac{1}{\omega - \omega_{1} - \varepsilon_{rp}} \times (\tilde{\varepsilon}_{r} + \tilde{\varepsilon}_{p}) \mathcal{A}_{rp}^{\delta} (f_{rp} - f_{qr}).$$
(118)

Here $\Pi^{(2),\beta\delta}$ is the intraband contribution, which is the generalized second-order Drude term. The others are the interband contributions which contain the Berry connection.

Now we consider the static state. The dominating terms are distinguished by the ω -dependent denominators of the integral kernels. For $\Pi^{(2),\beta\delta}$, it is proportional to $1/(\omega\omega_2)$ (considering $\omega_2 = \omega - \omega_1$), which diverges at DC limit (as ω_1 , ω_2 approaching zero). For $\Pi^{(2),\delta}$, it is proportional to $1/\omega_2$, which also diverges at DC limit. While for $\Pi^{(2),\beta}$ and $\Pi^{(2)}$, there

is no divergent dominator and can be safely omitted. Therefore, the dominating terms are from $\Pi^{(2),\beta\delta}$ and $\Pi^{(2),\delta}$ in the DC limit, and the second-order thermoelectric conductivity is given by

$$L_{\text{DC},12}^{\text{Kubo,}\alpha\beta\delta}(\omega;\omega_{1},\omega_{2}) = -\sum_{p,q} \int_{k} \left[\frac{1}{\omega\omega_{2}} v_{p}^{\alpha} \tilde{\varepsilon}_{p} \partial^{\beta} (\tilde{\varepsilon}_{p} \partial^{\delta} f_{p}) + \frac{i}{2\omega_{2}} \varepsilon_{p} (\varepsilon_{p} + \varepsilon_{q}) \frac{v_{pq}^{\alpha} v_{qp}^{\beta} - v_{pq}^{\beta} v_{qp}^{\alpha}}{\varepsilon_{pq}^{2}} \partial^{\delta} f_{p} \right].$$
(119)

By use of the identity (61), the DC second-order thermoelectric response can be written into the following more suggestive form:

$$L_{\text{DC},12}^{\text{Kubo,}\alpha\beta\delta}(\omega;\omega_{1},\omega_{2}) = -\sum_{p} \int_{k} \left[\frac{1}{\omega\omega_{2}} v_{p}^{\alpha} \tilde{\varepsilon}_{p} \partial^{\beta} (\tilde{\varepsilon}_{p} \partial^{\delta} f_{p}) + \frac{i}{\omega_{2}} (\tilde{\varepsilon}_{p} m_{p}^{\gamma} + \tilde{\varepsilon}_{p}^{2} \Omega_{p}^{\gamma}) \partial^{\delta} f_{p} \right].$$
(120)

Now we derive the second-order particle magnetization density, which is related to the first-order RDM:

$$M_N^{(2),\gamma}(\omega) = \operatorname{Tr}\left[\int_k \rho^{(1)}(\omega)m^{\gamma} + \frac{1}{e}\int d\varepsilon \,\sigma^{\gamma}(\varepsilon)\rho^{(1)}(\omega)\right].$$
(121)

Referring to Eq. (103), the second term of $\rho^{(1)}$ is omitted because it is subleading in the DC limit. Hence, the second-order thermoelectric magnetization response is given as

$$M_{12,\text{DC}}^{\gamma\delta}(\omega) = i \sum_{p} \int_{k} \frac{1}{\omega} \tilde{\varepsilon}_{p} m_{p}^{\gamma} \partial^{\delta} f_{p} + i \frac{1}{e} \sum_{p} \int d\varepsilon \frac{1}{\omega} \tilde{\varepsilon}_{p} \sigma^{\gamma}(\varepsilon) \partial^{\delta} f_{p}(\varepsilon).$$
(122)

Combining Eqs. (120) and (122), we obtain the second thermoelectric conductivity in the DC limit

$$L_{12,\text{DC}}^{\text{tr},\alpha\beta\delta}(\omega;\omega_1,\omega_2) = L_{12,D}^{\alpha\beta\delta}(\omega;\omega_1,\omega_2) + L_{12,A}^{\alpha\beta\delta}(\omega;\omega_1,\omega_2).$$
(123)

For the Drude term,

$$L_{12,D}^{\alpha\beta\delta} = -\sum_{p} \int_{k} \frac{1}{\omega\omega_{2}} v_{p}^{\alpha} \tilde{\varepsilon}_{p} \partial^{\beta} (\tilde{\varepsilon}_{p} \partial^{\delta} f_{p}), \qquad (124)$$

and the anomalous term is given as

$$L_{12,A}^{\alpha\beta\delta} = i\epsilon^{\alpha\beta\gamma} \sum_{p} \int d\varepsilon_{p} \frac{1}{\omega_{2}} v_{p}^{\delta} \sigma^{\gamma}(\varepsilon_{p}) \bigg[2\tilde{\varepsilon}_{p} \frac{\partial f_{p}}{\partial \varepsilon_{p}} + \tilde{\varepsilon}_{p}^{2} \frac{\partial^{2} f_{p}}{\partial \varepsilon_{p}^{2}} \bigg].$$
(125)

Noting that for the system with time-reversal symmetry, the Drude term vanishes and only the anomalous term survives.

Next, we study how the thermoelectric conductivity is related to the electric conductivity at the second order. The

second-order electric-electric response is written as

$$J_N^{\mathrm{tr},(2),\alpha}(\omega) = \int_{k} \mathrm{Tr} \big[j_N^{\alpha} \rho^{(2)}(\omega) \big].$$
(126)

The second- order RDM with an electric field perturbation is given as

$$\rho^{(2)} = -\int d\omega_1 \int d\omega_2 E^{\beta}(\omega_1) E^{\delta}(\omega_2) d(\omega)$$
$$\circ D^{\beta}[d(\omega - \omega_1) \circ D^{\delta}[\rho^{(0)}]] \delta(\omega_{[2]} - \omega). \quad (127)$$

Expanding $\rho^{(1)}$, the second-order electric-electric response becomes [38]

$$L_{11,\text{DC}}^{\text{tr},\alpha\beta\delta}(\omega;\omega_1,\omega_2) = L_{11,D}^{\alpha\beta\delta}(\omega;\omega_1,\omega_2) + L_{11,A}^{\alpha\beta\delta}(\omega;\omega_1,\omega_2),$$
(128)

with

$$L_{11,D}^{\alpha\beta\delta} = -\sum_{p} \int_{k} \frac{1}{\omega\omega_{2}} \partial^{\beta} v_{p}^{\alpha} \partial^{\delta} f_{p}, \qquad (129)$$

$$L_{11,A}^{\alpha\beta\delta} = -\epsilon^{\alpha\beta\gamma} \sum_{p} \int_{k} i \frac{1}{\omega_2} \Omega_p^{\gamma} \partial^{\delta} f_p.$$
(130)

First, we focus on the anomalous term $L_{11,A}^{\alpha\beta\delta}$. Integrating by part, it can be rewritten as

$$L_{11,A}^{\alpha\beta\delta} = -\frac{i}{\hbar^2} \epsilon^{\alpha\beta\gamma} \sum_p \int d\varepsilon_p \frac{1}{\omega_2} A^{\delta}(\varepsilon_p) \sigma^{\gamma}(\varepsilon_p), \quad (131)$$

in which we define $A^{\delta}(\varepsilon_p) \equiv \frac{\partial f_p}{\partial \varepsilon_p} \frac{\partial v^{\delta}(\varepsilon_p)}{\partial \varepsilon_p} + \frac{\partial^2 f_p}{\partial \varepsilon_p^2} v^{\delta}(\varepsilon_p)$. Using the identity

$$\frac{\partial f_0}{\partial \varepsilon_k} \frac{\partial v_k^{\alpha}}{\partial k_{\beta}} + \frac{\partial^2 f_0}{\partial \varepsilon_k^2} v_k^{\alpha} v_k^{\beta} = v_k^{\beta} \frac{\partial f_0}{\partial \varepsilon_k} \frac{\partial v_k^{\alpha}}{\partial \varepsilon_k} + \frac{\partial^2 f_0}{\partial \varepsilon_k^2} v_k^{\alpha} v_k^{\beta}, \quad (132)$$

we have

$$v_{k}^{\beta} \frac{\partial v_{k}^{\alpha}}{\partial \varepsilon_{k}} = \frac{\partial v_{k}^{\alpha}}{\partial k_{\beta}} = \frac{\partial^{2} \varepsilon_{k}}{\partial k_{\alpha} \partial k_{\beta}} = \frac{1}{m_{\alpha\beta}^{*}}.$$
 (133)

Here $m_{\alpha\beta}^*$ is the effective mass of the Bloch electrons. When we consider a limit case that v_k is independent of energy, namely, $\partial v_k / \partial \varepsilon = 0$ which indicates a large effective mass. The second-order anomalous Hall conductivity is approximated as

$$L_{11,A}^{\alpha\beta\delta} \approx -\frac{i}{\hbar^2} \epsilon^{\alpha\beta\gamma} \sum_p \int d\varepsilon_p \frac{1}{\omega_2} \frac{\partial^2 f_p}{\partial \varepsilon_p^2} v^{\delta}(\varepsilon_p) \sigma^{\gamma}(\varepsilon_p). \quad (134)$$

By inserting the low-temperature expansion formula (81) into (134) and (125), and considering that the electric conductivity $\sigma_{\text{DC}}^{\alpha\beta\delta}$ and thermoelectric conductivity $\eta_A^{\alpha\beta\delta}$ satisfy $\sigma_A^{\alpha\beta\delta} = L_{A,11}^{\text{tr},\alpha\beta\delta}$ and $\eta_A^{\alpha\beta\delta} = L_{12,A}^{\text{tr},\alpha\beta\delta}/T^2$, we obtain

$$\eta_A^{\alpha\beta\delta} = \frac{1}{3} \frac{\pi^2 k_B^2}{e^2} \sigma_A^{\alpha\beta\delta} = L \sigma_A^{\alpha\beta\delta}.$$
 (135)

It indicates that when the dispersion is weakly dependent on the velocity, the second-order thermoelectric conductivity (the second-order Nernst coefficient) is proportional to the second-order electric conductivity (the second-order particle Hall conductivity) at low temperatures, which is different from the Mott relation for the linear order. The linear Mott relation tells us that the linear Nernst coefficient is proportional to the derivative of linear Hall conductivity to the Fermi energy, which is $\eta_A^{\alpha\beta} = \frac{\pi^2}{3} \frac{k_B^2 T}{e} \frac{\partial \sigma_A^{\alpha\beta}(\mu)}{\partial \mu}$ [1]. This proportionality between second Nernst and Hall conductivity results from that the second-order thermoelectric conductivity has a power of ε^2/T^2 , and the nonzero contribution of the low-temperature Eq. (81) comes from the second-order Mott relation is derived in Refs. [44,45] by use of the semiclassical Boltzmann equation.

Now we demonstrate that the second-order Mott relation (135) applies to the Drude contribution. Integrating by part, the Drude contribution of the second thermoelectric conductivity (124) can be rewritten as

$$L_{12,D}^{\alpha\beta\delta} = -\sum_{p} \int d\varepsilon_{p} \frac{1}{\omega\omega_{2}} \left[2\tilde{\varepsilon}_{p} \frac{\partial f_{p}}{\partial\varepsilon_{p}} + \tilde{\varepsilon}_{p}^{2} \frac{\partial^{2} f_{p}}{\partial\varepsilon_{p}^{2}} \right] \int_{k} v_{p}^{\alpha} v_{p}^{\beta} \times \delta(\varepsilon_{p} - \varepsilon_{p,k}).$$
(136)

Using Eq. (132) and considering the large effective mass limit, the Drude contribution of the second electric conductivity is given as

$$L_{11,D}^{\alpha\beta\delta} \approx -\sum_{p} \int d\varepsilon_{p} \frac{1}{\omega\omega_{2}} \tilde{\varepsilon}_{p}^{2} \frac{\partial^{2} f_{p}}{\partial \varepsilon_{p}^{2}} \int_{k} v_{p}^{\alpha} v_{p}^{\beta} \delta(\varepsilon_{p} - \varepsilon_{p,k}).$$
(137)

By use of the Sommerfeld expansion (81), the second-order Mott relation (135) for the Drude term is directly testified.

