Effects of Berry curvature and orbital magnetic moment on the magnetothermoelectric transport of Bloch electron systems

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Thermoelectric transport coefficients up to linear order in the applied magnetic field are microscopically studied using Kubo-Luttinger linear response theory and thermal Green's functions. We derive exact formulas for the thermoelectric conductivity and thermal conductivity in the limit of small relaxation rates for Bloch electrons in terms of Bloch wave functions, which show that the Sommerfeld-Bethe relationship holds. Our final formula contains the Berry curvature contributions as well as the orbital magnetic moment contributions that arise naturally from the microscopic theory. We show that generalized f-sum rules containing the Berry curvature and orbital magnetic moment play essential roles in taking into account the interband effects of the magnetic field. As an application, we study a model of a gapped Dirac electron system with broken time-reversal symmetry and show the presence of a linear magnetothermopower in such systems.

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I. INTRODUCTION

Inspired by the anomalous velocity [1] related to the Berry curvature in the semiclassical Boltzmann transport equation [2,3], extensive studies of the contributions of the Berry curvature to transport properties [4–22], orbital magnetic moment [23–26], orbital magnetic susceptibility [27–29], and orbital-Zeeman susceptibility [30–32] have been conducted.

In addition to the quantum Hall effect [5,6] the Berry curvature contribution to the anomalous Hall effect was already obtained by Karplus and Luttinger microscopically using perturbation theory [4], although at that time it was not called *Berry curvature*. Similarly, in the case of the orbital magnetic susceptibility, the Berry curvature terms were included in the studies by Hebborn and Sondheimer [33] and by Blount [34]. Actually, the notation of $\mathbf{\Omega}$ for the Berry curvature originates from the paper by Blount [34].

The Berry curvature vanishes in the presence of both inversion symmetry and time-reversal symmetry. In the case of time-reversal symmetry breaking, the typical example of the Berry curvature contribution to the conductivity is the Hall conductivity σ_{xy} in the quantum Hall effect [5,6] and anomalous Hall effect [4]. In contrast, in the diagonal components of the conductivity tensor, such as σ_{xx} and σ_{zz}, anomalous contributions proportional to the applied magnetic field B can appear due to the Berry curvature [7–22,35,36]. [Note that conventional magnetoconductivity is proportional to B^2.]

Furthermore, it has been discussed that the Seebeck coefficient and figure of merit $ZT = S^2\sigma T/\kappa$ can also be enhanced in the presence of a magnetic field [37–40]. Therefore, a microscopic understanding of thermoelectric conductivity in the presence of a magnetic field is also important for applications such as thermoelectric devices.

Recently, we calculated the magnetoconductivity in terms of thermal Green's functions [15] based on Fukuyama's formula [41] and found that there are contributions from the Berry curvature $\Omega^a_{\mu\nu}$ and orbital magnetic moment $M^a_{\mu\nu}$ in $\sigma_{\mu\nu}(B)$ at linear order in B. Here, a represents the band index, and $\mu, \nu = x, y$, or z. The orbital magnetic moment $M^a_{\mu\nu}$ expressed by Eq. (19) is absent in the Boltzmann transport theory with anomalous velocities. To discuss transport properties, microscopic calculations using Kubo's linear response theory and thermal Green's functions are very important. A similar situation also appeared in the studies on orbital magnetic susceptibility $\chi_{\rm orb}$. Gao *et al.* [27] studied $\chi_{\rm orb}$ using the semiclassical Boltzmann transport theory with Berry curvature and found that $\chi_{\rm orb}$ can be expressed in terms of various contributions, including the Berry curvature contributions. However, it has been shown that some of the obtained coefficients of the contributions do not agree with the microscopically obtained results [29,33].

In this paper, we give a fully microscopic description of the thermoelectric transport coefficients that can be used to validate the results obtained using semiclassical Boltzmann transport theory [7–13,16,18,20–22]. We do this by extending our previous microscopic theory for the conductivity [15] to thermoelectric and thermal conductivities.

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In the classical Boltzmann transport theory, the following relation between the transport coefficients L_{11}, L_{12}, and L_{22} holds:

$$
\begin{aligned}
L_{11} &= \int_{-\infty}^{\infty} d\varepsilon[-f'(\varepsilon)]\sigma(\varepsilon, T),\\
L_{12} = L_{21} &= \frac{1}{e}\int_{-\infty}^{\infty} d\varepsilon(\varepsilon-\mu)[-f'(\varepsilon)]\sigma(\varepsilon, T),\\
L_{22} &= \frac{1}{e^2}\int_{-\infty}^{\infty} d\varepsilon(\varepsilon-\mu)^2[-f'(\varepsilon)]\sigma(\varepsilon, T),
\end{aligned}
\tag{1}
$$

which we call the Sommerfeld-Bethe relation. Here, e (< 0) is the charge of an electron, and $f(\varepsilon)$ is the Fermi distribution function, $f(\varepsilon) = 1/[e^{\beta(\varepsilon-\mu)} + 1]$, with $\beta = 1/k_{\rm B}T$. One of the issues to be studied is whether or not this kind of relation holds under the magnetic field and for the contributions from the Berry curvature that do not have $f'(\varepsilon)$ but $f(\varepsilon)$. In this paper, we derive $L^{12}_{\mu\nu}$ and $L^{22}_{\mu\nu}$ up to linear order in the external magnetic field using Kubo-Luttinger linear response theory and thermal Green's functions. Compared with the calculation of the magnetic susceptibility [29,42], which is a thermodynamic quantity, in the present calculation of $L^{ij}_{\mu\nu}$, the finite-frequency Green's functions will be carefully taken into account since $L^{ij}_{\mu\nu}$ is a dynamical quantity.

In Sec. II, we introduce our model and define the current and heat current operators, $\boldsymbol{j}(\boldsymbol{r})$ and $\boldsymbol{j}_Q(\boldsymbol{r})$. Using the imaginary time interaction representation, we show a specific relationship between $\boldsymbol{j}(\boldsymbol{r}, \tau, \tau')$ and $\boldsymbol{j}_Q(\boldsymbol{r}, \tau, \tau')$, which will be used later. In Sec. III, we define the electronic and thermoelectric linear response functions $L^{ij}_{\mu\nu}$ represented by the analytic continuation of the correlation functions. We show our final results in Eq. (17) before describing the details of the calculation. In Sec. IV, we calculate the correlation functions at linear order in the magnetic field. Since we use the general Bloch band representation, there are seven contributions depending on the interband matrix elements of the current operator, as shown in Fig. 1. Then, we calculate each contribution by taking the leading and subleading orders with respect to Γ^{ℓ} ($\ell = -2$ and -1) assuming for the relaxation rate Γ of electrons is small. The results at the leading order of $O(\Gamma^{-2})$ are shown in Sec. IV A, where we reproduce the results in the Boltzmann theory for the Hall conductivity. We also derive a generalized f-sum rule that contains the orbital magnetic moment, which is used for summing up the interband contributions. The results for the subleading order of $O(\Gamma^{-1})$ are summarized in Sec. IV B, where another generalized f-sum rule containing the Berry curvature is derived and used. In Sec. V, we study a simple two-band model that shows an anomalous linear-B behavior of the diagonal components of the linear response functions. We show the Seebeck coefficient, thermal conductivity, Lorenz number, power factor, and figure of merit zT for this model. We summarize our results in Sec. VI. The details of the calculations are shown in the Appendixes.