C. Second-order thermal conductivity and Wiedemann-Franz law

According to Eq. (100), the Kubo contribution to the second-order heat current is given by

$$J_Q^{\text{Kubo},(2),\alpha}(\omega) = \int_k \text{Tr}[\hat{j}_Q^{\alpha} \rho^{(2)}].$$
 (138)

By use of the expansion of the second RDM, the second-order thermoelectric response is expressed in form of four integral kernels

$$L_{22}^{\text{Kubo},\alpha\beta\delta} = \int_{k} [\Xi^{(2),\beta\delta} + \Xi^{(2),\beta} + \Xi^{(2),\delta} + \Xi^{(2)}], \quad (139)$$

where $\Xi^{(2),\beta\delta}$, $\Xi^{(2),\beta}$, $\Xi^{(2),\delta}$, and $\Xi^{(2)}$ are given by (see Appendix D for details)

$$\begin{split} \Xi^{(2),\beta\delta} &= \sum_{p} v_{p}^{\alpha} \frac{1}{\omega} \tilde{\varepsilon}_{p}^{2} \partial^{\beta} \bigg[\frac{1}{\omega - \omega_{1}} \tilde{\varepsilon}_{p} \partial^{\delta} f_{p} \bigg], \\ \Xi^{(2),\beta} &= \sum_{p,q} -i \frac{1}{2} v_{pq}^{\alpha} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q}) \frac{1}{\omega} \tilde{\varepsilon}_{p} \partial^{\beta} \bigg[\frac{1}{\omega - \omega_{1} - \varepsilon_{qp}} \\ &\times (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q}) \mathcal{A}_{qp}^{\delta} f_{pq} \bigg], \\ \Xi^{(2),\delta} &= \sum_{p,q} -i \frac{1}{4} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q}) v_{pq}^{\alpha} \frac{1}{(\omega - \varepsilon_{qp})} \frac{1}{(\omega - \omega_{1})} \\ &\times \mathcal{A}_{qp}^{\beta} (\tilde{\varepsilon}_{p} \tilde{\varepsilon}_{q} \partial^{\delta} f_{pq} + \tilde{\varepsilon}_{p}^{2} \partial^{\delta} f_{p} - \tilde{\varepsilon}_{q}^{2} \partial^{\delta} f_{q} \big), \end{split}$$

$$\Xi^{(2)} = \sum_{p,q,r} -\frac{1}{8} v_{pq}^{\alpha} (\tilde{\varepsilon}_p + \tilde{\varepsilon}_q) \frac{1}{\omega - \varepsilon_{qp}} (\tilde{\varepsilon}_q + \tilde{\varepsilon}_r) \mathcal{A}_{qr}^{\beta}$$
$$\times \frac{1}{\omega - \omega_1 - \varepsilon_{rp}} (\tilde{\varepsilon}_r + \tilde{\varepsilon}_p) \mathcal{A}_{rp}^{\delta} (f_{rp} - f_{qr}). \quad (140)$$

It can be seen that the poles $\Xi^{(2),...}$ are identical to that of $\Pi^{(2),...}$, with the leading term contributed by $\Xi^{(2),\beta\delta}$ and $\Xi^{(2),\delta}$. Hence, the Kubo contribution in DC limit is found as

$$L_{22,\text{DC}}^{\text{Kubo},\alpha\beta\delta}(\omega;\omega_{1},\omega_{2}) = -\sum_{p,q} \int_{k} \left[\frac{1}{\omega\omega_{2}} v_{p}^{\alpha} \tilde{\varepsilon}_{p}^{2} \partial^{\beta} (\tilde{\varepsilon}_{p} \partial^{\delta} f_{p}) + i \frac{1}{4\omega_{2}} \tilde{\varepsilon}_{p} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q})^{2} \right] \\ \times \frac{v_{pq}^{\alpha} v_{qp}^{\beta} - v_{pq}^{\beta} v_{qp}^{\alpha}}{\varepsilon_{pq}^{2}} \partial^{\delta} f_{p} \left].$$
(141)

By use of the quantity w_p^{γ} introduced in Eq. (74), it can be rewritten as

$$L_{22,\text{DC}}^{\text{Kubo},\alpha\beta\delta}(\omega;\omega_1,\omega_2) = -\sum_{p,q} \int_{k} \left[\frac{1}{\omega\omega_2} v_p^{\alpha} \tilde{\varepsilon}_p^2 \partial^{\beta} (\tilde{\varepsilon}_q \partial^{\delta} f_p) + i \frac{1}{\omega_2} \tilde{\varepsilon}_p w_p^{\gamma} \partial^{\delta} f_p \right].$$
(142)

The second-order heat magnetization is written as

$$M_Q^{(2),\gamma}(\omega) = \operatorname{Tr}\left[\int_k w^{\gamma} \rho^{(1)}(\omega) - \frac{1}{e^2} \int d\varepsilon \,\tilde{\varepsilon} \sigma^{\gamma}(\varepsilon) \rho^{(1)}(\omega)\right].$$
(143)

Hence, we obtain the second-order thermal-thermal magnetization response

$$M_{22,\text{DC}}^{\gamma\delta}(\omega) = i \sum_{p} \int_{k} \frac{1}{\omega} \tilde{\varepsilon}_{p} w_{p}^{\gamma} \partial^{\delta} f_{p} -i \frac{1}{e^{2}} \sum_{p} \int d\varepsilon \frac{1}{\omega} \tilde{\varepsilon}_{p}^{2} \sigma^{\gamma}(\varepsilon) \partial^{\delta} f_{p}(\varepsilon).$$
(144)

From Eqs. (141) and (144), we obtain the second-order thermal-thermal response

$$L_{22,\text{DC}}^{\text{tr},\alpha\beta\delta}(\omega;\omega_1,\omega_2) = L_{22,D}^{\alpha\beta\delta}(\omega;\omega_1,\omega_2) + L_{22,A}^{\alpha\beta\delta}(\omega;\omega_1,\omega_2)$$
(145)

with

$$L_{22,D}^{\alpha\beta\delta} = -\sum_{p} \int_{k} \frac{1}{\omega\omega_{2}} v_{p}^{\alpha} \tilde{\varepsilon}_{p}^{2} \partial^{\beta} (\tilde{\varepsilon}_{p} \partial^{\delta} f_{p}), \qquad (146)$$

$$L_{22,A}^{\alpha\beta\delta} = i\epsilon^{\alpha\beta\gamma} \sum_{p} \int d\varepsilon_{p} \frac{1}{\omega_{2}} v_{p}^{\delta} \sigma^{\gamma} (\varepsilon_{p}) \bigg[2\tilde{\varepsilon}_{p}^{2} \frac{\partial f_{p}}{\partial \varepsilon_{p}} + \tilde{\varepsilon}_{p}^{3} \frac{\partial^{2} f_{p}}{\partial \varepsilon_{p}^{2}} \bigg]. \qquad (147)$$

By use of the Sommerfeld expansion (81) and the identity $\kappa^{\alpha\beta\delta} = L_{22}^{\text{tr},\alpha\beta\delta}/T^2$, it yields

$$\sigma^{\alpha\beta\delta} = -\frac{e}{2L} \frac{\partial \kappa^{\alpha\beta\delta}(\mu)}{\partial \mu}.$$
 (148)

We call Eq. (148) as the second-order WF law. We see that the relation between the second-order thermal conductivity $\kappa^{\alpha\beta\delta}$ and the second-order electric conductivity $\sigma^{\alpha\beta\delta}(\mu)$ does not obey the linear WF law in Eq. (84), which is $\kappa^{\alpha\beta} = LT\sigma^{\alpha\beta}$. In the second-order response, the second-order electric conductivity $\sigma^{\alpha\beta\delta}$ is proportional to the first derivative of the second-order thermal conductivity $\kappa^{\alpha\beta\delta}(\mu)$ to the chemical potential, rather than to $\kappa^{\alpha\beta\delta}(\mu)$ itself.

D. Third-order thermal response

The Kubo contribution of the third-order electric current is written as

$$J_N^{\text{Kubo},(3),\alpha}(\omega) = \int_k \text{Tr}[j_N^{\alpha} \rho^{(3)}], \qquad (149)$$

where the third-order RDM is given by

$$\rho^{(3)}(\omega) = i^3 \int d\omega_1 \int d\omega_2 \int d\omega_3 E_T^{\alpha_1}(\omega_1) E_T^{\alpha_2}(\omega_2) E_T^{\alpha_3}(\omega_3) (d(\omega) \circ [\mathcal{D}^{\beta}[d(\omega - \omega_1) \circ [\mathcal{D}^{\delta}[d(\omega - \omega_{[2]}) \circ [\mathcal{D}^{\zeta}[\rho^{(0)}]]]])]), \quad (150)$$

in which the expansion of the third-order RDM results in eight terms, hence, the third Kubo thermoelectric response can be rewritten as (for details see Appendix E)

$$L_{12}^{\text{Kubo},\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3) = \int_{\boldsymbol{k}} [\Pi^{(3),\beta\delta\zeta} + \Pi^{(3),\beta\delta} + \Pi^{(3),\beta\zeta} + \Pi^{(3),\delta\zeta} + \Pi^{(3),\delta} + \Pi^{(3),\delta} + \Pi^{(3),\zeta} + \Pi^{(3)}].$$
(151)

The expressions of the $\Pi^{(3),\dots}$ s are shown in Appendix E. The derivation of the third-order thermoelectric conductivity in the DC limit can be done by calculating the poles of the denominator of $\Pi^{(3),\dots}$. The divergent terms are $\Pi^{(3),\beta\delta\zeta}$ (with poles of 0, ω_1 , and $\omega_1 + \omega_2$), $\Pi^{(3),\beta\zeta}$ (with poles of $\omega_1 + \omega_2$), and $\Pi^{(3),\alpha\delta\zeta}$ (with poles of ω_1 and $\omega_1 + \omega_2$). Reserving the leading terms of $O(\omega^{-3})$ ($\Pi^{(3),\beta\delta\zeta}$) and $O(\omega^{-2})$ ($\Pi^{(3),\delta\zeta}$), we obtain the third-order thermoelectric conductivity in the DC limit as

$$L_{12,\text{DC}}^{\text{Kubo},\alpha\beta\delta\zeta}(\omega;\omega_{1},\omega_{2},\omega_{3}) = \sum_{p} \int_{k} \left\{ -i\frac{1}{\omega\omega_{[2]}\omega_{3}} v_{p}^{\alpha}\tilde{\varepsilon}_{p}\partial^{\beta}[\tilde{\varepsilon}_{p}\partial^{\delta}(\tilde{\varepsilon}_{p}\partial^{\zeta}f_{p})] - \frac{1}{2\omega_{[2]}\omega_{3}} \frac{v_{pq}^{\alpha}v_{qp}^{\beta}}{\varepsilon_{pq}^{2}} [\tilde{\varepsilon}_{q}\tilde{\varepsilon}_{p}\partial^{\delta}(\tilde{\varepsilon}_{p}\partial^{\zeta}f_{p}) - \tilde{\varepsilon}_{q}^{2}\partial^{\delta}(\tilde{\varepsilon}_{q}\partial^{\zeta}f_{q})] \right\},$$

$$(152)$$

which can be written in a more compact form

$$L_{12,\text{DC}}^{\text{Kubo},\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3) = \sum_p \int_k \left\{ -i \frac{1}{\omega\omega_{[2]}\omega_3} v_p^{\alpha} \tilde{\varepsilon}_p \partial^{\beta} [\tilde{\varepsilon}_p \partial^{\delta} (\tilde{\varepsilon}_p \partial^{\zeta} f_p)] - \frac{1}{\omega_{[2]}\omega_3} (\tilde{\varepsilon}_p m_p^{\gamma} + \tilde{\varepsilon}_p^2 \Omega_p^{\gamma}) \partial^{\delta} (\tilde{\varepsilon}_p \partial^{\zeta} f_p) \right\}.$$
(153)

The third-order particle magnetization is given as

$$M_N^{(3),\gamma}(\omega) = \operatorname{Tr}\left[\int_k \rho^{(2)}(\omega)m^{\gamma} + \frac{1}{e}\int d\varepsilon \,\sigma^{\gamma}(\varepsilon)\rho^{(2)}(\omega)\right].$$
(154)

Note that only the terms up to $O(\omega^{-2})$ are retained. By use of the expansion of $\rho^{(2)}$ (see Appendix E for details), the leading term is proportional to $\Pi^{(2),\beta\delta}$. Hence, we obtain the third-order thermoelectric magnetization response

$$M_{12}^{\gamma\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3) = \sum_p \int_k \frac{1}{\omega\omega_2} \tilde{\varepsilon}_p m^{\gamma} \partial^{\delta}(\tilde{\varepsilon}_p \partial^{\zeta} f_p) + \frac{1}{e} \int d\varepsilon \frac{1}{\omega\omega_2} \tilde{\varepsilon}_p \sigma_p^{\gamma}(\varepsilon) \partial^{\delta}(\tilde{\varepsilon}_p \partial^{\zeta} f_p).$$
(155)

Combining Eqs. (155) and (153), we finally obtain the third-order thermoelectric response

$$L_{12,\text{DC}}^{\text{tr},\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3) = L_{12,D}^{\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3) + L_{12,A}^{\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3)$$
(156)

with

$$L_{12,D}^{\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3) = \sum_p \int_k -i\frac{1}{\omega\omega_{[2]}\omega_3} v_p^{\alpha}\tilde{\varepsilon}_p \partial^{\beta}[\tilde{\varepsilon}_p \partial^{\delta}(\tilde{\varepsilon}_p \partial^{\zeta}f_p)],$$
(157)

$$L_{12,A}^{\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3) = \epsilon^{\alpha\beta\gamma} \sum_p \int d\varepsilon_p \frac{1}{\omega\omega_2} \bigg[6\tilde{\varepsilon}_p \frac{\partial f_p}{\partial \varepsilon_p} + 6\tilde{\varepsilon}_p^2 \frac{\partial^2 f_p}{\partial \varepsilon_p^2} + \tilde{\varepsilon}_p^3 \frac{\partial^3 f}{\partial \varepsilon_p^3} \bigg] v^{\delta}(\varepsilon_p) v^{\zeta}(\varepsilon_p) \sigma^{\gamma}(\varepsilon_p).$$
(158)

Following the similar process, the Drude part and the anomalous part of the third-order electric conductivity is given as

$$L_{11,D}^{\alpha\beta\delta\zeta}(\omega;\omega_{1},\omega_{2},\omega_{3}) = \sum_{p} \int_{k} \frac{-i}{\omega\omega_{[2]}\omega_{3}} v_{p}^{\alpha} \partial^{\beta} [\partial^{\delta}(\partial^{\zeta}f_{p})],$$

$$L_{11,A}^{\alpha\beta\delta\zeta}(\omega;\omega_{1},\omega_{2},\omega_{3}) = \epsilon^{\alpha\beta\gamma} \sum_{p} \int_{k} \frac{1}{\omega_{[2]}\omega_{3}} \Omega_{p}^{\gamma} \partial^{\delta}(\partial^{\zeta}f_{p}).$$
(159)

In the limit of large effective mass, the anomalous part is approximated as

$$\mathcal{L}_{11,A}^{\alpha\beta\delta\zeta}(\omega;\omega_{1},\omega_{2},\omega_{3}) \approx -\epsilon^{\alpha\beta\gamma}\sum_{p}\int d\varepsilon_{p}\frac{1}{\omega_{[2]}\omega_{3}}\frac{\partial^{3}f_{p}}{\partial\varepsilon_{p}^{3}}v_{p}^{\delta}v_{p}^{\xi}\sigma^{\beta}(\varepsilon_{p}).$$
(160)

By use of the Sommerfeld expansion (81) and considering that $\sigma^{\alpha\beta\delta\zeta} = L_{\text{DC},11}^{\text{tr},\alpha\beta\delta\zeta}, \eta^{\alpha\beta\delta\zeta} = L_{\text{DC},12}^{\text{tr},\alpha\beta\delta\zeta}/T^3$, we obtain

$$\sigma^{\alpha\beta\delta\xi} = \frac{e}{9TL} \frac{\partial \eta^{\alpha\beta\delta\xi}(\mu)}{\partial \mu}.$$
 (161)

After a similar derivation for the third-order thermal conductivity (see Appendix F), we obtain

$$\sigma^{\alpha\beta\delta\xi} = \frac{e^2}{42TL} \frac{\partial^2 \kappa^{\alpha\beta\delta\xi}(\mu)}{\partial\mu^2}.$$
 (162)

Interestingly, it is found that at third order the electric conductivity is proportional to the first derivative of the third-order thermoelectric conductivity. Analogously, the third-order electric conductivity is proportional to the second derivative of the third-order thermal conductivity. According to the expression of the thermally expanded Hamiltonian (13), it is seen that expanding one more order of E_T is accompanied by one more order of the band energy. Given the fact that the order of band energy in response functions determines the leading terms in low-temperature expansion, hence we reach the conclusion that for the non-linear Mott relation, the *n*th-order electric conductivity is proportional to the (n - 2)th-order derivative of the *n*th-order thermoelectric conductivity with respect to the chemical potential. For the nonlinear WF law, the *n*th-order electric conductivity is proportional to the (n - 1)th derivative of the *n*th-order thermal conductivity with respect to the chemical potential (see Table III). Here, by invoking the semiclassical Boltzmann equation, the above transport coefficients are further testified (see Appendix G).

IV. NONLINEAR THERMAL RESPONSE OF MAGNONS

Based on the analytical formula of nonlinear thermal conductivity, we attempt to find a system in which the nonlinear response dominates over the linear effect. Note that although we start from a fermionic Hamiltonian to derive the thermal response, the formulas are general and can be directly extended to bosonic or other systems.

We consider the magnon transport driven by temperature gradient in a collinear antiferromagnet on a honeycomb lattice. The Hamiltonian is

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + g_J \mu_B \sum_i S_i \cdot \mathbf{B} + K \sum_i S_{iz}^2, \quad (163)$$

where J > 0 is the nearest-neighbor antiferromagnetic exchange interaction. The second term is the Zeeman coupling to the external magnetic field applied parallel to the magnetic ordering direction, in which g_J is the Lande's g factor and μ_B

Order	Thermal-electric (Mott)	Thermal-thermal (Wiedemann-Franz)
First Second Third	$\sigma^{lphaeta} = rac{1}{eLT} \int_{-\infty}^{\mu} darepsilon \eta^{lphaeta}(arepsilon) \ \sigma^{lphaeta\delta} = rac{1}{L} \eta^{lphaeta\delta} \ \sigma^{lphaeta\delta\xi} = rac{e}{e^{\alpha\mu}} rac{\partial\eta^{lphaeta\delta\xi}(\mu)}{\partial\eta^{lphaeta\delta\xi}(\mu)}$	$\sigma^{lphaeta} = rac{1}{LT} \kappa^{lphaeta} \ \sigma^{lphaeta} = -rac{e}{2L} rac{\partial \kappa^{lphaeta}(\mu)}{\partial \mu} \ \sigma^{lphaeta\delta} = rac{e^2}{2L} rac{\partial \kappa^{lphaeta\delta}(\mu)}{\partial \mu}$

TABLE III. The high order of thermal to electric conductivity, and thermal to thermal conductivity, i.e.. the higher-order Mott relation and values of WF law are summarized up to the third order. $L = \frac{1}{3} \left(\frac{k_B \pi}{e}\right)^2 = 2.44 \times 10^{-8} \text{ W}\Omega/K^2$ is the well-known first-order Lorentz number.

is the Bohr magneton. The third term (K < 0) is the easy-axis anisotropy which ensures the Néel vector in the *z* direction.

As the ground state of Eq. (163) is a fully aligned antiferromagnetic order, we describe the underlying magnetic excitations by the Holstein-Primakoff transformation

$$S_{iA}^+ \approx \sqrt{2S}a_i, \quad S_{iA}^- \approx \sqrt{2S}a_i^\dagger, \quad S_{iA}^z = S - a_i^\dagger a_i, \quad (164)$$

$$S_{iB}^+ \approx \sqrt{2S} b_i^\dagger, \quad S_{iB}^- \approx \sqrt{2S} b_i, \quad S_{iB}^z = b_i^\dagger b_i - S.$$
 (165)

Performing a Fourier transformation, the bosonic Bogoliubov-de Gennes (BdG) Hamiltonian defined in the 2 × 2 form with a vector $\Psi_{k} = (a_{k}, b_{k}^{\dagger})^{T}$ as

$$H_0(\boldsymbol{k}) = S \begin{bmatrix} 3J - K + g_J \mu_B B & \gamma^*(\boldsymbol{k}) \\ \gamma(\boldsymbol{k}) & 3J - K - g_J \mu_B B \end{bmatrix}.$$
(166)

We define $\gamma(\mathbf{k}) = \sum_{i} e^{i\mathbf{k}\cdot\boldsymbol{\delta}_{i}}$, $\boldsymbol{\delta}_{1} = (0, 1)l$, $\boldsymbol{\delta}_{2} = (\frac{\sqrt{3}}{2}, -\frac{1}{2})l$, and $\boldsymbol{\delta}_{2} = (-\frac{\sqrt{3}}{2}, -\frac{1}{2})l$ are the vectors connecting the nearest neighbors. For simplicity, we set $l = \frac{1}{\sqrt{3}}$.

As the next step, the Bogoliubov transformation $c_k = u_k a_k - v_k b_k^{\dagger}$ and $d_k = u_k b_k - v_k a_k^{\dagger}$ is used to diagonalize $H_0(k)$. We need to solve the eigenvalue equation

$$H_0(\mathbf{k})\mathbf{t}_{\pm}(\mathbf{k}) = \sigma_z \varepsilon_{\pm}(\mathbf{k})\mathbf{t}_{\pm}(\mathbf{k}),$$

$$H_0(\mathbf{k})\mathbf{t}_{\pm}(\mathbf{k})\sigma_z = \varepsilon_{\pm}(\mathbf{k})\mathbf{t}_{\pm}(\mathbf{k}).$$
 (167)

We only keep the particle branch (positive excitation), and the dispersions of the two branch magnons of the unstrained Hamiltonian are given by

$$\varepsilon_{p=\uparrow,\downarrow} = S\sqrt{(3J-K)^2 - |J\gamma(k)|^2} \pm g_J\mu_B B, \qquad (168)$$

in which \uparrow (\downarrow) denotes *z*-direction spin angular momentum carried by the magnons. In the absence of Dzyaloshinskii-Moriya interaction (DMI), the two branches of magnons are degenerate. The linear spin Nernst coefficient of magnons is given by

$$\eta^{\alpha\beta} = \sum_{p=\uparrow,\downarrow} \frac{ek_B}{\hbar} \epsilon^{\alpha\beta\gamma} \int_k S(g_p) \Omega_p^{\gamma}.$$
 (169)

Distinguished from that of electrons, here g_p is the Bose-Einstein distribution and $S(g_p) = g_p \ln g_p - (1 + g_p) \ln(1 + g_p)$ is the entropy density of *p*-band magnons. The thermal Hall conductivity is given as [46,47]

$$\kappa^{\alpha\beta} = -\sum_{p=\uparrow,\downarrow} \frac{k_B^2 T}{\hbar} \epsilon^{\alpha\beta\gamma} \int_k c_2(g_p) \Omega_p^{\gamma}, \qquad (170)$$

where the bosonic c_2 function is $c_2(g_p) = (1 + g_p)(\ln \frac{1+g_p}{g_p})^2 - (\ln g_p)^2 - 2\operatorname{Li}_2(-g_p)$ [46].

In the absence of DMI, it is demonstrated in Ref. [48] the quadratic order expanded Hamiltonian of Eq. (163) is invariant under combined symmetry of time reversal (\mathcal{T}) and a 180° rotation around the *x* axis in the spin space (c_x). Under $\mathcal{T}c_x$, $\varepsilon_p(\mathbf{k}) = \varepsilon_p(-\mathbf{k})$ and $\Omega_p(\mathbf{k}) = -\Omega_p(-\mathbf{k})$, hence, the integrand in Eq. (169) is odd and indicates a zero linear spin Nernst coefficient (i.e., $\eta_{\text{DC}}^{\alpha\beta} = 0$). We shall emphasize that the spin Nernst effect of magnon does not exist at any order if there is no DMI. If the DMI is introduced, it breaks $\mathcal{T}c_x$ symmetry and changes the dispersion, leaving a nonzero linear spin Nernst coefficient as the leading order [48]. Since we focus on zero DMI case, we will not discuss the spin Nernst effect of magnon in the following.

For the magnon thermal Hall effect (MTHE), things are different. Although the linear MTHE disappears for both zero and nonzero DMI (the two branches of magnons with opposite spin angular momentum flow in opposite transverse directions), the second-order nonlinear MTHE should exist (even for zero DMI) giving rise to a leading-order contribution to the MTHE. Assuming that the temperature gradient is applied along the *y* direction, according to Eq. (G28) the second-order magnon thermal Hall conductivity is

$$\kappa^{xyy} \cong \frac{\tau}{T^2} \sum_p \int_{\boldsymbol{k}} \varepsilon_p^3 \partial^y g_p \Omega_p^z(\boldsymbol{k}).$$
(171)

In deriving Eq. (171), the relaxation-time approximation for steady state $\lim_{\omega\to 0} -i/(\omega + i\Gamma) \cong \tau$ is indicated and the negligible external magnetic field is adopted. It should be noted that κ_{DC}^{xyy} becomes zero when *T* approaches zero [49].

It has been shown that the largest symmetry of a twodimensional (2D) crystal that allows for nonvanishing Berry curvature dipole is a mirror symmetry [7]. The mirror symmetry M_y is perpendicular to the mirror line, and the mirror symmetry M_y requires $\Omega_p^z(k_x, k_y) = -\Omega_p^z(k_x, -k_y)$. Together with $\mathcal{T}c_x$, we get $\Omega_p^z(k_x, k_y) = \Omega_p^z(-k_x, k_y)$. The mirror symmetry M_y leads to $\varepsilon_p(k_x, k_y) = \varepsilon_p(k_x, -k_y)$, When combining $\mathcal{T}c_x$ and M_y , it requires $\varepsilon_p(k_x, k_y) = \varepsilon_p(-k_x, k_y)$. Therefore, the partial derivative of Bose function distribution $\partial^x g_p$ and $\partial^y g_p$ is both an odd function.

To reduce the c_{3v} space-group symmetry of Hamiltonian (163) to the single mirror symmetry M_y , we apply a uniaxial tensile strain along the *y* direction. Hence, only the interaction along the *y* axis changes, without lattice deformation. Hence, antiferromagnetic coupling on the d_1 bonds is changed to $J(1 + \delta)$, and the correction to the Hamiltonian is

$$H_{s}(\boldsymbol{k}) = \begin{bmatrix} \delta J & \delta J \exp(i\boldsymbol{k} \cdot \boldsymbol{\delta}_{1}) \\ \delta J \exp(-i\boldsymbol{k} \cdot \boldsymbol{\delta}_{1}) & \delta J \end{bmatrix}.$$
 (172)



FIG. 3. (a), (b) Berry curvature $\Omega_{\uparrow}^{z}(\mathbf{k})$ of the spin-up magnon mode without strain $\delta J = 0$ (a) and with uniform uniaxial strain $\delta J = 0.5$ (b). The gray circles denote the locations of maximum value for the unstrained $\Omega_{\uparrow}^{z}(\mathbf{k})$, which correspond to *K* and *K'*. The yellow circle denotes locations of maximum value for strained $\Omega_{\uparrow}^{z}(\mathbf{k})$. (c), (d) $\partial g_{\uparrow}/\partial k_{y}$ without strain $\delta J = 0$ in (c) and with strain $\delta J = 0.5$ in (d). The gray (yellow) circles denote the locations of maximum value for the unstrained (strained) $\partial g_{\uparrow}/\partial k_{y}$. Parameters are J = 2, K = -0.2, $k_{B}T = 0.5$, and $g_{J}\mu_{B}B = 0.01$. Numbers are in units of meV.