II. MODEL, CURRENT, AND HEAT CURRENT OPERATORS

We consider Bloch electrons in a periodic potential $V(\boldsymbol{r})$ and spin-orbit interactions using the following Hamiltonian

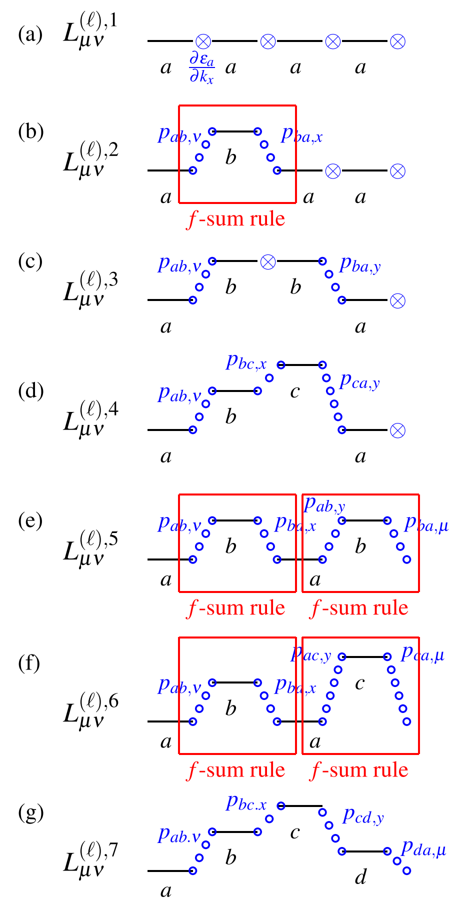

FIG. 1. Schematic representation of the contributions to $L^{(\ell),1}_{\mu\nu}$-$L^{(\ell),7}_{\mu\nu}$: The solid lines with band indices a, b, etc., represent the Green's functions. The height of these lines represents the energy level ε_a. The array of blue circles connecting the two lines represents the off-diagonal (or interband) matrix elements of γ_μ, i.e., $p_{ab,\mu}$. The symbol $\otimes$ between two solid lines represents the diagonal (or intraband) component of γ_μ, i.e., $\partial\varepsilon_a/\partial k_\mu$. The right side of each diagram is connected to its left side because of the trace in (25). The red squares indicate the parts of the diagrams which can be expressed by the f-sum rule in Eq. (34).

derived from the Dirac equation with nonrelativistic expansion:

$$
\begin{aligned}
\mathcal{H} &= \int d\boldsymbol{r}\psi^{\dagger}(\boldsymbol{r})H(\boldsymbol{r})\psi(\boldsymbol{r}),\\
H(\boldsymbol{r}) &= \frac{1}{2m}\boldsymbol{p}^2 + V(\boldsymbol{r}) + \frac{\hbar^2}{8m^2c^2}\nabla^2 V(\boldsymbol{r}) - \frac{e\hbar}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{b}(\boldsymbol{r})\\
&\quad + \frac{\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot\nabla V\times\boldsymbol{p},
\end{aligned}
\tag{2}
$$

where $\boldsymbol{p} = -i\hbar\nabla$, σ_i are the Pauli matrices representing spin, and $\psi(\boldsymbol{r})$ $[\psi^{\dagger}(\boldsymbol{r})]$ is the two-component electron annihilation (creation) field operator. An effective field $\boldsymbol{b}(\boldsymbol{r})$ is phenomenologically introduced which breaks time-reversal symmetry. The last term represents the spin-orbit interaction in a general form. We treat the general case where $V(\boldsymbol{r})$ is a noncentrosymmetric potential [i.e., $V(-\boldsymbol{r}) \neq V(\boldsymbol{r})$], similar to what was done in Ref. [29].

We take the Bloch wave functions in the form $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_{a,\boldsymbol{k}}(\boldsymbol{r})$, which satisfy

$$H_{\boldsymbol{k}}u_{a,\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon_a(\boldsymbol{k})u_{a,\boldsymbol{k}}(\boldsymbol{r}). \tag{3}$$

Here, a indicates the band index including the pseudospin degrees of freedom, and $H_{\boldsymbol{k}} := e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}H(\boldsymbol{r})e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ is given by

$$\begin{aligned} H_{\boldsymbol{k}} = {}& \frac{\hbar^2k^2}{2m} - \frac{i\hbar^2}{m}\boldsymbol{k}\cdot\nabla - \frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) + \frac{\hbar^2}{8m^2c^2}\nabla^2 V \\ & - \frac{e\hbar}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{b} + \frac{\hbar^2}{4m^2c^2}\boldsymbol{\sigma}\cdot\nabla V\times(\boldsymbol{k}-i\nabla) \end{aligned} \tag{4}$$

in the present Hamiltonian in Eq. (2). Note that the function $u_{a,\boldsymbol{k}}(\boldsymbol{r})$ is a two-component vector (representing the spin degrees of freedom), which is periodic with the same period as $V(\boldsymbol{r})$.

The current operator $\boldsymbol{j}(\boldsymbol{r})$ and the energy current operator $\boldsymbol{j}_E(\boldsymbol{r})$ are defined via the continuity equations [43]

$$\begin{aligned} &\frac{d}{dt}e\rho(\boldsymbol{r}) + \mathrm{div}\boldsymbol{j}(\boldsymbol{r}) = 0, \\ &\frac{d}{dt}h(\boldsymbol{r}) + \mathrm{div}\boldsymbol{j}_E(\boldsymbol{r}) = 0, \end{aligned} \tag{5}$$

where $\rho(\boldsymbol{r}) = \psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})$ represents the electron density operator and $h(\boldsymbol{r}) = \frac{1}{2}\psi^\dagger(\boldsymbol{r})\{H(\boldsymbol{r}) + \overleftarrow{H}(\boldsymbol{r})\}\psi(\boldsymbol{r})$ is the symmetrized Hamiltonian density operator. Here, $\overleftarrow{H}(\boldsymbol{r})$ is defined by replacing the operator $p_j = -i\hbar\partial_j$ $(j = x, y, z)$ in $H(\boldsymbol{r})$ with $\overleftarrow{p_j} := i\hbar\overleftarrow{\partial_j}$, where $\overleftarrow{\partial_j}$ represents the partial derivative with respect to j that acts on the functions and operators on its left-hand side. The heat current operator is given by $\boldsymbol{j}_Q(\boldsymbol{r}) = \boldsymbol{j}_E(\boldsymbol{r}) - \mu\boldsymbol{j}(\boldsymbol{r})/e$, with μ being the chemical potential.

Using the continuity equations, we obtain

$$\begin{aligned} &\boldsymbol{j}(\boldsymbol{r}) = e\psi^\dagger(\boldsymbol{r})\overleftrightarrow{\boldsymbol{j}_0}(\boldsymbol{r})\psi(\boldsymbol{r}), \\ &\boldsymbol{j}_E(\boldsymbol{r}) = \tfrac{1}{2}\psi^\dagger(\boldsymbol{r})\{\overleftrightarrow{\boldsymbol{j}_0}(\boldsymbol{r})H(\boldsymbol{r}) + \overleftarrow{H}(\boldsymbol{r})\overleftrightarrow{\boldsymbol{j}_0}(\boldsymbol{r})\}\psi(\boldsymbol{r}), \end{aligned} \tag{6}$$

with

$$\overleftrightarrow{\boldsymbol{j}_0}(\boldsymbol{r}) = \frac{1}{2m}(-i\hbar\nabla + i\hbar\overleftarrow{\nabla}) + \frac{\hbar}{4m^2c^2}\boldsymbol{\sigma}\times\nabla V. \tag{7}$$

The derivation including the case with the vector potential is given in Appendix A. We can show that the heat current and the electric current operator are related to each other [44,45]. Defining the imaginary time interaction representation of the electric current operator as

$$\boldsymbol{j}(\boldsymbol{r},\tau,\tau') = e\psi^\dagger(\boldsymbol{r},\tau)\overleftrightarrow{\boldsymbol{j}_0}(\boldsymbol{r})\psi(\boldsymbol{r},\tau'), \tag{8}$$

with $\psi^\dagger(\boldsymbol{r},\tau) = e^{\tau(\mathcal{H}-\mu N)}\psi^\dagger(\boldsymbol{r})e^{-\tau(\mathcal{H}-\mu N)}$ and $\psi(\boldsymbol{r},\tau') = e^{\tau'(\mathcal{H}-\mu N)}\psi(\boldsymbol{r})e^{-\tau'(\mathcal{H}-\mu N)}$, it can be shown that

$$\frac{1}{2e}\left(\frac{\partial}{\partial\tau} - \frac{\partial}{\partial\tau'}\right)\boldsymbol{j}(\boldsymbol{r},\tau,\tau') = \boldsymbol{j}_Q(\boldsymbol{r},\tau,\tau'), \tag{9}$$

where $\boldsymbol{j}_Q(\boldsymbol{r},\tau,\tau')$ is the similarly defined imaginary time interaction representation of the heat current operator, $\boldsymbol{j}_Q(\boldsymbol{r}) = \boldsymbol{j}_E(\boldsymbol{r}) - \mu\boldsymbol{j}(\boldsymbol{r})/e$ (see also Appendix A). This type of relationship was used by Jonson and Mahan [44] to show the Sommerfeld-Bethe relationship (1) between the electric conductivity and thermoelectric conductivity [45]. Note that, when there is electron-phonon interaction or finite-range mutual interaction between electrons, the relation in Eq. (9) does not hold [45]. In the Hamiltonian (2), Eq. (9) does hold even in the presence of the spin-orbit interaction. In the following sections, we will show that the Sommerfeld-Bethe relationship in Eq. (1) holds even in the presence of a magnetic field, where the heat current operator also depends on the magnetic field.

The current density in terms of the Bloch wave functions is

$$(j_\mu)_{ab} = e\int u^\dagger_{a,\boldsymbol{k}}(\boldsymbol{r})e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\overleftrightarrow{j_{0,\mu}}(\boldsymbol{r})e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_{b,\boldsymbol{k}}(\boldsymbol{r})d\boldsymbol{r}. \tag{10}$$

We define $(\gamma_\mu)_{ab} = \frac{\hbar}{e}(j_\mu)_{ab}$. Using the definition of $H_{\boldsymbol{k}}$ in Eq. (4) and the k_μ derivative of $(\varepsilon_a - H)|a\rangle = 0$, we obtain

$$\begin{aligned} &(\gamma_\mu)_{ab} = \langle a|\partial_\mu H|b\rangle = \partial_\mu\varepsilon_a\delta_{ab} + p_{ab,\mu}, \\ &p_{ab,\mu} := (\varepsilon_b - \varepsilon_a)\langle a|\partial_\mu b\rangle, \end{aligned} \tag{11}$$

where $|a\rangle = u_{a,\boldsymbol{k}}(\boldsymbol{r})$, $\partial_\mu H = \partial H_{\boldsymbol{k}}/\partial k_\mu$, $\partial_\mu\varepsilon_a = \partial\varepsilon_a/\partial k_\mu$, $|\partial_\mu a\rangle = \partial u_{a,\boldsymbol{k}}(\boldsymbol{r})/\partial k_\mu$, and the wave number $\boldsymbol{k}$ dependence is not shown explicitly since it is common in all the expressions. Apparently, $p_{ab,\mu}$ is closely related to the interband Berry connection.

III. TRANSPORT COEFFICIENTS

The electric and thermoelectric linear response functions are defined as

$$\begin{aligned} &\langle j_\mu\rangle = \sum_\nu L^{11}_{\mu\nu}E_\nu + L^{12}_{\mu\nu}\left(-\frac{\partial_\nu T}{T}\right), \\ &\langle j_{Q,\mu}\rangle = \sum_\nu L^{21}_{\mu\nu}E_\nu + L^{22}_{\mu\nu}\left(-\frac{\partial_\nu T}{T}\right) \end{aligned} \tag{12}$$

for $\mu,\nu = x, y, z$, where $L^{11}_{\mu\nu}$ is the usual electric conductivity tensor, $L^{12}_{\mu\nu}$ and $L^{21}_{\mu\nu}$ are the thermoelectric and electrothermal conductivities, and the thermal conductivity is obtained from $L^{22}_{\mu\nu}$. The observable quantities can be computed as

$$\begin{aligned} \sigma &= \mathbf{L}_{11}, \\ S &= \frac{1}{T}\mathbf{L}^{-1}_{11}\mathbf{L}_{12}, \\ \kappa &= \frac{1}{T}[\mathbf{L}_{22} - \mathbf{L}_{21}\mathbf{L}^{-1}_{11}\mathbf{L}_{12}], \end{aligned} \tag{13}$$

where σ is the electric conductivity tensor, S is the Seebeck tensor, and κ is the thermal conductivity tensor.

In the linear response theory or in the Kubo formula, the conductivity $L^{11}_{\mu\nu}$ is obtained as

$$L^{11}_{\mu\nu} = \lim_{\omega\to 0}\frac{1}{i(\omega+i\delta)}\{\tilde{\Phi}^{11}_{\mu\nu}(\omega+i\delta) - \tilde{\Phi}^{11}_{\mu\nu}(0)\}, \tag{14}$$

where $\tilde{\Phi}^{11}_{\mu\nu}(\omega+i\delta)$ is the analytic continuation of the current-current correlation function

$$\Phi^{11}_{\mu\nu}(i\omega_\lambda) = \frac{1}{V}\int_0^\beta d\tau\langle j_{\boldsymbol{k}=\boldsymbol{0},\mu}(\tau)j_{\boldsymbol{k}=\boldsymbol{0},\nu}(0)\rangle e^{i\omega_\lambda\tau}, \tag{15}$$

with $i\omega_\lambda \to \hbar(\omega+i\delta)$ and δ being an infinitesimally small parameter. Here, $\beta = 1/k_\mathrm{B}T$, $\omega_\lambda = 2\pi\lambda k_\mathrm{B}T$ is the Matsubara frequency, with $\lambda \in \mathbb{Z}$, and $j_{\boldsymbol{k},\mu}(\tau)$ is the μ component of the Fourier transform of the current density operator, defined as

$$\boldsymbol{j}_{\boldsymbol{k}}(\tau) = \int d\boldsymbol{r}\boldsymbol{j}(\boldsymbol{r},\tau,\tau)e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}. \tag{16}$$

The other linear response coefficients, $L^{12}_{\mu\nu} = L^{21}_{\mu\nu}$ and $L^{22}_{\mu\nu}$, are similarly obtained using the heat current operators. We calculate them at linear order in the applied magnetic field B in the z direction. Since the calculation is lengthy and complicated, we show our final results beforehand. Expressing $L^{11}_{\mu\nu}$, $L^{12}_{\mu\nu}$, and $L^{22}_{\mu\nu}$ as $L^{(0)}_{\mu\nu}$, $L^{(1)}_{\mu\nu}$, and $L^{(2)}_{\mu\nu}$, respectively, we obtain

$$\begin{aligned} L^{(\ell)}_{\mu\nu} = &-\frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a}(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)\bigg[\frac{1}{8\Gamma^2}\{\partial_\mu\varepsilon_a\partial_x\varepsilon_a(\partial_\nu\partial_y\varepsilon_a) - \partial_\mu\varepsilon_a\partial_y\varepsilon_a(\partial_\nu\partial_x\varepsilon_a) \\ &- \partial_\nu\varepsilon_a\partial_x\varepsilon_a(\partial_\mu\partial_y\varepsilon_a) + \partial_\nu\varepsilon_a\partial_y\varepsilon_a(\partial_\mu\partial_x\varepsilon_a)\} - \frac{1}{2\Gamma}\big(\partial_\mu\varepsilon_a\partial_\nu\varepsilon_a\Omega^a_{xy} - \partial_\mu\varepsilon_a\partial_x\varepsilon_a\Omega^a_{\nu y} + \partial_\mu\varepsilon_a\partial_y\varepsilon_a\Omega^a_{\nu x} \\ &- \partial_\nu\varepsilon_a\partial_x\varepsilon_a\Omega^a_{\mu y} + \partial_\nu\varepsilon_a\partial_y\varepsilon_a\Omega^a_{\mu x}\big) - \frac{1}{4\Gamma}\{\partial_\mu\varepsilon_a\partial_\nu M_{xy} + \partial_\nu\varepsilon_a\partial_\mu M_{xy} - 2(\partial_\mu\partial_\nu\varepsilon_a)M_{xy}\}\bigg] + O(\Gamma^0) \quad (\ell = 0,1,2), \end{aligned} \tag{17}$$

where Γ is the relaxation rate of electrons and ∂_μ represents the partial derivative $\partial/\partial k_\mu$. Here, we calculate the transport coefficients $L^{(\ell)}_{\mu\nu}$ in the power expansion with respect to Γ^{-n} assuming Γ is small compared with the Fermi energy. The contribution proportional to $1/\Gamma^2$ is exactly the same as the result of the Boltzmann transport theory. The contributions proportional to $1/\Gamma$ are related to the Berry curvature for band a,

$$\Omega^a_{\mu\nu} := -2\mathrm{Im}\langle\partial_\mu a|\partial_\nu a\rangle = i\{\langle\partial_\mu a|\partial_\nu a\rangle - \langle\partial_\nu a|\partial_\mu a\rangle\}, \tag{18}$$

as well as the orbital magnetic moment,

$$\begin{aligned} M^a_{\mu\nu} &:= \mathrm{Im}\langle\partial_\mu a|\varepsilon_a - H_{\boldsymbol{k}}|\partial_\nu a\rangle \\ &= \frac{1}{2i}\big(\langle\partial_\mu a|\varepsilon_a - H_{\boldsymbol{k}}|\partial_\nu a\rangle - \langle\partial_\nu a|\varepsilon_a - H_{\boldsymbol{k}}|\partial_\mu a\rangle\big). \end{aligned} \tag{19}$$

When we define

$$\begin{aligned} \sigma(\varepsilon,T) = &-\frac{e^3B}{\hbar^2 V}\sum_{\boldsymbol{k},a}\delta(\varepsilon-\varepsilon_a)\bigg[\frac{1}{8\Gamma^2}\{\partial_\mu\varepsilon_a\partial_x\varepsilon_a(\partial_\nu\partial_y\varepsilon_a) - \partial_\mu\varepsilon_a\partial_y\varepsilon_a(\partial_\nu\partial_x\varepsilon_a) \\ &- \partial_\nu\varepsilon_a\partial_x\varepsilon_a(\partial_\mu\partial_y\varepsilon_a) + \partial_\nu\varepsilon_a\partial_y\varepsilon_a(\partial_\mu\partial_x\varepsilon_a)\} - \frac{1}{2\Gamma}\big(\partial_\mu\varepsilon_a\partial_\nu\varepsilon_a\Omega^a_{xy} - \partial_\mu\varepsilon_a\partial_x\varepsilon_a\Omega^a_{\nu y} + \partial_\mu\varepsilon_a\partial_y\varepsilon_a\Omega^a_{\nu x} \\ &- \partial_\nu\varepsilon_a\partial_x\varepsilon_a\Omega^a_{\mu y} + \partial_\nu\varepsilon_a\partial_y\varepsilon_a\Omega^a_{\mu x}\big) - \frac{1}{4\Gamma}\{\partial_\mu\varepsilon_a\partial_\nu M_{xy} + \partial_\nu\varepsilon_a\partial_\mu M_{xy} - 2(\partial_\mu\partial_\nu\varepsilon_a)M_{xy}\}\bigg], \end{aligned} \tag{20}$$

we can easily see that the Sommerfeld-Bethe relation in Eq. (1) holds.