The total Hamiltonian is $H = H_0 + H_s$, and the magnon dispersion is given by

$$\varepsilon_{p=\uparrow,\downarrow} = S\sqrt{(3J+\delta J-K)^2 - |J\gamma(\mathbf{k})+\delta Je^{i\mathbf{k}\cdot\delta_1}|^2} \pm g_J\mu_B B.$$
(173)

Figure 3 shows the unstrained (strained) Berry curvature of spin-up magnon and the associated $\partial g_{\uparrow}/\partial k_y$ distribution. Considering that the integral in Eq. (171) is mostly contributed from the region around *K* and *K'*. In the absence of strain [see Fig. 3(a)], the maximum values of Berry curvature $\Omega_{\uparrow}^z(k)$ locate at *K* and *K'*. Meanwhile, the zero points of $\partial g_{\uparrow}/\partial k_y$ also locate at *K* and *K'* [see Fig. 3(c)], resulting in the cancellation of the integral around each *K* and *K'* and zero κ^{xyy} . However, when applying the uniaxial strain along the *y* direction, the maximum values of Berry curvature $\Omega_{\uparrow}^z(k)$ are shifted from the original *K* (*K'*) towards $-k_x (k_x)$ direction [see Fig. 3(b)]. The zero points of $\partial g_{\uparrow}/\partial k_y$ are also shifted from the original *K* (*K'*) towards $k_x (-k_x)$ direction [see Fig. 3(d)]. Therefore, the integral around each *K* and *K'* can not be canceled, leading to a finite second-order magnon thermal Hall conductivity κ^{xyy} .

To further illustrate the above picture, we show the dependence of κ^{xyy} on the temperature and the strain-induced coupling δJ , which is plotted in Fig. 4(a). Notice that κ^{xyy} approaches zero as *T* approaches zero. For fixed *T*, κ^{xyy} increases monotonically with increasing δJ , suggesting the appearance of the nonlinear MTHE induced by the strain. It should be noted that our analysis based on the linear spin-wave theory is only valid in the temperature range much lower than the Néel temperature, which is estimated to be around 200 K in MnPS₃ [50]. However, κ^{xyy} is not monotonic in



FIG. 4. (a) The magnon thermal Hall conductivity up to the second order (i.e., κ^{xyy} , and first order disappears) as a function of strain-induced coupling δJ and temperature of a collinear antiferromagnets. J = 2, K = -0.2, and $g_J \mu_B B = 0.01$. (b) The *T*-dependent factor \mathcal{F} for different δJ . ε_p is taken to be -0.2. Numbers are in units of meV.

T. For fixed δJ , κ^{xyy} increases at first and then decreases with a maximum around 22 K. To understand this nonmonotonicity, we extract the temperature dependence of Eq. (171). The T-dependent factor of Eq. (171) is expressed as $\mathcal{F} =$ $\frac{1}{(k_B T)^2} \frac{\exp(\beta \varepsilon_p)}{[\exp(\beta \varepsilon_p) - 1]^2}.$ In Fig. 4(b) we depict the *T*-dependent factor \mathcal{F} as a function of T. For different δJ , \mathcal{F} is maximized around 22 K, hence, we conclude that the temperature nonmonotonicity of κ^{xyy} is determined by \mathcal{F} . As shown in Fig. 4(b), the temperature position T_{max} of the maximum of \mathcal{F} decreases from 25 to 18 K as δJ increases from 0.5 to 0.7 meV. In Fig. 4(a) we indicate the position T_{max} of the maximum of κ^{xyy} by the dashed-dotted line. As a contrast, T_{max} increases slightly with the increment δJ . This is because the T dependent \mathcal{F} indicates that all momentum k is weighted equally for fixed T. However, according to Eq. (171), the final temperature dependence of κ^{xyy} should be weighted by $\varepsilon_p^3 \Omega_p^z$ additionally.

V. CONCLUDING REMARKS AND DISCUSSIONS

In summary, a nonlinear thermal response theory is developed through perturbed expansion approach in favor of thermal vector potential. Based on the diagram rules and values of vertices connecting the propagator of temperature gradient, the general expressions of the dynamical thermoelectric and thermal conductivity are obtained. The central results for the linear-order [the thermoelectric response (64) and the thermal-thermal response (76)], the second-order [the thermoelectric responses (124) and (125) and the thermal-thermal response (146) and (147)], and the third-order responses [(157) and (158)] are explicitly derived.

The choice of the gauge depends on convenience. It is easy to give a cleaner resonance structure and is easier to implement numerically in velocity gauge. For the DC limit and semiclassical limits, it is better to apply the length gauge. By providing the DC limit formula in length gauge, we demonstrate the relations among the thermal response coefficients beyond the linear order (cf. Table III). For linear transport, the Mott relation and WF law tell us that the thermoelectric (thermal) conductivity is proportional to the first (zero) derivative of the linear electric conductivity to the Fermi energy. Beyond the linear order, it is found that there exist higher-order Mott relation and WF law. The second-order Mott relation and WF law say that the second-order electric conductivity is proportional to zero (the first) derivative of the thermoelectric (thermal) conductivity with respect to the chemical potential. And the third-order Mott relation and WF law show that the third-order electric conductivity is proportional to the first (second) derivative of the thermoelectric (thermal) conductivity with respect to the chemical potential. It is found that the derivative on the thermoelectric and the thermal conductivity increases linearly with the nonlinear order. The derivative in the WF law is one order higher than that of the Mott relation. We call this structure as a "hierarchy rule." Although we only explicitly calculate the nonlinear response up to the third order, we speculate that this "hierarchy rule" between Mott relation and the WF law exists to higher order, revealing a deeper relationship between them. Moreover, it is discovered that the Lorentz number characterizing the relation of linear thermoelectric and thermal-thermal response applies to the nonlinear order.

An interesting and important fact is that for the secondorder response, the Mott relation is only proportional to the second-order electric conductivity by the linear Lorentz number. Since the off-diagonal element of the second electric conductivity is just the nonlinear Hall conductivity which has been measured in experiments, the off-diagonal element of the second thermoelectric conductivity (i.e., the secondorder Nernst coefficient) can be obtained immediately by using the experimental data of the nonlinear Hall conductivity. We estimate that the transverse charge current density can be the order of 10^{-6} A/(cm)² for a temperature gradient of 0.01 K/cm based on few layers WTe₂ [51]. This charge-current density induced by a temperature gradient can be explored in experiments. For the second-order WF law, the electric conductivity is proportional to the first derivative of the second-order thermal conductivity with respect to the chemical potential. The proportional factor is related to the Lorentz number, and the second thermal conductivity can be sizable. Therefore, the quantities from the second-order response can be measured in experiments without introducing more difficulties. We expect that our predictions can be tested in the near future experiments.

Although the derived quantum theory of nonlinear thermal response is based on a formalism for fermions, it can be utilized to boson systems. As an application, we specifically calculate the magnon thermal Hall conductivity in a strained collinear antiferromagnet model. We predict that with the combined $\mathcal{T}c_x$ symmetry and broken inversion symmetry, the linear magnon thermal Hall conductivity vanishes and the second-order thermal Hall effect dominates.

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APPENDIX A: DETAILS OF DERIVATION FOR EQ. (21), DEFINITION OF HEAT CURRENT, AND THE RELATION TO ENTROPY FLUX

The definition of heat current in the presence of the "gravitational" potential, has been presented previously [33]. However, since it is important to the rest of our discussion, we shall review it here. Considering a noninteracting electron system, the energy density is written as

$$\hat{h}^{\Psi}(\boldsymbol{r}) = [1 + \Psi(\boldsymbol{r})] \left\{ \frac{m}{2} [\hat{\boldsymbol{v}}\hat{\boldsymbol{\varphi}}(\boldsymbol{r})]^{\dagger} \cdot [\hat{\boldsymbol{\varphi}}(\boldsymbol{r})\hat{\boldsymbol{v}}] + \hat{\boldsymbol{\varphi}}^{\dagger}(\boldsymbol{r})[V(\boldsymbol{r})]\hat{\boldsymbol{\varphi}}(\boldsymbol{r}) \right\},\tag{A1}$$

where $\hat{\varphi}(\mathbf{r}) [\hat{\varphi}^{\dagger}(\mathbf{r})]$ is the electron annihilation (creation) field operator. The energy current operator is defined by the conservation equation

$$\frac{\partial \hat{h}^{\Psi}(\boldsymbol{r})}{\partial t} = \frac{1}{i\hbar} [\hat{h}^{\Psi}(\boldsymbol{r}), \hat{H}^{\Psi}] = -\nabla \cdot \boldsymbol{J}_{E}^{\Psi}(\boldsymbol{r}), \tag{A2}$$

where $\hat{H}^{\Psi} = \frac{m}{2}\hat{v}[1 + \Psi(r)]\hat{v} + [1 + \Psi(r)]V(r)$. Substituting the energy density operator into the conservation equation, it yields

$$\frac{\partial \hat{h}^{\Psi}(\boldsymbol{r})}{\partial t} = -\boldsymbol{\nabla} \cdot \left\{ \frac{1}{2} [1 + \Psi(\boldsymbol{r})] \left([\hat{\boldsymbol{v}}\hat{\boldsymbol{\varphi}}(\boldsymbol{r})]^{\dagger} [\hat{H}^{\Psi}\hat{\boldsymbol{\varphi}}(\boldsymbol{r})] + [\hat{H}^{\Psi}\hat{\boldsymbol{\varphi}}(\boldsymbol{r})]^{\dagger} [\hat{\boldsymbol{v}}\hat{\boldsymbol{\varphi}}(\boldsymbol{r})] \right) \right\}.$$
(A3)

Therefore, the energy current operator is identified as

$$J_{E}^{\Psi}(\mathbf{r}) = \left\{ \frac{1}{2} [1 + \Psi(\mathbf{r})] \left([\hat{v}\hat{\varphi}(\mathbf{r})]^{\dagger} [\hat{H}^{\Psi}\hat{\varphi}(\mathbf{r})] + [\hat{H}^{\Psi}\hat{\varphi}(\mathbf{r})]^{\dagger} [\hat{v}\hat{\varphi}(\mathbf{r})] \right) \right\} \\ = \frac{1}{2} [1 + \Psi(\mathbf{r})]^{2} \{ ([\hat{v}\hat{\varphi}(\mathbf{r})]^{\dagger} [\hat{H}_{0}\hat{\varphi}(\mathbf{r})] + [\hat{H}_{0}\hat{\varphi}(\mathbf{r})]^{\dagger} [\hat{v}\hat{\varphi}(\mathbf{r})]) \} + \nabla [1 + \Psi(\mathbf{r})]^{2} \times \hat{\Lambda},$$
(A4)

where $\hat{\Lambda} = -\frac{i\hbar}{8} [\hat{v}\hat{\varphi}(\mathbf{r})]^{\dagger} \times [\hat{v}\hat{\varphi}(\mathbf{r})]$. Noting that the current operator is only defined up to a curl by the equation of continuity. The form of the energy current can be determined by the scaling law

$$\boldsymbol{I}_{E}^{\Psi}(\boldsymbol{r}) = [1 + \Psi(\boldsymbol{r})]^{2} \boldsymbol{J}_{E}(\boldsymbol{r}), \tag{A5}$$

therefore the energy current operator becomes

$$\boldsymbol{J}_{E}^{\Psi}(\boldsymbol{r}) \to \boldsymbol{J}_{E}^{\Psi}(\boldsymbol{r}) - \boldsymbol{\nabla}[1 + \Psi(\boldsymbol{r})]^{2} \times \hat{\boldsymbol{\Lambda}},\tag{A6}$$

$$J_E(\mathbf{r}) \to J_E(\mathbf{r}) + \nabla \times \hat{\mathbf{\Lambda}}.$$
 (A7)

The heat current is defined as $J_Q(\mathbf{r}) \equiv J_E(\mathbf{r}) - \mu J_N(\mathbf{r})$. In the absence of temperature gradient field, the zero-field heat current operator is given by

$$\boldsymbol{J}_{\mathcal{Q}}(\boldsymbol{r}) = \frac{1}{2} \left[\left[\hat{\boldsymbol{v}} \hat{\boldsymbol{\varphi}}(\boldsymbol{r}) \right]^{\dagger} \left[\hat{K}_{0} \hat{\boldsymbol{\varphi}}(\boldsymbol{r}) \right] + \left[\hat{K}_{0} \hat{\boldsymbol{\varphi}}(\boldsymbol{r}) \right]^{\dagger} \left[\hat{\boldsymbol{v}} \hat{\boldsymbol{\varphi}}(\boldsymbol{r}) \right] \right) - \nabla \times \hat{\boldsymbol{\Lambda}}, \tag{A8}$$

where $\hat{K}_0 = \hat{H}_0 - \mu_0 \hat{N}$. Noting that apart from the first term which is recognized as the usual anticommutator representation of the heat current, the second term appears is essential for satisfying the scaling law. It has been proved that in calculating the Kubo formula, the second term cancels out [27,33]; this could be the reason why the anticommutator representation usually leads to the right results.

Alternatively, the heat current can be defined through the thermodynamics of entropy flux [52], and it is equivalent to the definition via conservation equation. To see this we start form the Luttinger's Hamiltonian. The particle-number conservation equation is given as

$$\frac{\partial \hat{n}^{\Psi}(\boldsymbol{r})}{\partial t} = \frac{1}{i\hbar} [\hat{n}^{\Psi}(\boldsymbol{r}), \hat{H}^{\Psi}] = -\nabla \cdot \boldsymbol{J}_{N}^{\Psi}(\boldsymbol{r}).$$
(A9)

Combining Eqs. (A2) and (A9), the conservation equation of heat is written as

$$\frac{\partial \hat{k}^{\Psi}(\boldsymbol{r})}{\partial t} = \frac{1}{i\hbar} [\hat{k}^{\Psi}(\boldsymbol{r}), \hat{H}^{\Psi}] = -\nabla \cdot \boldsymbol{J}_{Q}^{\Psi}(\boldsymbol{r}), \tag{A10}$$

in which $\hat{k}^{\Psi}(\mathbf{r}) = \hat{h}^{\Psi}(\mathbf{r}) - \mu \hat{n}^{\Psi}(\mathbf{r})$ is the grand-canonical ensemble energy density. The Luttinger's Hamiltonian can be rewritten as

$$H_L(t) = \int d^3r \int_{-\infty}^t dt' \boldsymbol{J}_Q(t') \cdot \boldsymbol{\nabla} \Psi(\boldsymbol{r}, t).$$
(A11)

By converting the "gravitational" potential in form of thermal vector potential $\partial A_T(\mathbf{r}, t)/\partial t = \nabla \Psi(\mathbf{r}, t) = \nabla T/T$, the perturbation Hamiltonian is written as

$$H_L(t) = -\int d^3 r J_Q(t') \cdot A_T(\mathbf{r}, t).$$
(A12)

The rate of the change of the entropy *S* due to a heat current is [53]

$$\frac{dS}{dt} = -\int d^3r \frac{1}{T} \nabla \cdot \boldsymbol{J}_{\mathcal{Q}} = -\int d^3r \frac{\nabla T}{T^2} \cdot \boldsymbol{J}_{\mathcal{Q}}.$$
(A13)

The change of entropy modifies the thermodynamic potential $E - TS - \mu N$ (*E* is the internal energy). The perturbation Hamiltonian induced by the temperature gradient field becomes

$$H_{S} = \frac{1}{T} \int d^{3}r \int_{-\infty}^{t} dt' \boldsymbol{J}_{\mathcal{Q}}(t') \cdot \boldsymbol{\nabla} T.$$
(A14)

It recovers the Luttinger's Hamiltonian after the replacement $\nabla \Psi(\mathbf{r}, t) = \nabla T/T$. Similar definition of the heat current can be found in [54].

APPENDIX B: EXPANSION OF THE HERMITIAN DERIVATIVES

The second-order Hermitian derivative on the unperturbed Hamiltonian is expanded as

$$\hat{\mathcal{K}}^{\alpha\beta} = \hat{\mathcal{D}}^{\alpha}\hat{\mathcal{D}}^{\beta}[\hat{K}_{0}] = \frac{1}{4} \big(\hat{K}_{0}\hat{h}^{\alpha}\hat{h}^{\beta} + \hat{K}_{0}^{2}\hat{h}^{\alpha\beta} + 2\hat{K}_{0}\hat{h}^{\alpha\beta}\hat{K}_{0} + \hat{K}_{0}\hat{h}^{\beta}\hat{h}^{\alpha} + \hat{h}^{\alpha}\hat{h}^{\beta}\hat{K}_{0} + \hat{h}^{\alpha\beta}\hat{K}_{0}^{2} + \hat{h}^{\beta}\hat{h}^{\alpha}\hat{K}_{0} \big). \tag{B1}$$

Its normal derivative is given by

$$\hat{D}^{\mu}[\hat{\mathcal{K}}^{\alpha\beta}] = \frac{1}{4} (\hat{h}^{\mu}\hat{h}^{\alpha}\hat{h}^{\beta} + \hat{K}_{0}\hat{h}^{\mu\alpha}\hat{h}^{\beta} + \hat{K}_{0}\hat{h}^{\alpha}\hat{h}^{\mu\beta} + \hat{h}^{\mu}\hat{K}_{0}\hat{h}^{\alpha\beta} + \hat{K}_{0}\hat{h}^{\mu}\hat{h}^{\alpha\beta} + \hat{K}_{0}\hat{h}^{\mu}\hat{h}^{\alpha\beta} + \hat{K}_{0}\hat{h}^{\mu}\hat{h}^{\alpha\beta} + \hat{K}_{0}\hat{h}^{\mu}\hat{h}^{\alpha\beta} + \hat{K}_{0}\hat{h}^{\mu}\hat{h}^{\alpha\beta} + \hat{h}^{\mu\alpha}\hat{h}^{\beta}\hat{K}_{0} + \hat{h}^{\alpha}\hat{h}^{\mu\beta}\hat{K}_{0} + \hat{h}^{\alpha}\hat{h}^{\beta}\hat{h}^{\mu} + \hat{h}^{\mu\alpha\beta}\hat{K}_{0}^{2} \\ + \hat{h}^{\alpha\beta}\hat{h}^{\mu}\hat{K}_{0} + \hat{h}^{\alpha\beta}\hat{K}_{0}\hat{h}^{\mu} + \hat{h}^{\mu\beta}\hat{h}^{\alpha}\hat{K}_{0} + \hat{h}^{\beta}\hat{h}^{\mu\alpha}\hat{K}_{0} + \hat{h}^{\beta}\hat{h}^{\alpha}\hat{h}^{\mu}).$$
(B2)

APPENDIX C: DERIVATION OF EQS. (59) AND (72)

Using the relations (42) and (43), and the following identities

$$\int_{\beta}^{\infty} f(\varepsilon) d\lambda = \frac{\beta}{\varepsilon} \ln(1 + e^{-\beta\varepsilon}) / \beta,$$
(C1)

$$\int_{\beta}^{\infty} \frac{\partial f(\varepsilon)}{\partial \varepsilon} d\lambda = -\frac{\beta}{\varepsilon} f(\varepsilon) + \frac{\beta}{\varepsilon^2} \int_{\varepsilon}^{\infty} f(\lambda) d\lambda, \tag{C2}$$

the first-order particle magnetization response (59) and heat magnetization response (72) are obtained by integrating the auxiliary particle magnetization with respect to β .

APPENDIX D: EXPANSION OF THE INTEGRAL KERNELS USED IN LENGTH GAUGE

For the Kubo contribution of the linear thermoelectric response, the integrand is calculated as

$$\operatorname{Tr}\{v^{\alpha}(d(\omega) \circ \mathcal{D}^{\beta}[\rho^{(0)}])\} = \sum_{p,q} \frac{1}{2} v^{\alpha}_{pq} d_{qp}(\omega) [H_0, D^{\beta}[\rho^{(0)}]]_{+,qp}$$
$$= \sum_{p,q} \frac{1}{2} v^{\alpha}_{pq} d_{qp}(\omega) \left\{ [H_0, \partial^{\beta} \rho^{(0)}]_{+,qp} - i \frac{1}{2} [H_0, [\mathcal{A}^{\beta}, \rho^{(0)}]_{-}]_{+,qp} \right\}$$
$$= \sum_{p} \frac{1}{\omega} v^{\alpha}_{p} \varepsilon_{p} \partial^{\beta} f_p - \sum_{p,q} i \frac{1}{2(\omega - \varepsilon_{qp})} (\varepsilon_{p} + \varepsilon_{q}) v^{\alpha}_{pq} \mathcal{A}^{\beta}_{qp} f_{pq}.$$
(D1)

The integrand in the second-order thermoelectric response is calculated as

$$Tr\{v^{\alpha}(d(\omega) \circ \mathcal{D}^{\beta}[d(\omega - \omega_{1}) \circ \mathcal{D}^{\gamma}[\rho^{(0)}]])\} = \sum_{p,q} \frac{1}{4} v^{\alpha}_{pq} d_{qp}(\omega) [H_{0}, D^{\beta}[d(\omega - \omega_{1}) \circ [H_{0}, D^{\gamma}[\rho^{(0)}]]_{+}]]_{+,qp}$$
$$= \Pi^{(2),\beta\gamma} + \Pi^{(2),\beta} + \Pi^{(2),\gamma} + \Pi^{(2)},$$
(D2)

where

$$\Pi^{(2),\beta\gamma} = \sum_{p,q} \frac{1}{4} v_{pq}^{\alpha} d_{qp}(\omega) [H_0, \partial^{\beta} [d(\omega - \omega_1) \circ [H_0, \partial^{\gamma} [\rho^{(0)}]]_+]]_{+,qp} = \sum_p v_p^{\alpha} \frac{1}{\omega} \varepsilon_p \frac{1}{\omega - \omega_1} \partial^{\beta} (\varepsilon_p \partial^{\gamma} f_p), \tag{D3}$$

$$\Pi^{(2),\beta} = \sum_{p,q} \frac{1}{4} v_{pq}^{\alpha} d_{qp}(\omega) [H_0, \partial^{\beta} [d(\omega - \omega_1) \circ [H_0, [\mathcal{A}^{\gamma}, \rho^{(0)}]_-]_+]]_{+,qp}$$

$$= \sum_{p,q} -i \frac{1}{4} v_{pq}^{\alpha} \frac{1}{\omega - \varepsilon_{qp}} (\varepsilon_p + \varepsilon_q) \partial^{\beta} \left\{ \frac{1}{\omega - \omega_1 - \varepsilon_{qp}} \times (\varepsilon_p + \varepsilon_q) \mathcal{A}_{qp}^{\gamma} f_{pq} \right\}, \tag{D4}$$

$$\Pi^{(2),\gamma} = \sum_{p,q} \frac{1}{4} v_{pq}^{\alpha} d_{qp}(\omega) [H_0, [\mathcal{A}^{\beta}, [d(\omega - \omega_1) \circ [H_0, \partial^{\gamma} [\rho^{(0)}]]_+]]_-]_{+,qp}$$

$$= \sum_{p,q} -i \frac{1}{2} v_{pq}^{\alpha} \frac{1}{(\omega - \varepsilon_{qp})} \frac{1}{(\omega - \omega_1)} \mathcal{A}_{qp}^{\beta} (\varepsilon_p \varepsilon_q \partial^{\gamma} f_{pq} + \varepsilon_p^2 \partial^{\gamma} f_p - \varepsilon_q^2 \partial^{\gamma} f_q), \tag{D5}$$

$$\Pi^{(2)} = \sum_{p,q,r} \frac{1}{4} v_{pq}^{\alpha} d_{qp}(\omega) [H_0, [\mathcal{A}^{\beta}, [d(\omega - \omega_1) \circ [H_0, [\mathcal{A}^{\gamma}, \rho^{(0)}]_-]_+]]_-]_{+,qp}$$

$$= \sum_{p,q,r} -\frac{1}{4} v_{pq}^{\alpha} \frac{1}{\omega - \varepsilon_{qp}} (\varepsilon_q + \varepsilon_p) \bigg[\frac{1}{\omega - \omega_1 - \varepsilon_{rp}} \mathcal{A}_{qr}^{\beta} \mathcal{A}_{rp}^{\gamma} \varepsilon_p (\varepsilon_r + \varepsilon_p) - \frac{1}{\omega - \omega_1 - \varepsilon_{qr}} \mathcal{A}_{qr}^{\gamma} \mathcal{A}_{rp}^{\beta} \varepsilon_p (\varepsilon_r + \varepsilon_q) \bigg].$$
(D6)