Let us note here a problem in transverse thermoelectric transport [46–51]. In the case of transverse thermoelectric transport, a term appears which diverges as $1/T$ as $T \to 0$. This nonphysical divergence is removed by considering the local equilibrium current [51], which is of order Γ^0 since the local equilibrium current does not depend on the relaxation. Although the same problem will appear in the present formalism, it appears only at orders higher than the ones discussed in this paper, Γ^{-2} and Γ^{-1}, as shown in Eq. (17).

IV. CORRELATION FUNCTIONS AT LINEAR ORDER IN THE MAGNETIC FIELD

In the presence of a magnetic field, Fukuyama [41,52] obtained an exact formula for the Hall conductivity, or $\Phi^{11}_{xy}(i\omega_\lambda)$, expressed in terms of thermal Green's functions in a gauge-invariant form using a finite-momentum vector potential $\boldsymbol{A}(\boldsymbol{r}) = e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\boldsymbol{A}_{\boldsymbol{q}}$. Recently, in Ref. [15] we simplified the formula of $\Phi^{11}_{xy}(i\omega_\lambda)$ and furthermore calculated the formula for the other components such as $\Phi^{11}_{zz}(i\omega_\lambda)$. In the present paper, we study $\Phi^{11}_{\mu\nu}(i\omega_\lambda)$, $\Phi^{12}_{\mu\nu}(i\omega_\lambda)$, and $\Phi^{22}_{\mu\nu}(i\omega_\lambda)$ for all the components $\mu,\nu = x,y,z$ in a unified way. As shown in Appendix B, the correlation function $\Phi^{11}_{\mu\nu}(i\omega_\lambda)$ at linear order in the magnetic field can be simplified as

$$\begin{aligned} \Phi^{11}_{\mu\nu}(i\omega_\lambda) &= -\frac{k_BT}{V}\sum_{n,\boldsymbol{k}}\frac{ie^3B}{\hbar^3}\mathrm{Tr}\,F(\boldsymbol{k},i\varepsilon_n,i\omega_\lambda), \\ F(\boldsymbol{k},i\varepsilon_n,i\omega_\lambda) &= \frac{\hbar^2}{2m}\big[\delta_{\mu y}(\mathcal{G}_+\gamma_\nu\mathcal{G}\gamma_x\mathcal{G} - \mathcal{G}_+\gamma_x\mathcal{G}_+\gamma_\nu\mathcal{G}) \\ &\quad + \delta_{\nu x}(\gamma_\mu\mathcal{G}_+\mathcal{G}\gamma_y\mathcal{G} - \gamma_\mu\mathcal{G}_+\gamma_y\mathcal{G}_+\mathcal{G})\big] \\ &\quad + \gamma_\mu\mathcal{G}_+\gamma_\nu\mathcal{G}\gamma_x\mathcal{G}\gamma_y\mathcal{G} - \gamma_\mu\mathcal{G}_+\gamma_y\mathcal{G}_+\gamma_x\mathcal{G}_+\gamma_\nu\mathcal{G}, \end{aligned} \tag{21}$$

where the magnetic field B is applied in the z direction without loss of generality. The summation of the wave vector $\boldsymbol{k}$ is taken within the first Brillouin zone, the summation of n represents the Matsubara frequency summation, and the trace (Tr) is taken over all the eigenstates of the Bloch states including the spin degrees of freedom. Note that the simplified formula for $\Phi_{xy}^{11}(i\omega_\lambda)$ enables us to show the close relationship between the orbital magnetic susceptibility and part of the Hall conductivity [53].

The thermal Green's function $\mathcal{G}$ is band-index diagonal, which has the form

$$\mathcal{G}_a(\boldsymbol{k}, \varepsilon_n) = \frac{1}{i\varepsilon_n - \varepsilon_a(\boldsymbol{k}) + \mu + i\Gamma \mathrm{sign}(\varepsilon_n)}, \tag{22}$$

where $\varepsilon_n = (2n+1)\pi k_{\mathrm{B}}T$ is the fermion Matsubara frequency and we have abbreviated $\mathcal{G}(\boldsymbol{k}, i\varepsilon_n + i\omega_\lambda) \to \mathcal{G}_+$ as $\mathcal{G}(\boldsymbol{k}, i\varepsilon_n) \to \mathcal{G}$. Here, we have assumed the case with simple random impurities that have δ-function potentials for simplicity. In this case, the self-energy can be approximated as $-i\Gamma \mathrm{sgn}(\varepsilon_n)$, and the vertex corrections due to impurity scattering are safely neglected. This is the simplest assumption, and for actual models, we have to modify the self-energy depending on the explicit model, which remains as an extension of the present theory. In the following, we evaluate the transport coefficients in the expansion with respect to Γ^n assuming that $\Gamma \ll \varepsilon_{\mathrm{F}}$.

In Ref. [15] we calculated the conductivity tensors $L_{\mu\nu}^{11}$ using Eq. (21). In the present paper, we discuss $L_{\mu\nu}^{12}$, $L_{\mu\nu}^{21}$, and $L_{\mu\nu}^{22}$. For example, the electrothermal conductivity $L_{\mu\nu}^{21}$ can be obtained from the analytic continuation $[i\omega_\lambda \to \hbar(\omega + i\delta)]$ of

$$\Phi_{\mu\nu}^{21}(i\omega_\lambda) = \frac{1}{V}\int_0^\beta d\tau \langle j_{Q,\boldsymbol{k}=\boldsymbol{0},\mu}(\tau) j_{\boldsymbol{k}=\boldsymbol{0},\nu}(0)\rangle e^{i\omega_\lambda \tau}, \tag{23}$$

where $j_{Q,\boldsymbol{k},\mu}(\tau)$ is defined as

$$\boldsymbol{j}_{Q,\boldsymbol{k}}(\tau) = \int d\boldsymbol{r} \boldsymbol{j}_Q(\boldsymbol{r}, \tau, \tau) e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}. \tag{24}$$

Because $\boldsymbol{j}_Q(\boldsymbol{r}, \tau, \tau)$ is related to the current operator $\boldsymbol{j}(\boldsymbol{r}, \tau, \tau)$ as in Eq. (9), we can show that each Feynman diagram to calculate Eq. (23) contains the τ derivatives of the thermal Green's functions. [Note that the relation in Eq. (9) also holds even in the presence of magnetic field, as shown in Appendix A.] Since the τ derivatives yield the Matsubara frequencies of the Green's functions, we find

$$\begin{aligned}
\Phi_{\mu\nu}^{12}(i\omega_\lambda) &= -\frac{k_{\mathrm{B}}T}{V}\sum_{n,\boldsymbol{k}} \frac{ie^2 B}{\hbar^3}\left(i\varepsilon_n + \frac{i\omega_\lambda}{2}\right) \mathrm{Tr}\, F(\boldsymbol{k}, i\varepsilon_n, i\omega_\lambda), \\
\Phi_{\mu\nu}^{21}(i\omega_\lambda) &= \Phi_{\mu\nu}^{12}(i\omega_\lambda), \\
\Phi_{\mu\nu}^{22}(i\omega_\lambda) &= -\frac{k_{\mathrm{B}}T}{V}\sum_{n,\boldsymbol{k}} \frac{ieB}{\hbar^3}\left(i\varepsilon_n + \frac{i\omega_\lambda}{2}\right)^2 \mathrm{Tr}\, F(\boldsymbol{k}, i\varepsilon_n, i\omega_\lambda).
\end{aligned} \tag{25}$$

Note that the additional factor $(i\varepsilon_n + i\omega_\lambda/2)^\ell$ ($\ell = 1, 2$) does not depend on the wave numbers, so the gauge-invariance argument in Ref. [41] that uses the $\boldsymbol{k}$ dependence of Green's functions and current operators is not affected.