The integrand in the second-order thermal-thermal response is calculated as

$$\operatorname{Tr}\left\{\frac{1}{2}[H_{0}, v^{\alpha}]_{+} \times (d(\omega) \circ \mathcal{D}^{\beta}[d(\omega - \omega_{1}) \circ \mathcal{D}^{\gamma}[\rho^{(0)}]])\right\}$$
$$= \sum_{p,q} \frac{1}{4} v^{\alpha}_{pq} d_{qp}(\omega)[H_{0}, D^{\beta}[d(\omega - \omega_{1}) \circ [H_{0}, D^{\gamma}[\rho^{(0)}]]_{+}]]_{+,qp} = \Xi^{(2),\beta\gamma} + \Xi^{(2),\beta} + \Xi^{(2),\gamma} + \Xi^{(2)}, \tag{D7}$$

where

$$\Xi^{(2),\beta\gamma} = \sum_{p,q} \frac{1}{8} [H_0, v^{\alpha}]_{+,pq} d_{qp}(\omega) [H_0, \partial^{\beta} [d(\omega - \omega_1) \circ [H_0, \partial^{\gamma} [\rho^{(0)}]]_{+}]]_{+,qp}$$

$$= \sum_{p} v^{\alpha}_{p} \frac{1}{\omega} \tilde{\varepsilon}^2_{p} \partial^{\beta} \left[\frac{1}{\omega - \omega_1} \tilde{\varepsilon}_{q} \partial^{\gamma} f_p \right], \qquad (D8)$$

$$\Xi^{(2),\beta} = \sum_{p,q} \frac{1}{8} [H_0, v^{\alpha}]_{+,pq} d_{qp}(\omega) [H_0, \partial^{\beta} [d(\omega - \omega_1) \circ [H_0, [\mathcal{A}^{\gamma}, \rho^{(0)}]_{-}]_{+}]]_{+,qp}$$

$$= \sum_{p,q} -i \frac{1}{8} v^{\alpha}_{pq} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q})^2 \frac{1}{\omega - \varepsilon_{pq}} \partial^{\beta} \left[\frac{1}{\omega - \omega_1 - \varepsilon_{qp}} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q}) \mathcal{A}^{\gamma}_{qp} f_{pq} \right], \qquad (D9)$$

$$\Xi^{(2),\gamma} = \sum_{p,q} \frac{1}{8} [H_0, v^{\alpha}]_{+,pq} d_{qp}(\omega) [H_0, [\mathcal{A}^{\beta}, [d(\omega - \omega_1) \circ [H_0, \partial^{\gamma} [\rho^{(0)}]]_{+}]]_{-}]_{+,qp}$$

$$= \sum_{p,q} -i \frac{1}{8} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q})^2 v^{\alpha}_{pq} \frac{1}{(\omega - \varepsilon_{p})} \frac{1}{(\omega - \omega_1)} \mathcal{A}^{\beta}_{qp} [\tilde{\varepsilon}_{p} \tilde{\varepsilon}_{q} \partial^{\gamma} f_{pq} + \tilde{\varepsilon}^2_{p} \partial^{\gamma} f_{p} - \tilde{\varepsilon}^2_{q} \partial^{\gamma} f_{q}), \qquad (D10)$$

$$\Xi^{(2)} = \sum_{p,q} \frac{1}{8} [H_0, v^{\alpha}]_{+,pq} d_{qp}(\omega) [H_0, [\mathcal{A}^{\beta}, [d(\omega - \omega_1) \circ [H_0, [\mathcal{A}^{\gamma}, \rho^{(0)}]_-]_+]]_-]_{+,qp}$$
$$= \sum_{p,q,r} -\frac{1}{8} v^{\alpha}_{pq} \frac{1}{\omega - \varepsilon_{qp}} (\varepsilon_q + \varepsilon_p)^2 \left[\frac{1}{\omega - \omega_1 - \varepsilon_{rp}} \mathcal{A}^{\beta}_{qr} \mathcal{A}^{\gamma}_{rp} \varepsilon_p (\varepsilon_r + \varepsilon_p) - \frac{1}{\omega - \omega_1 - \varepsilon_{qr}} \mathcal{A}^{\gamma}_{qr} \mathcal{A}^{\beta}_{rp} \varepsilon_p (\varepsilon_r + \varepsilon_q) \right].$$
(D11)

APPENDIX E: EXPANSION OF THE INTEGRAL KERNELS AT THE THIRD ORDER

The integrand in the third-order thermoelectric response is calculated as

$$Tr\{v^{\alpha}(d(\omega) \circ \mathcal{D}^{\beta}[d(\omega - \omega_{1}) \circ \mathcal{D}^{\gamma}[d(\omega - \omega_{[2]}) \circ \mathcal{D}^{\delta}[\rho^{(0)}]]])\} = \sum_{p,q} \frac{1}{8} v^{\alpha}_{pq} d_{qp}(\omega)[H_{0}, D^{\beta}[d(\omega - \omega_{1}) \circ [H_{0}, D^{\gamma}[d(\omega - \omega_{[2]}) \circ [H_{0}, D^{\delta}[\rho^{(0)}]]_{+}]]_{+}]]_{+,qp} = \Pi^{(3),\beta\gamma\delta} + \Pi^{(3),\beta\gamma} + \Pi^{(3),\gamma\delta} + \Pi^{(3),\beta} + \Pi^{(3),\gamma} + \Pi^{(3),\delta} + \Pi^{(3)},$$
(E1)

where

$$\Pi^{(3),\beta\gamma\delta} = \sum_{p,q} \frac{1}{8} v_{pq}^{a} d_{qp}(\omega) [H_{0}, \partial^{\beta} [d(\omega - \omega_{1}) \circ [H_{0}, \partial^{\gamma} [d(\omega - \omega_{[2]}) \circ [H_{0}, [\partial^{\delta} [\rho^{(0)}]]_{+}]]_{+}]]_{+,qp}$$

$$= \sum_{p} v_{p}^{a} \frac{1}{\omega} \frac{1}{\omega - \omega_{1}} \frac{1}{\omega - \omega_{[2]}} \varepsilon_{p} \partial^{\beta} [\varepsilon_{p} \partial^{\gamma} (\varepsilon_{p} \partial^{\delta} f_{p})],$$
(E2)
$$\Pi^{(3),\beta\gamma} = \sum_{p,q} \frac{1}{8} v_{pq}^{a} d_{qp}(\omega) [H_{0}, \partial^{\beta} [d(\omega - \omega_{1}) \circ [H_{0}, \partial^{\gamma} [d(\omega - \omega_{[2]}) \circ [H_{0}, [\mathcal{A}^{\delta}, \rho^{(0)}]_{-}]_{+}]]_{+}]]_{+,qp}$$

$$= \sum_{p,q,r} -i \frac{1}{8} v_{pq}^{a} \frac{1}{\omega - \varepsilon_{qp}} (\varepsilon_{p} + \varepsilon_{q}) \partial^{\beta} \left[\frac{1}{\omega - \omega_{1} - \varepsilon_{qp}} (\varepsilon_{p} + \varepsilon_{q}) \left[\partial^{\gamma} \frac{1}{\omega - \omega_{[2]} - \varepsilon_{pq}} (\varepsilon_{p} + \varepsilon_{q}) \mathcal{A}_{qp}^{\delta} f_{pq} \right] \right],$$
(E3)
$$\Pi^{(3),\beta\delta} = \sum_{p,q} \frac{1}{8} v_{pq}^{a} d_{qp}(\omega) [H_{0}, \partial^{\beta} [d(\omega - \omega_{1}) \circ [H_{0}, [\mathcal{A}^{\gamma}, [d(\omega - \omega_{[2]}) \circ [H_{0}, \partial^{\delta} [\rho^{(0)}]]_{+}]]_{-}]_{+}]]_{+,qp}$$

$$= \sum_{p,q} -i \frac{1}{8} v_{pq}^{a} \frac{1}{\omega - \varepsilon_{qp}} (\varepsilon_{p} + \varepsilon_{q}) \frac{1}{\omega - \omega_{[2]}} \partial^{\beta} \left[\frac{1}{\omega - \omega_{1} - \varepsilon_{qp}} \mathcal{A}_{qp}^{\gamma} (\varepsilon_{p} \varepsilon_{q} \partial^{\delta} f_{pq} + \varepsilon_{p}^{2} \partial^{\delta} f_{p} - \varepsilon_{q}^{2} \partial^{\delta} f_{q}) \right],$$
(E4)
$$\Pi^{(3),\gamma\delta} = \sum_{p,q} \frac{1}{8} v_{pq}^{a} d_{qp}(\omega) [H_{0}, [\mathcal{A}^{\beta}, [d(\omega - \omega_{1}) \circ [H_{0}, [\partial^{\gamma} [d(\omega - \omega_{[2]}) \circ [H_{0}, \partial^{\delta} [\rho^{(0)}]]_{+}]]_{-}]_{+}]]_{-}]_{+,qp}$$

$$= \sum_{p,q} -i \frac{1}{8} v_{pq}^{a} d_{qp}(\omega) [H_{0}, [\mathcal{A}^{\beta}, [d(\omega - \omega_{1}) \circ [H_{0}, [\partial^{\gamma} [d(\omega - \omega_{[2]}) \circ [H_{0}, \partial^{\delta} [\rho^{(0)}]]_{+}]]_{-}]_{+}]]_{-}]_{+,qp}$$

The integrand in the third-order thermal-thermal response is calculated as

$$\operatorname{Tr}\left\{\frac{1}{2}[H_{0}, v^{\alpha}]_{+} \times (d(\omega) \circ \mathcal{D}^{\beta}[d(\omega - \omega_{1}) \circ \mathcal{D}^{\gamma}[d(\omega - \omega_{[2]}) \circ \mathcal{D}^{\delta}[\rho^{(0)}]]])\right\}$$

$$= \sum_{p,q} \frac{1}{16}[H_{0}, v^{\alpha}]_{+,pq} d_{qp}(\omega)[H_{0}, \mathcal{D}^{\beta}[d(\omega - \omega_{1}) \circ [H_{0}, \mathcal{D}^{\gamma}[d(\omega - \omega_{[2]}) \circ [H_{0}, \mathcal{D}^{\delta}[\rho^{(0)}]]_{+}]]_{+}]]_{+,qp}$$

$$= \Xi^{(3),\beta\gamma\delta} + \Xi^{(3),\beta\gamma} + \Xi^{(3),\beta\delta} + \Xi^{(3),\gamma\delta} + \Xi^{(3),\beta} + \Xi^{(3),\gamma} + \Xi^{(3),\beta} + \Xi^{(3),\delta} + \Xi^{(3)}, \qquad (E10)$$

where

$$\Xi^{(3),\beta\gamma\delta} = \sum_{p,q} \frac{1}{16} [H_0, v^{\alpha}]_{+,pq} d_{qp}(\omega) [H_0, \partial^{\beta} [d(\omega - \omega_1) \circ [H_0, \partial^{\gamma} [d(\omega - \omega_{[2]}) \circ [H_0, [\partial^{\delta} [\rho^{(0)}]]_+]]_+]]_{+,qp}$$

$$= \sum_p v_p^{\alpha} \frac{1}{\omega} \frac{1}{\omega - \omega_1} \frac{1}{\omega - \omega_{[2]}} \varepsilon_p^2 \partial^{\beta} [\varepsilon_p \partial^{\gamma} (\varepsilon_p \partial^{\delta} f_p)],$$

$$\Xi^{(3),\beta\gamma} = \sum_{p,q} \frac{1}{16} [H_0, v^{\alpha}]_{+,pq} d_{qp}(\omega) [H_0, \partial^{\beta} [d(\omega - \omega_1) \circ [H_0, \partial^{\gamma} [d(\omega - \omega_{[2]}) \circ [H_0, [\mathcal{A}^{\delta}, \rho^{(0)}]_-]_+]]_+]]_{+,qp}$$
(E11)

$$=\sum_{p,q,r}-i\frac{1}{8}v_{pq}^{\alpha}\frac{1}{\omega-\varepsilon_{qp}}(\varepsilon_{p}+\varepsilon_{q})^{2}\partial^{\beta}\left[\frac{1}{\omega-\omega_{1}-\varepsilon_{qp}}(\varepsilon_{p}+\varepsilon_{q})\left[\partial^{\gamma}\frac{1}{\omega-\omega_{[2]}-\varepsilon_{pq}}(\varepsilon_{p}+\varepsilon_{q})\mathcal{A}_{qp}^{\delta}f_{pq}\right]\right],\quad(E12)$$

$$\Xi^{(3),\beta\delta} = \sum_{p,q} \frac{1}{16} [H_0, v^{\alpha}]_{+,pq} d_{qp}(\omega) [H_0, \partial^{\beta} [d(\omega - \omega_1) \circ [H_0, [\mathcal{A}^{\gamma}, [d(\omega - \omega_{[2]}) \circ [H_0, \partial^{\delta} [\rho^{(0)}]]_+]]_-]_+]]_{+,qp}$$

$$= \sum_{p,q} -i \frac{1}{16} v^{\alpha}_{pq} \frac{1}{\omega - \varepsilon_{qp}} (\varepsilon_p + \varepsilon_q)^2 \frac{1}{\omega - \omega_{[2]}} \partial^{\beta} \left[\frac{1}{\omega - \omega_1 - \varepsilon_{qp}} \mathcal{A}^{\gamma}_{qp} (\varepsilon_p \varepsilon_q \partial^{\delta} f_{pq} + \varepsilon_p^2 \partial^{\delta} f_p - \varepsilon_q^2 \partial^{\delta} f_q) \right], \quad (E13)$$

$$\begin{split} \Xi^{(3),\gamma\delta} &= \sum_{p,q} \frac{1}{16} [H_0, v^g]_{+,pq} d_{qp}(\omega) [H_0, [A^{\beta}, [d(\omega - \omega_1) \circ [H_0, [\partial^{\gamma}[d(\omega - \omega_{[2]}) \circ [H_0, \partial^{\delta}[p^{(0)}]]_+]]_-]_+]_-]_{+,qp} \\ &= \sum_{p,q} -i \frac{1}{16} v_{pq}^{\alpha} (\varepsilon_p + \varepsilon_q) \frac{1}{\omega - \varepsilon_{qp}} \frac{1}{\omega - \omega_{12}} \frac{1}{\omega - \omega_{12}} A_{qp}^{\beta} [\varepsilon_q \varepsilon_p \partial^{\gamma}(\varepsilon_p \partial^{\delta} f_p) - \varepsilon_q \varepsilon_p \partial^{\gamma}(\varepsilon_q \partial^{\delta} f_q) + \varepsilon_p^2 \partial^{\gamma}(\varepsilon_p \partial^{\delta} f_p) \\ &- \varepsilon_q^2 \partial^{\gamma}(\varepsilon_q \partial^{\delta} f_q)], \end{split}$$
(E14)
$$\Xi^{(3),\delta} &= \sum_{p,q} \frac{1}{16} [H_0, v^g]_{+,pq} d_{qp}(\omega) [H_0, [A^{\beta}, [d(\omega - \omega_1) \circ [H_0, [A^{\gamma}, [d(\omega - \omega_{22}]) \circ [H_0, \partial^{\delta}[\rho^{(0)}]]_+]]_-]_+]_+]_{+,qp} \\ &= \sum_{p,q,r} -i \frac{1}{16} v_{pq}^{\alpha} \frac{1}{\omega - \varepsilon_{qp}} (\varepsilon_p + \varepsilon_q)^2 \left[\frac{1}{\omega - \omega_1 - \varepsilon_{rq}} \frac{1}{\omega - \omega_{12} - \varepsilon_{rp}} A_{qr}^{\beta} A_{rp}^{\gamma} (\varepsilon_p \varepsilon_p \partial^{\delta} f_p) - \varepsilon_q^2 \partial^{\delta} f_p \right], \end{aligned}$$
(E15)
$$\Xi^{(3),\gamma} &= \sum_{p,q,r} \frac{1}{16} [H_0, v^g]_{+,pq} d_{qp}(\omega) [H_0, [A^{\beta}, [d(\omega - \omega_1) \circ [H_0, \partial^{\gamma}[d(\omega - \omega_{21}) \circ [H_0, \partial^{\delta}[\rho^{(0)}]]_+]]_-]_+]_+]_{+,qp} \\ &= \sum_{p,q,r} -i \frac{1}{16} v_{pq}^{\alpha} \frac{1}{\omega - \varepsilon_{qp}} A_{qr}^{\gamma} A_{rp}^{\beta} (\varepsilon_q \varepsilon_r \partial^{\delta} f_r + \varepsilon_r^2 \partial^{\delta} f_r) - \varepsilon_r^2 \partial^{\delta} f_p \right], \end{aligned}$$
(E15)
$$\Xi^{(3),\gamma} &= \sum_{p,q} \frac{1}{16} [H_0, v^a]_{+,pq} d_{qp}(\omega) [H_0, [A^{\beta}, [d(\omega - \omega_1) \circ [H_0, \partial^{\gamma}[d(\omega - \omega_{21}) \circ [H_0, [A^{\delta}, \rho^{(0)}]_-]_+]]_+]_+]_{+,qp} \\ &= \sum_{p,q,r} -i \frac{1}{16} v_{pq}^{\alpha} \frac{1}{\omega - \omega_{12} - \varepsilon_{rp}} A_{qr}^{\delta} (\varepsilon_q + \varepsilon_r) f_{qq} A_{pp}^{\delta} \right], \qquad$$
(E16)
$$\Xi^{(3),\beta} &= \sum_{p,q} \frac{1}{16} [H_0, v^a]_{+,pq} d_{qp}(\omega) [H_0, \partial^{\beta}[d(\omega - \omega_1) \circ [H_0, [A^{\gamma}, [d(\omega - \omega_{21}) \circ [H_0, [A^{\delta}, \rho^{(0)}]_-]_+]]_+]_+]_{+,qp} \\ &= \sum_{p,q,r} -i \frac{1}{16} v_{pq}^{\alpha} \frac{1}{\omega - \varepsilon_{qp}} A_{qr}^{\delta} (\varepsilon_q + \varepsilon_r) f_{qq} A_{pp}^{\delta} B_{p} (\varepsilon_r + \varepsilon_p) \partial^{\gamma} \left[\frac{1}{\omega - \omega_{12} - \varepsilon_r} A_{qr}^{\delta} A_{qr}^{\delta} B_{p} (\varepsilon_r + \varepsilon_p) - \frac{1}{\omega - \omega_{12} - \varepsilon_r} A_{qr}^{\delta} A_{qr}^{\delta} A_{qr}^{\delta} B_{p} (\varepsilon_r + \varepsilon_p) \right], \qquad$$
(E16)
$$\Xi^{(3),\beta} &= \sum_{p,q} \frac{1}{16} [H_0, v^a]_{+,pq} d_{qp}(\omega) [H_0, \partial^{\beta}[d(\omega - \omega_1) \circ [H_0, [A^{\gamma}, [d(\omega - \omega_{21}) \circ [H_0, [A^{\delta}, \rho^{(0)}]_-]_+]]_+]_+]_{+,qp} \\ &= \sum_{p,q,r,s} -i \frac{1}{16} v_{pq}^{\alpha} \frac{1}{\omega - \varepsilon_{qq}} (\varepsilon_q + \varepsilon_q)^2 \partial^{\beta} \left[\frac{1}{\omega - \omega_{1} - \varepsilon_r} A_{qr}^{\delta}$$

APPENDIX F: THIRD-ORDER THERMAL-THERMAL RESPONSE

The third-order thermal-thermal response is calculated in an similar way. The Kubo contribution in this case to the heat current is

$$J_h^{\text{Kubo},(3),\alpha}(\omega) = \int_k \text{Tr}[j_h^{\alpha} \rho^{(3)}].$$
(F1)

Following the same steps in calculating $L_{12}^{\text{Kubo},\alpha\beta\delta\zeta}$, the third-order Kubo thermal-thermal response is rewritten as

$$L_{22}^{\text{Kubo},\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3) = \int_{k} [\Xi^{(3),\beta\delta\zeta} + \Xi^{(3),\beta\delta} + \Xi^{(3),\beta\zeta} + \Xi^{(3),\delta\zeta} + \Xi^{(3),\beta} + \Pi^{(3),\delta} + \Xi^{(3),\zeta} + \Xi^{(3)}].$$
(F2)

The poles of $\Xi^{(3),...}$ are identical to those of $\Pi^{(3),...}$, with the leading term contributed by $\Xi^{(3),\beta\delta\zeta}$ and $\Xi^{(3),\delta\zeta}$. Hence, the Kubo contribution in DC limit is found as

$$L_{22}^{\text{Kubo},\alpha\beta\delta\zeta}(\omega;\omega_{1},\omega_{2},\omega_{3}) = \sum_{p} \int_{k} \left\{ \frac{-i}{\omega\omega_{[2]}\omega_{3}} v_{p}^{\alpha} \tilde{\varepsilon}_{p}^{2} \partial^{\beta} [\tilde{\varepsilon}_{p} \partial^{\delta} (\tilde{\varepsilon}_{p} \partial^{\zeta} f_{p})] + \frac{1}{4\omega_{[2]}\omega_{3}} (\tilde{\varepsilon}_{p} + \tilde{\varepsilon}_{q}) \mathcal{A}_{qp}^{\beta} [\tilde{\varepsilon}_{q} \tilde{\varepsilon}_{p} \partial^{\delta} (\tilde{\varepsilon}_{p} \partial^{\zeta} f_{p}) - \tilde{\varepsilon}_{q}^{2} \partial^{\delta} (\tilde{\varepsilon}_{q} \partial^{\zeta} f_{q})] \right\},$$

$$-\tilde{\varepsilon}_{q} \tilde{\varepsilon}_{p} \partial^{\delta} (\tilde{\varepsilon}_{q} \partial^{\zeta} f_{q}) + \tilde{\varepsilon}_{p}^{2} \partial^{\delta} (\tilde{\varepsilon}_{p} \partial^{\zeta} f_{p}) - \tilde{\varepsilon}_{q}^{2} \partial^{\delta} (\tilde{\varepsilon}_{q} \partial^{\zeta} f_{q})] \bigg\},$$
(F3)

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which can be written as

$$L_{22,\text{DC}}^{\text{Kubo},\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3) = \sum_p \int_k \left\{ -i \frac{1}{\omega\omega_{[2]}\omega_3} v_p^{\alpha} \tilde{\varepsilon}_p^2 \partial^{\beta} [\tilde{\varepsilon}_p \partial^{\delta} (\tilde{\varepsilon}_p \partial^{\zeta} f_p)] - \frac{1}{\omega_{[2]}\omega_3} \tilde{\varepsilon}_p w_p^{\gamma} \partial^{\delta} (\tilde{\varepsilon}_p \partial^{\zeta} f_p) \right\}.$$
(F4)

The third-order heat magnetization is given as

$$M_Q^{(3),\gamma}(\omega) = \operatorname{Tr}\left[\int_k \rho^{(2)}(\omega)w^{\gamma} - \frac{1}{e^2} \int d\varepsilon \,\tilde{\varepsilon}\sigma^{\gamma}(\varepsilon)\rho^{(2)}(\omega)\right],\tag{F5}$$

and we obtain the third-order thermal-thermal magnetization response

$$L_{22,\text{DC}}^{\text{tr},\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3) = L_{22,D}^{\text{tr},\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3) + L_{22,A}^{\text{tr},\alpha\beta\delta\zeta}(\omega;\omega_1,\omega_2,\omega_3)$$
(F6)

with

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$$L_{22,D}^{\mathrm{tr},\alpha\beta\delta\zeta}(\omega;\omega_{1},\omega_{2},\omega_{3}) = \sum_{p} \int_{k} \frac{-i}{\omega\omega_{[2]}\omega_{3}} v_{p}^{\alpha} \tilde{\varepsilon}_{p}^{2} \partial^{\beta} [\tilde{\varepsilon}_{p} \partial^{\delta} (\tilde{\varepsilon}_{p} \partial^{\zeta} f_{p})],$$

$$L_{22,A}^{\mathrm{tr},\alpha\beta\delta\zeta}(\omega;\omega_{1},\omega_{2},\omega_{3}) = \sum_{p} \int d\varepsilon_{p} \frac{1}{\omega\omega_{2}} \bigg[6\tilde{\varepsilon}_{p}^{2} \frac{\partial f_{p}}{\partial\varepsilon_{p}} + 6\tilde{\varepsilon}_{p}^{3} \frac{\partial^{2} f_{p}}{\partial\varepsilon_{p}^{2}} + \tilde{\varepsilon}_{p}^{4} \frac{\partial^{3} f}{\partial\varepsilon_{p}^{3}} \bigg] v^{\delta}(\varepsilon_{p}) v^{\zeta}(\varepsilon_{p}) \sigma_{p}^{\gamma}(\varepsilon).$$
(F7)

APPENDIX G: SEMICLASSICAL APPROACH

In this Appendix we carefully give the derivation of the nonlinear thermal response through the semiclassical approach. We start with the semiclassical Boltzmann equation, then show that it matches the results from the quantum approach in previous sections. In the last we discuss the symmetries of the nonlinear currents.

The local particle or heat current is contributed by two parts: one is from the motion of the wave-packet center, the other is from the self-rotation of the wave packet, which can be written as

$$J_{N} = \int_{k} f(\varepsilon_{k})\dot{r} + \nabla_{r} \times \int_{k} f(\varepsilon_{k})\boldsymbol{m}(\boldsymbol{k}),$$

$$J_{Q} = \int_{k} (\varepsilon - \mu)f(\varepsilon_{k})\dot{r} + \nabla \times \int_{k} f(\varepsilon_{k})\boldsymbol{m}^{Q}(\boldsymbol{k}), \quad (G1)$$

in which we introduce the energy and thermal magnetic moment

$$\boldsymbol{m}^{E}(\boldsymbol{k}) = \varepsilon_{\boldsymbol{k}}\boldsymbol{m}(\boldsymbol{k}), \quad \boldsymbol{m}^{Q}(\boldsymbol{k}) = \boldsymbol{m}^{E}(\boldsymbol{k}) - \mu \boldsymbol{m}(\boldsymbol{k}).$$
 (G2)

We write the formula of the transport currents again

$$\boldsymbol{J}_{N(Q)}^{\mathrm{tr}} = \boldsymbol{J}_{N(Q)} - \boldsymbol{\nabla} \times \boldsymbol{M}_{N(Q)}. \tag{G3}$$

The total particle magnetization can be derived based on the wave-packet theory using a confining potential [28]

$$\boldsymbol{M}_{N} = \int_{\boldsymbol{k}} f(\varepsilon_{\boldsymbol{k}}) \boldsymbol{m}(\boldsymbol{k}) - \frac{1}{e^{2}} \int d\varepsilon f(\varepsilon) \boldsymbol{\sigma}(\varepsilon), \qquad (\text{G4})$$

in which $\sigma(\varepsilon) = \frac{e^2}{\hbar} \int_k \Theta(\varepsilon - \varepsilon_k) \Omega(k)$ is the zero-temperature Hall conductivity with Fermi energy ε . The thermal magnetization is written as [30]

$$\mathbf{M}^{Q} = \int_{\mathbf{k}} f(\varepsilon_{\mathbf{k}}) \mathbf{m}^{Q}(\mathbf{k}) - \frac{1}{e^{2}} \int d\varepsilon (\varepsilon - \mu) f(\varepsilon) \boldsymbol{\sigma}(\varepsilon). \quad (G5)$$