Like for the conductivity expressed in Ref. [15], we express the transport coefficients as

$$\begin{aligned}
L_{\mu\nu}^{(\ell)} = \frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k}} &\frac{\hbar^2}{2m}\delta_{\mu y}\left\{(\gamma_\nu)_{ab}(\gamma_x)_{ba}C_{aba}^{(\ell)} - (\gamma_x)_{ab}(\gamma_\nu)_{ba}\tilde{C}_{aba}^{(\ell)}\right\} + \frac{\hbar^2}{2m}\delta_{\nu x}\left\{(\gamma_y)_{ab}(\gamma_\mu)_{ba}C_{aab}^{(\ell)} - (\gamma_\mu)_{ab}(\gamma_y)_{ba}\tilde{C}_{baa}^{(\ell)}\right\} \\
&+ (\gamma_\mu)_{da}(\gamma_\nu)_{ab}(\gamma_x)_{bc}(\gamma_y)_{cd}D_{abcd}^{(\ell)} - (\gamma_\mu)_{ad}(\gamma_y)_{dc}(\gamma_x)_{cb}(\gamma_\nu)_{ba}\tilde{D}_{dcba}^{(\ell)},
\end{aligned} \tag{26}$$

where ℓ is defined using the indices of the transport coefficients $\mathbf{L}_{ij}$ as $\ell = i + j - 2$. The $C_{abc}^{(\ell)}$ and $D_{abcd}^{(\ell)}$ ($\ell = 0, 1, 2$) functions are defined as

$$\begin{aligned}
C_{abc}^{(\ell)} &= -\lim_{\omega\to 0}\frac{k_{\mathrm{B}}T}{\hbar\omega}\sum_n \left(i\varepsilon_n + \frac{i\omega_\lambda}{2}\right)^\ell (\mathcal{G}_+)_a(\mathcal{G})_b(\mathcal{G})_c, \\
\tilde{C}_{cba}^{(\ell)} &= -\lim_{\omega\to 0}\frac{k_{\mathrm{B}}T}{\hbar\omega}\sum_n \left(i\varepsilon_n + \frac{i\omega_\lambda}{2}\right)^\ell (\mathcal{G}_+)_c(\mathcal{G}_+)_b(\mathcal{G})_a, \\
D_{abcd}^{(\ell)} &= -\lim_{\omega\to 0}\frac{k_{\mathrm{B}}T}{\hbar\omega}\sum_n \left(i\varepsilon_n + \frac{i\omega_\lambda}{2}\right)^\ell (\mathcal{G}_+)_a(\mathcal{G})_b(\mathcal{G})_c(\mathcal{G})_d, \\
\tilde{D}_{dcba}^{(\ell)} &= -\lim_{\omega\to 0}\frac{k_{\mathrm{B}}T}{\hbar\omega}\sum_n \left(i\varepsilon_n + \frac{i\omega_\lambda}{2}\right)^\ell (\mathcal{G}_+)_d(\mathcal{G}_+)_c(\mathcal{G}_+)_b(\mathcal{G})_a,
\end{aligned} \tag{27}$$

where the substitution of $i\omega_\lambda \to \hbar(\omega + i\delta)$ should be made in the thermal Green's functions after taking the Matsubara summations.

The explicit forms of these functions are shown in Appendix C, where they are expressed in terms of the retarded and advanced Green's functions and the Fermi distribution function. We can see that the relations

$$\left[\tilde{C}_{cba}^{(\ell)}\right]^* = -C_{\mathrm{abc}}^{(\ell)}, \quad \left[\tilde{D}_{dcba}^{(\ell)}\right]^* = -D_{abcd}^{(\ell)} \tag{28}$$

hold, which guarantees that the transport coefficients are real.

Because the matrix elements of γ_μ in Eq. (11) have two terms, several types of contributions in $L_{\mu\nu}^{(\ell)}$ in Eq. (26) come from different combinations of these two terms. In particular, the contributions containing $D_{abcd}^{(\ell)}$ (i.e., the case with four Green's functions) are shown in Fig. 1. (Similar diagrams for $C_{abc}^{(\ell)}$ and $\tilde{C}_{abc}^{(\ell)}$ can be drawn, which we do not show here.) The diagrams in Fig. 1 are similar to those discussed in the case of the orbital magnetic susceptibility [42]. As we will see later, part of the infinite summations is carried out by using the f-sum rule, which is indicated by the red squares in Fig. 1.

When we add all the diagrams in Fig. 1, we obtain the transport coefficients, which are valid for any strength of the scattering rate Γ. We noted in Ref. [15] that, if we take the leading and subleading order contributions with respect to Γ^ℓ, we can express $L_{\mu\nu}^{(0)}$ in terms of the Berry curvature and the orbital magnetic moment. In the following, we use a similar procedure to obtain $L_{\mu\nu}^{(1)}$ and $L_{\mu\nu}^{(2)}$ in general. Note that, in the case of the orbital magnetic susceptibility [42], the contributions of the diagrams like those in Fig. 1 can be summed. In that case, it is not necessary to introduce the relaxation rate Γ because the susceptibility is a thermodynamic quantity. In other words, the calculation for the susceptibility is carried out at order Γ^0. In contrast, for the transport quantities, transport coefficients diverge for $\Gamma \to 0$, and we have to take into account the contributions proportional to Γ^{-2} and Γ^{-1}, as we show below.

First, we evaluate $C^{(\ell)}_{abc}$ and $D^{(\ell)}_{abcd}$ in the small Γ expansion ($\Gamma \ll \varepsilon_{\rm F}$). Equations (D7), (D8), and (D10) in Appendix D show their contributions are of order Γ^{-2} and Γ^{-1}. As in the usual transport theory, the contributions containing both the retarded Green's function G^R_a and the advanced Green's function G^A_a have singularities of order Γ^{-2} and Γ^{-1}. Substituting the matrix elements in Eq. (11) for γ_μ and the small Γ expansions of $C^{(\ell)}_{abc}$ and $D^{(\ell)}_{abcd}$ into Eq. (26), we obtain each contribution $L^{(\ell),1}_{\mu\nu}$ to $L^{(\ell),7}_{\mu\nu}$ shown in Fig. 1. Their explicit expressions are shown in Eqs. (D13)–(D18) in Appendix D. (Note that $L^{(\ell),7}_{\mu\nu}$ does not appear since $D^{(\ell)}_{abcd}$ is of order Γ^0.) As a result, the transport coefficient can be obtained as

$$L^{(\ell)}_{\mu\nu} = \sum_{n=1}^{2} L^{(\ell)C,n}_{\mu\nu} + \sum_{n=1}^{6} L^{(\ell),n}_{\mu\nu} + O(\Gamma^0). \tag{29}$$

A. Leading order of $O(\Gamma^{-2})$

First, we consider the leading order terms in $L^{(\ell)}_{\mu\nu}$ in Eq. (29); they are proportional to Γ^{-2}. As shown in Appendix D, they are $L^{(\ell)C,1}_{\mu\nu}$ in Eq. (D11), $L^{(\ell),1}_{\mu\nu}$ in Eq. (D13), and the first term in $L^{(\ell),2}_{\mu\nu}$ in Eq. (D14). According to the different denominators in Eq. (D14), we divide $L^{(\ell),2}_{\mu\nu}$ as

$$L^{(\ell),2}_{\mu\nu} = L^{(\ell),2;1}_{\mu\nu} + L^{(\ell),2;2}_{\mu\nu} + L^{(\ell),2;3}_{\mu\nu}. \tag{30}$$

These terms have the denominators $\Gamma^2(\varepsilon_a - \varepsilon_b)$, $\Gamma(\varepsilon_a - \varepsilon_b)$, and $\Gamma(\varepsilon_a - \varepsilon_b)^2$, respectively.

As we can see from Fig. 1(a), $L^{(\ell),1}_{\mu\nu}$ is a purely intraband contribution because only the intraband matrix elements of γ_μ are involved. Considering that $\partial_x\varepsilon_a\partial[(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)]/\partial\varepsilon_a = \partial_x[(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)]$ and carrying out integration by parts with respect to k_x and k_y symmetrically, we obtain

$$\begin{aligned} L^{(\ell),1}_{\mu\nu} = &-\frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a}\frac{(\varepsilon-\mu)^\ell f'(\varepsilon_a)}{8\Gamma^2}\{2\partial_\mu\varepsilon_a\partial_\nu\varepsilon_a(\partial_x\partial_y\varepsilon_a) \\ &+ \partial_\mu\varepsilon_a\partial_x\varepsilon_a(\partial_\nu\partial_y\varepsilon_a) + \partial_\mu\varepsilon_a\partial_y\varepsilon_a(\partial_\nu\partial_x\varepsilon_a) \\ &+ \partial_\nu\varepsilon_a\partial_x\varepsilon_a(\partial_\mu\partial_y\varepsilon_a) + \partial_\nu\varepsilon_a\partial_y\varepsilon_a(\partial_\mu\partial_x\varepsilon_a)\}, \end{aligned} \tag{31}$$

where $f(\varepsilon_a) = 1/(e^{\beta(\varepsilon_a-\mu)}+1)$ is the Fermi distribution function. In particular, when $\ell = 0$ and $\mu = x$, $\nu = y$, i.e., in the case of Hall conductivity, this becomes

$$\begin{aligned} L^{(0),1}_{xy} = &-\frac{e^3B}{\hbar^2V}\sum_{\boldsymbol{k},a}\frac{f'(\varepsilon_a)}{8\Gamma^2}\{4\partial_x\varepsilon_a\partial_y\varepsilon_a(\partial_x\partial_y\varepsilon_a) \\ &+ (\partial_x\varepsilon_a)^2(\partial_y^2\varepsilon_a) + (\partial_y\varepsilon_a)^2(\partial_x^2\varepsilon_a)\}, \end{aligned} \tag{32}$$

which is similar to the result in the Boltzmann transport theory,

$$\begin{aligned} \sigma^{\rm Boltzmann}_{xy} = &-\frac{e^3B}{\hbar^2V}\sum_{\boldsymbol{k},a}\frac{f'(\varepsilon_a)}{8\Gamma^2}\{(\partial_x\varepsilon_a)^2(\partial_y^2\varepsilon_a) \\ &+ (\partial_y\varepsilon_a)^2(\partial_x^2\varepsilon_a) - 2\partial_x\varepsilon_a\partial_y\varepsilon_a(\partial_x\partial_y\varepsilon_a)\}, \end{aligned} \tag{33}$$

but the coefficient of the term $\partial_x\varepsilon_a\partial_y\varepsilon_a(\partial_x\partial_y\varepsilon_a)$ is different. We will show shortly that the result in the Boltzmann theory is obtained by adding other contributions from $L^{(0)C,1}_{\mu\nu}$ and $L^{(0),2:1}_{\mu\nu}$ that are proportional to $1/\Gamma^2$. This means that one should not pick up only $L^{(0),1}_{\mu\nu}$ in discussing the Hall conductivity in a single-band model. This situation is the same as in the case of orbital magnetic susceptibility, where χ_1 that looks like a purely intraband contribution gives a different result than the Landau-Peierls orbital magnetic susceptibility [42,54].

The first term of $L^{(\ell),2}_{\mu\nu}$ in Eq. (D14) (i.e., $L^{(\ell),2;1}_{\mu\nu}$) has the summation over the band indices a and b ($b \neq a$) [see also Fig. 1(b)]. Therefore, one may think that this term is an interband contribution. However, the summation over b can be carried out exactly, and then this term can be regarded as an intraband contribution, which should be added to Eq. (31). For this purpose, we use the generalized f-sum rule,

$$\sum_{b,(b\neq a)}\frac{p_{ab,\mu}p_{ba,\nu}}{\varepsilon_a-\varepsilon_b} = \frac{1}{2}\left(\partial_\mu\partial_\nu\varepsilon_a - \frac{\hbar^2}{m}\delta_{\mu\nu}\right) + i\,M^a_{\mu\nu}, \tag{34}$$

where $M^a_{\mu\nu}$ is the orbital magnetic moment for band a defined before in Eq. (19). The proof of this identity is given in Appendix E. When we use this generalized f-sum rule, we obtain

$$\begin{aligned} L^{(\ell),2;1}_{\mu\nu} = &\frac{e^{3-\ell}B}{\hbar^2V}\sum_{\boldsymbol{k},a}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{4\Gamma^2} \\ &\times\left[\partial_\nu\varepsilon_a\partial_x\varepsilon_a\left(\partial_y\partial_\mu\varepsilon_a - \frac{\hbar^2}{m}\delta_{\mu y}\right) + \partial_\mu\varepsilon_a\partial_\nu\varepsilon_a(\partial_x\partial_y\varepsilon_a)\right. \\ &\left.+\,\partial_\mu\varepsilon_a\partial_y\varepsilon_a\left(\partial_\nu\partial_x\varepsilon_a - \frac{\hbar^2}{m}\delta_{\nu x}\right)\right]. \end{aligned} \tag{35}$$

This f-sum rule is schematically shown in Fig. 1(b), where the red squares indicate the parts of the diagram representing the f-sum rule.

Thus, the total of Eqs. (D11), (31), and (35) becomes

$$\begin{aligned} &L^{(\ell),C1}_{\mu\nu} + L^{(\ell),1}_{\mu\nu} + L^{(\ell),2;1}_{\mu\nu} \\ &= -\frac{e^{3-\ell}B}{\hbar^2V}\sum_{\boldsymbol{k},a}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{8\Gamma^2}\{\partial_\mu\varepsilon_a\partial_x\varepsilon_a(\partial_\nu\partial_y\varepsilon_a) \\ &\quad - \partial_\mu\varepsilon_a\partial_y\varepsilon_a(\partial_\nu\partial_x\varepsilon_a) - \partial_\nu\varepsilon_a\partial_x\varepsilon_a(\partial_\mu\partial_y\varepsilon_a) \\ &\quad + \partial_\nu\varepsilon_a\partial_y\varepsilon_a(\partial_\mu\partial_x\varepsilon_a)\}. \end{aligned} \tag{36}$$

In particular, when $\ell = 0$, $\mu = x$, and $\nu = y$, i.e., in the case of Hall conductivity, this total becomes equal to the result obtained using Boltzmann theory.

The generalized f-sum rule in Eq. (34) results from the completeness property of $u_{b\boldsymbol{k}}$ (see Appendix A of Ref. [42]). One may call the left-hand side of (34) "interband" since it contains the off-diagonal matrix element $p_{ab,\mu}$. On the other hand, the right-hand side of (34) is expressed by a single-band property, ε_a, and as a result, $L_{\mu\nu}^{(\ell),2;1}$ looks like an "intraband" contribution. This indicates that the naive classification of "intraband" and "interband" does not apply, as discussed for the case of orbital magnetic susceptibility [42].

B. Subleading order of $O(\Gamma^{-1})$

Next, we discuss the subleading order of $O(\Gamma^{-1})$. The second term of $L_{\mu\nu}^{(\ell),2}$ in Eq. (D14) (i.e., $L_{\mu\nu}^{(\ell),2;2}$) can be calculated in a way similar to $L_{\mu\nu}^{(\ell),2;1}$, which yields

$$L_{\mu\nu}^{(\ell),2;2} = \frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a}\frac{\frac{\partial}{\partial\varepsilon_a}[(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)]}{2\Gamma}\big[\partial_\nu\varepsilon_a\partial_x\varepsilon_a M^a_{y\mu} + \partial_\mu\varepsilon_a\partial_\nu\varepsilon_a M^a_{xy} + \partial_\mu\varepsilon_a\partial_y\varepsilon_a M^a_{\nu x}\big]. \tag{37}$$

The third term of $L_{\mu\nu}^{(\ell),2}$ (i.e., $L_{\mu\nu}^{(\ell),2;3}$) has the denominator $(\varepsilon_a-\varepsilon_b)^2$, which is different from $L_{\mu\nu}^{(\ell),2;1}$ and $L_{\mu\nu}^{(\ell),2;2}$ discussed above. In this case, instead of Eq. (34), we use another generalized f-sum rule (see Appendix E),

$$\sum_{b,(b\neq a)}\frac{p_{ab,\mu}p_{ba,\nu}}{(\varepsilon_a-\varepsilon_b)^2} = \mathrm{Re}\langle\partial_\mu a|\partial_\nu a\rangle - \langle\partial_\mu a|a\rangle\langle a|\partial_\nu a\rangle - \frac{i}{2}\,\Omega^a_{\mu\nu}, \tag{38}$$

where $\Omega^a_{\mu\nu}$ is the Berry curvature for band a defined before in Eq. (18).

Using this second generalized f-sum rule, we obtain

$$L_{\mu\nu}^{(\ell),2;3} = \frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{2\Gamma}\big[\partial_\nu\varepsilon_a\partial_x\varepsilon_a\Omega^a_{y\mu} + \partial_\mu\varepsilon_a\partial_\nu\varepsilon_a\Omega^a_{xy} + \partial_\mu\varepsilon_a\partial_y\varepsilon_a\Omega^a_{\nu x}\big]. \tag{39}$$

Note that we have used the fact that $\langle\partial_\mu a|b\rangle = -\langle a|\partial_\mu b\rangle$ and it is purely imaginary for any μ when a is equal to b.