Note that the first term is from the self-rotation of the wave packet, while the second term is contributed by the edge, as it vanishes in the bulk for a uniform system. Using Eqs. (G4)

and (G5), the transport current is found as

$$\boldsymbol{J}_{N(Q)}^{\text{tr}} = \boldsymbol{J}_{N(Q)}^{D} + \boldsymbol{J}_{N(Q)}^{A}, \tag{G6}$$

where the first term is the Drude contribution

$$\boldsymbol{J}_{N}^{D} = \int_{\boldsymbol{k}} f(\varepsilon_{\boldsymbol{k}})\boldsymbol{v}_{\boldsymbol{k}}, \tag{G7}$$

$$\boldsymbol{I}_{Q}^{D} = \int_{\boldsymbol{k}} (\varepsilon_{\boldsymbol{k}} - \mu) f(\varepsilon_{\boldsymbol{k}}) \boldsymbol{v}_{\boldsymbol{k}}.$$
 (G8)

The second term is from the anomalous term, manifesting itself as the anomalous Nernst (thermal Hall) effect:

$$\boldsymbol{J}_{N}^{A} = -\frac{1}{e^{2}}\boldsymbol{\nabla}\times\int d\varepsilon\,f(\varepsilon)\boldsymbol{\sigma}(\varepsilon),\tag{G9}$$

$$\boldsymbol{J}_{Q}^{A} = -\frac{1}{e^{2}}\boldsymbol{\nabla}\times\int d\boldsymbol{\varepsilon}(\boldsymbol{\varepsilon}-\boldsymbol{\mu})f(\boldsymbol{\varepsilon})\boldsymbol{\sigma}(\boldsymbol{\varepsilon}),\qquad(\text{G10})$$

and the anomalous Hall effect

$$\boldsymbol{J}_{N}^{A} = \frac{e}{\hbar} \boldsymbol{E} \times \int_{\boldsymbol{k}} f(\varepsilon_{\boldsymbol{k}}) \boldsymbol{\Omega}(\boldsymbol{k}). \tag{G11}$$

It is worth noting that the contribution from the particle magnetic moment m(k) cancels out since it is localized and does not contribute to transport.

The Boltzmann equation is given as

$$(\partial t + \dot{\mathbf{r}} \cdot \nabla_{\mathbf{r}} + \dot{\mathbf{k}} \cdot \nabla_{\mathbf{k}})f(\mathbf{r}, \mathbf{k}, t) = \mathcal{I}_{\text{coll}}[f(\mathbf{r}, \mathbf{k}, t)], \quad (G12)$$

where the collision integral $\mathcal{I}_{coll}[f(\mathbf{r}, \mathbf{k}, t)]$ captures the effect of scattering. In the absence of the magnetic field, the equations of motion are given by

$$\dot{\mathbf{r}} = \frac{\partial \varepsilon_k}{\hbar \partial \mathbf{k}} - \dot{\mathbf{k}} \times \mathbf{\Omega}(\mathbf{k}),$$

$$\hbar \dot{\mathbf{k}} = -eE. \qquad (G13)$$

By expanding the distribution function $f = \sum_{n=0}^{\infty} f_n$ by order of temperature gradient ∇T or electric field E, the Hall current at each order is obtained by replacing the distribution function by f_n . Since we are interested in the steady-state solution, the *t* dependence of $f(\mathbf{r}, \mathbf{k}, t)$ is dropped. Perturbed by homogeneous electric field, the Boltzmann equations is

$$-\frac{e}{\hbar}\boldsymbol{E}\cdot\boldsymbol{\nabla}_{\boldsymbol{k}}f(\boldsymbol{k}) = \frac{f_0 - f(\boldsymbol{k})}{\tau}, \qquad (\text{G14})$$

where τ is the relaxation time. The iteration relation is found as

$$f_n^E = \frac{e}{\hbar} \tau E \cdot \nabla_k f_{n-1}^E. \tag{G15}$$

The first two order distribution functions are directly obtained as

$$f_1^E = \frac{e\tau}{\hbar} \frac{\partial f_0}{\partial \varepsilon_k} v_k^{\alpha} E^{\alpha},$$

$$f_2^E = \frac{e^2 \tau^2}{\hbar^2} \left(\frac{\partial f_0}{\partial \varepsilon_k} \frac{\partial v_k^{\alpha}}{\partial k_{\beta}} + \frac{\partial^2 f_0}{\partial \varepsilon_k^2} v_k^{\alpha} v_k^{\beta} \right) E^{\alpha} E^{\beta}. \quad (G16)$$

Following the same procedure, the Boltzmann equation in the presence of temperature gradient is

$$\dot{\boldsymbol{r}} \cdot \boldsymbol{\nabla}_{\boldsymbol{r}} f(\boldsymbol{r}, \boldsymbol{k}) = \frac{f_0 - f(\boldsymbol{r}, \boldsymbol{k})}{\tau}, \qquad (G17)$$

and the iteration relation is found as

$$f_n^T = -\tau \boldsymbol{v}_k \cdot \nabla_r f_{n-1}^T = (-\tau \boldsymbol{v}_k \cdot \nabla_r)^n f_0.$$
 (G18)

The first two order distribution functions are written as

$$f_1^T = \frac{\iota}{\hbar T} \mathcal{F}_1(\varepsilon_k) v_k^{\alpha} \nabla^{\alpha} T,$$

$$f_2^T = \frac{\tau^2}{\hbar T^2} \mathcal{F}_2(\varepsilon_k) v_k^{\alpha} v_k^{\beta} \nabla^{\alpha} T \nabla^{\beta} T,$$
 (G19)

where we define

$$\mathcal{F}_{1}^{T}(\varepsilon_{k}) = (\varepsilon_{k} - \mu) \frac{\partial f_{0}}{\partial \varepsilon_{k}},$$
$$\mathcal{F}_{2}^{T}(\varepsilon_{k}) = \left[2\mathcal{F}_{1}^{T}(\varepsilon_{k}) + (\varepsilon_{k} - \mu)^{2} \frac{\partial^{2} f_{0}}{\partial \varepsilon_{k}^{2}} \right].$$
(G20)

By use of the relation

$$\nabla_r f_0 = -\frac{1}{T} (\varepsilon_k - \mu) \frac{\partial f_0}{\partial \varepsilon_k} \nabla T \qquad (G21)$$

and substituting the formula of f_n^T of Eq. (G19) into Eqs. (G9) and (G10), one obtains the second-order anomalous Nernst (thermal Hall) conductivity

$$\eta^{\gamma\alpha\delta} = -\frac{e\tau}{\hbar^2 T^2} \epsilon^{\alpha\beta\gamma} \int d\varepsilon \, \mathcal{F}_2^T(\varepsilon) v^{\delta}(\varepsilon) \sigma^{\beta}(\varepsilon),$$

$$\kappa^{\gamma\alpha\delta} = \frac{\tau}{\hbar^2 T^2} \epsilon^{\alpha\beta\gamma} \int d\varepsilon (\varepsilon - \mu) \mathcal{F}_2^T(\varepsilon) v^{\delta}(\varepsilon) \sigma^{\beta}(\varepsilon), \quad (G22)$$

in which we assume the temperature is slowly varying in space, and omit the terms that are of nonlinear temperature gradient. Equation (G22) reproduces the formulas derived from the quantum approach in Sec. III.

Now we investigate how the large effective mass limit changes the thermal transport coefficient. According to Eq. (G9), the *n*th-order anomalous currents are given as

$$\mathbf{J}_{N}^{A,(n)} = \frac{1}{\hbar} \nabla \times \int d\varepsilon \, F^{(n-1)}(\varepsilon) \int_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}}) \mathbf{\Omega}(\mathbf{k}), \\
\mathbf{J}_{Q}^{A,(n)} = \frac{1}{\hbar} \nabla \times \int d\varepsilon \, G^{(n-1)}(\varepsilon) \int_{\mathbf{k}} \delta(\varepsilon - \varepsilon_{\mathbf{k}}) \mathbf{\Omega}(\mathbf{k}), \\$$
(G23)

where $F^{(n)}$ and $G^{(n)}$ are the primitive functions of f_1^T and $(\varepsilon - \mu)f_1^T$:

$$F^{(n)} = \int_{-\infty}^{\varepsilon} f^{(n)}(\varepsilon')d\varepsilon', \quad G^{(n)} = \int_{-\infty}^{\varepsilon} (\varepsilon' - \mu)f^{(n)}(\varepsilon')d\varepsilon'.$$
(G24)

Under the large effective mass limit, $F^{(1)}$ and $G^{(1)}$ are found as

$$F^{(1)} \approx \frac{\tau}{T} S(f_0) \boldsymbol{v}_k \cdot \boldsymbol{\nabla} T,$$

$$G^{(1)} \approx \frac{\tau}{T} C(f_0) \boldsymbol{v}_k \cdot \boldsymbol{\nabla} T,$$
(G25)

where we define

$$S(f_0) = f_0 \ln f_0 + (1 - f_0) \ln(1 - f_0),$$

$$C(f_0) = (f_0 - 1) \ln^2(f_0^{-1} - 1) + \ln^2 f_0 + 2 \operatorname{Li}_2 f_0. \quad (G26)$$

Therefore, we have

$$\eta^{\alpha\beta\delta} \approx -\frac{e\tau}{\hbar^2 T^2} \epsilon^{\alpha\beta\gamma} \int d\varepsilon (\varepsilon - \mu)^2 \frac{\partial f_0}{\partial \varepsilon} \\ \times \int_k \delta(\varepsilon - \varepsilon_k) v_k^\delta \Omega(k)^\gamma, \qquad (G27)$$
$$\kappa^{\alpha\beta\delta} \approx \frac{\tau}{\hbar^2 T^2} \epsilon^{\alpha\beta\gamma} \int d\varepsilon (\varepsilon - \mu)^3 \frac{\partial f_0}{\partial \varepsilon} \\ \times \int_k \delta(\varepsilon - \varepsilon_k) v_k^\delta \Omega(k)^\gamma, \qquad (G28)$$

which recovers the results in Ref. [9].

As it is shown above, a group velocity term and a topological term together constitute the conductivity in the DC limit. Let us consider the transformation of these two terms under time-reversal symmetry \mathcal{T} and inversion symmetry \mathcal{I} . For the group velocity term, it is composed of the group velocity or its higher-order derivatives. With the definition $v_p^{\alpha_1...\alpha_n}(\mathbf{k}) \equiv$ $[\prod_{i=1}^n \partial k^{\alpha_i}]\varepsilon_p(\mathbf{k})$, the time reversal \mathcal{T} or the inversion I give

$$v_p^{\alpha_1\dots\alpha_n}(\boldsymbol{k}) = (-)^n v_p^{\alpha_1\dots\alpha_n}(-\boldsymbol{k}).$$
 (G29)

Therefore, the group velocity term in odd-order conductivity is even, leaving the momentum integral vanishes. For example, the group velocity term in the second thermoelectric conductivity is $\Pi^{(2),\beta\delta}$ given by Eq. (118), which is expanded as

$$\Pi^{(2),\beta\delta} = \sum_{p} v_{p}^{\alpha} \frac{1}{\omega} \frac{1}{\omega - \omega_{1}} \bigg(\tilde{\varepsilon}_{p} v_{p}^{\beta} v_{p}^{\delta} \frac{\partial f_{p}}{\partial \varepsilon_{p}} + \tilde{\varepsilon}_{p}^{2} v_{p}^{\beta} v_{p}^{\delta} \frac{\partial^{2} f_{p}}{\partial \varepsilon_{p}^{2}} + \tilde{\varepsilon}_{p}^{2} v_{p}^{\beta\delta} \frac{\partial f_{p}}{\partial \varepsilon_{p}} \bigg).$$
(G30)

Referring to Eq. (G30), it is easy to see that $\Pi^{(2),\beta\delta}$ is odd. The topological terms are functions of Ω_p , m_p , and w_p . The time reversal \mathcal{T} gives

$$\mathbf{\Omega}_p(\mathbf{k}) = -\mathbf{\Omega}_p(-\mathbf{k}), \tag{G31}$$

$$\boldsymbol{m}_p(\boldsymbol{k}) = -\boldsymbol{m}_p(-\boldsymbol{k}), \qquad (G32)$$

$$\boldsymbol{w}_p(\boldsymbol{k}) = -\boldsymbol{w}_p(-\boldsymbol{k}), \tag{G33}$$

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and the inversion \mathcal{I} gives

$$\boldsymbol{\Omega}_p(\boldsymbol{k}) = \boldsymbol{\Omega}_p(-\boldsymbol{k}), \tag{G34}$$

$$\boldsymbol{m}_p(\boldsymbol{k}) = \boldsymbol{m}_p(-\boldsymbol{k}), \tag{G35}$$

$$\boldsymbol{w}_p(\boldsymbol{k}) = \boldsymbol{w}_p(-\boldsymbol{k}). \tag{G36}$$

Therefore, the topological term in odd-order conductivities is odd (even) under $\mathcal{T}(\mathcal{I})$, while this term in even-order conductivities is even (odd) under $\mathcal{T}(\mathcal{I})$.

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