Features similar to $L_{\mu\nu}^{(\ell),2}$ are present in $L_{\mu\nu}^{(\ell),5}$ and $L_{\mu\nu}^{(\ell),6}$, as seen in Fig. 1, where the excluded term of $b=c$ in $L_{\mu\nu}^{(\ell),6}$ is supplemented by $L_{\mu\nu}^{(\ell),5}$, leading to the independent summations over b and c. Other terms are calculated similarly; the details are shown in Appendix F.

Combining the leading and subleading order terms, we obtain the total thermoelectric conductivities, as shown in Eq. (17). Note that this final formula does not contain the terms proportional to $\hbar^2/m$ which appeared in Eq. (29) as $L_{\mu\nu}^{(\ell)C,1}$ and $L_{\mu\nu}^{(\ell)C,2}$. For example, for the Hall conductivity

$$\begin{aligned}L_{xy}^{(\ell)} = -\frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a}(\varepsilon_a-\mu)^\ell f'(\varepsilon_a) &\times\bigg[\frac{1}{8\Gamma^2}\big\{(\partial_x\varepsilon_a)^2(\partial_y^2\varepsilon_a) + (\partial_y\varepsilon_a)^2(\partial_x^2\varepsilon_a) \\ &- 2\partial_x\varepsilon_a\partial_y\varepsilon_a(\partial_x\partial_y\varepsilon_a)\big\} + \frac{1}{2\Gamma}\partial_x\varepsilon_a\partial_y\varepsilon_a\Omega^a_{xy} \\ &- \frac{1}{4\Gamma}\{\partial_x\varepsilon_a\partial_y M_{xy} + \partial_y\varepsilon_a\partial_x M_{xy} - 2(\partial_x\partial_y\varepsilon_a)M_{xy}\}\bigg],\end{aligned} \tag{40}$$

and for the xx and zz components,

$$\begin{aligned}L_{xx}^{(\ell)} &= -\frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a}(\varepsilon_a-\mu)^\ell f'(\varepsilon_a) \\ &\quad\times\bigg[\frac{1}{2\Gamma}(\partial_x\varepsilon_a)^2\Omega^a_{xy} - \frac{1}{2\Gamma}\big\{\partial_x\varepsilon_a\partial_x M_{xy} - \big(\partial_x^2\varepsilon_a\big)M_{xy}\big\}\bigg], \\ L_{zz}^{(\ell)} &= -\frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a}(\varepsilon_a-\mu)^\ell f'(\varepsilon_a) \\ &\quad\times\bigg[-\frac{1}{2\Gamma}\big\{(\partial_z\varepsilon_a)^2\Omega^a_{xy} + 2\partial_x\varepsilon_a\partial_z\varepsilon_a\Omega^a_{yz} + 2\partial_y\varepsilon_a\partial_z\varepsilon_a\Omega^a_{zx}\big\} \\ &\quad - \frac{1}{2\Gamma}\big\{\partial_z\varepsilon_a\partial_z M_{xy} - \big(\partial_z^2\varepsilon_a\big)M_{xy}\big\}\bigg].\end{aligned} \tag{41}$$

These results are consistent with our previous result for $\ell=0$ obtained in Ref. [15].

V. LINEAR MAGNETOTHERMOPOWER

In this section we study a simple two-band model that shows nontrivial effects, such as linear magnetoconductivity and magnetothermopower. We consider the following gapped model with broken time-reversal symmetry:

$$H = v\hbar k_x\sigma_x + v\hbar k_y\sigma_y + \Delta(1+\delta k_z^2)\sigma_z. \tag{42}$$

The dispersion relation of this model is

$$E_\pm = \pm\Delta\sqrt{\frac{v^2\hbar^2}{\Delta^2}\big(k_x^2+k_y^2\big) + \big(1+\delta k_z^2\big)^2}. \tag{43}$$

If time-reversal symmetry is present in the system and the only time-reversal symmetry breaking term is the magnetic field B, the transport coefficients obey $L_{\mu\nu}^{(\ell)}(\mathbf{B}) = L_{\nu\mu}^{(\ell)}(-\mathbf{B})$ due to the Onsager relations. In order to observe nontrivial effects that violate this equality (e.g., a diagonal term linear in the magnetic field), time-reversal symmetry must be broken already at zero magnetic field.

In the case of a completely gapless linear spectrum the conductivity will be chemical potential independent [15]; this leads to a vanishing thermopower. The presence of the gap leads to a finite thermopower caused by the diverging density of states around the gap.

The system in Eq. (42) has a nonvanishing Berry curvature and orbital magnetic moment, expressed as

$$\Omega^\pm_{xy} = -\hbar^2v^2\Delta\frac{1+\delta k_z^2}{2E_\pm^3},\quad \Omega^\pm_{yz} = -\hbar^2v^2\Delta\frac{\delta k_x k_z}{E_\pm^3}, \tag{44}$$

$$\Omega^\pm_{zx} = -\hbar^2v^2\Delta\frac{\delta k_y k_z}{E_\pm^3},\quad M^\pm_{xy} = \hbar^2v^2\Delta\frac{1+\delta k_z^2}{2E_\pm^2}. \tag{45}$$

Considering the symmetries of the system, the magnetoconductivity has the form

$$\sigma = \begin{pmatrix}\sigma_{xx} & \sigma_{xy} & 0\\ -\sigma_{xy} & \sigma_{xx} & 0\\ 0 & 0 & \sigma_{zz}\end{pmatrix}. \tag{46}$$

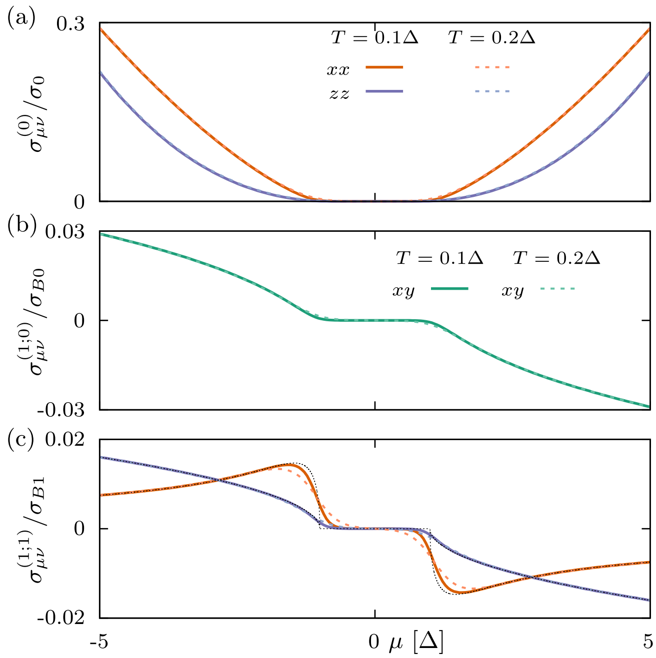

FIG. 2. Different components of the conductivity tensor of Eq. (42) as a function of the chemical potential up to linear order in the magnetic field. (a) Conductivity for $B = 0$ in units of $\sigma_0 = e^2\Delta^2/\Gamma v\hbar^2$. (b) Hall conductivity in units of $\sigma_{B0} = e^3 B\Delta v/\Gamma^2\hbar$. (c) Longitudinal and transverse linear magnetoconductivities for three different temperatures in units of $\sigma_{B1} = e^3 Bv/\Gamma\hbar$. In all panels $\delta = 0.1(\hbar v)^2/\Delta^2$, and only the nonzero components are shown.

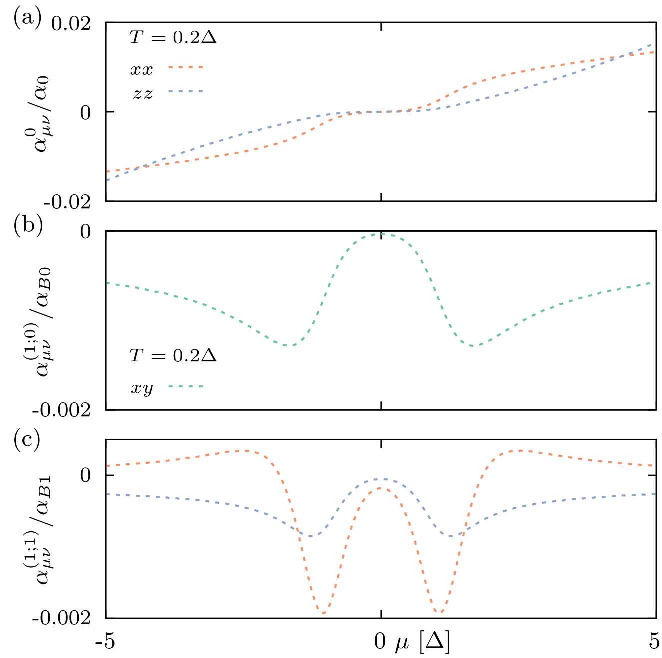

FIG. 3. Different components of the thermoelectric conductivity tensor of Eq. (42) as a function of the chemical potential up to linear order of the magnetic field. All panels correspond to the panels in Fig. 2, with the same parameters. The thermoelectric conductivity is measured in units of $\alpha_{0/B0/B1} = (\Delta/e)\sigma_{0/B0/B1}$.

There are three independent components. At linear order in the magnetic field they can be divided as

$$\sigma_{xx} = \sigma^{(0)}_{xx} + \sigma^{(1;1)}_{xx}, \tag{47a}$$

$$\sigma_{zz} = \sigma^{(0)}_{zz} + \sigma^{(1;1)}_{zz}, \tag{47b}$$

$$\sigma_{xy} = \sigma^{(1;0)}_{xy}, \tag{47c}$$

where (0) is the $B = 0$ result, $(1;0)$ is the B linear term with Γ^{-2}, and $(1;1)$ is the B linear term with Γ^{-1}.

The $B = 0$ result can be computed using Boltzmann theory [discarding $O(\Gamma^0)$ terms]. The rest of the terms can be computed using Eq. (17). All terms are computed numerically using Monte Carlo integration. The results as a function of the chemical potential are shown in Fig. 2. Figures 2(a) and 2(b) show the normal conductivity with symmetric diagonal elements and antisymmetric Hall conductivity. Figure 2(c) shows the linear magnetoconductivity terms that are forbidden in time-reversal-symmetric systems which satisfy $\sigma_{\mu\nu}(\mathbf{B}) = \sigma_{\nu\mu}(-\mathbf{B})$.

Similar to the conductivity, the thermoelectric conductivity ($\alpha = \mathbf{L}_{12}$) will have the form

$$\alpha = \begin{pmatrix} \alpha_{xx} & \alpha_{xy} & 0 \\ -\alpha_{xy} & \alpha_{xx} & 0 \\ 0 & 0 & \alpha_{zz} \end{pmatrix}, \tag{48}$$

with

$$\alpha_{xx} = \alpha^{(0)}_{xx} + \alpha^{(1;1)}_{xx}, \tag{49a}$$

$$\alpha_{zz} = \alpha^{(0)}_{zz} + \alpha^{(1;1)}_{zz}, \tag{49b}$$

$$\alpha_{xy} = \alpha^{(1;0)}_{xy}. \tag{49c}$$

This is computed similarly to the conductivity, and the results as a function of the chemical potential are shown in Fig. 3. The results for the thermoelectric conductivity also show finite $\alpha^{(1;1)}_{\mu\mu}$ terms that are classically forbidden; they appear because of the nonconstant chemical potential dependence of the $\sigma^{(1;1)}_{\mu\mu}$ terms. We see that if the conductivity is an even (odd) function of the chemical potential, the thermoelectric conductivity is odd (even). This is related to the charge carriers being electrons or holes with opposite charge.

Using Eq. (13), we can obtain the Seebeck coefficient tensor from the conductivity and thermoelectric conductivity, which will have the same structure as the former two, with

$$S_{xx} = \frac{1}{T}\frac{\alpha_{xx}\sigma_{xx} + \alpha_{xy}\sigma_{xy}}{\sigma^2_{xx} + \sigma^2_{xy}}, \tag{50a}$$

$$S_{zz} = \frac{1}{T}\frac{\alpha_{zz}}{\sigma_{zz}}, \tag{50b}$$

$$S_{xy} = \frac{1}{T}\frac{\alpha_{xx}\sigma_{xy} - \alpha_{xy}\sigma_{xx}}{\sigma^2_{xx} + \sigma^2_{xy}}. \tag{50c}$$

Using the previously computed results and choosing realistic parameters ($v = 10^6\,\mathrm{ms}^{-1}$, $\Delta = 0.1\,\mathrm{eV}$, $\Gamma = 0.01\Delta$), we calculate the thermopower, which is shown in Fig. 4 as a function of the chemical potential, temperature, and magnetic field.

We can see that the Seebeck tensor gets enhanced close to the band gap. We get a finite but small Nernst coefficient S_{xy}.

If the B-linear terms such as $\sigma^{(1;1)}$ and $\alpha^{(1;1)}$ are zero, $S_{xx}(B) - S_{xx}(0) \propto B^2$, and $S_{zz} = \text{const}$. If these nontrivial terms exist, the magnetothermopower can have a linear contribution in both cases. In the case of S_{zz} we can see this linear

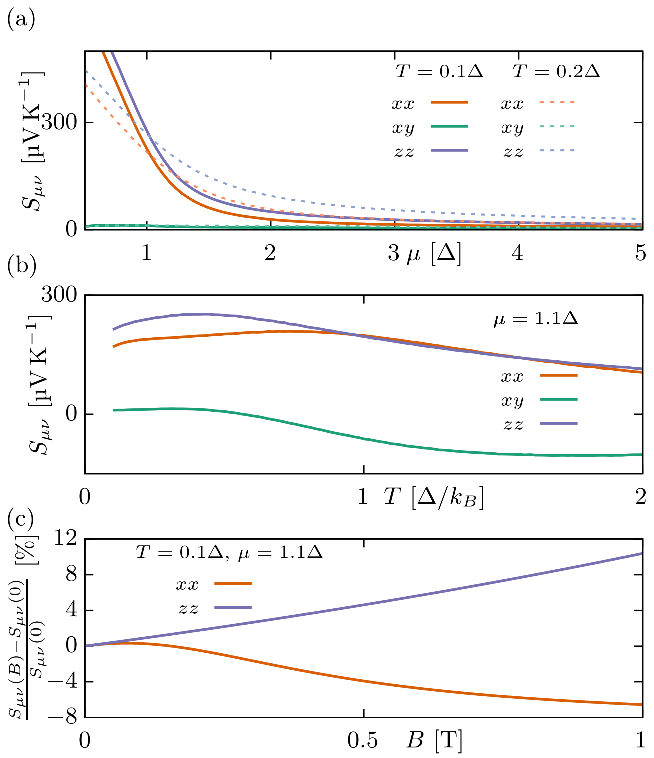

FIG. 4. Different components of the Seebeck tensor of (42) up to linear order in the magnetic field as a function of (a) the chemical potential at $B = 1$ T, (b) temperature at $B = 1$ T, and (c) magnetic field. The parameters used are $v = 10^6\,\mathrm{m\,s^{-1}}$, $\Delta = 0.1$ eV, $\Gamma = 0.01\Delta$, and $\delta = 0.1(\hbar v)^2/\Delta^2$.

dependence in Fig. 4(c). For S_{xx} we get a more complicated magnetic field dependence.

To see the gap dependence we compute the Seebeck coefficients as a function of Δ, as shown in Fig. 5. We can see that the Seebeck coefficient in the x direction is less sensitive to the gap size, while in the z direction it is strongly enhanced for small gaps.

We also compute the thermal conductivity (see Fig. 6) and the ratio of thermal conductivity to electric conductivity, also known as the Lorentz number (see Fig. 7). Far away from the gap at large μ we recover the Wiedemann-Franz law, with $L = \kappa/\sigma T = \pi^2 k_B^2/3e^2$. Closer to the band gap the Lorentz number gets enhanced and takes large values. As a function of magnetic field [see Fig. 7(c)], we get a weak linear increase.

Finally, we compute the power factor defined as σS^2 (see Fig. 8) and the figure of merit $zT = \sigma S^2 T/\kappa$ (see Fig. 9).

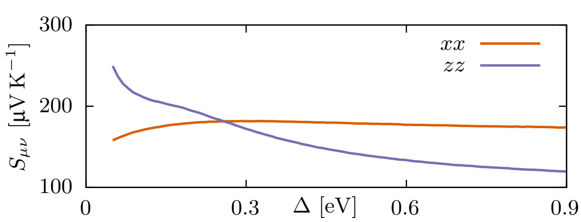

FIG. 5. Seebeck tensor as a function of the gap Δ. The parameters used are $v = 10^6\,\mathrm{m\,s^{-1}}$, $\Gamma = 0.001$ eV, $\mu = \Delta + 0.01$ eV, $k_B T = 0.1$ eV, and $\delta = 10(\hbar v)^2/\,\mathrm{eV}^2$.

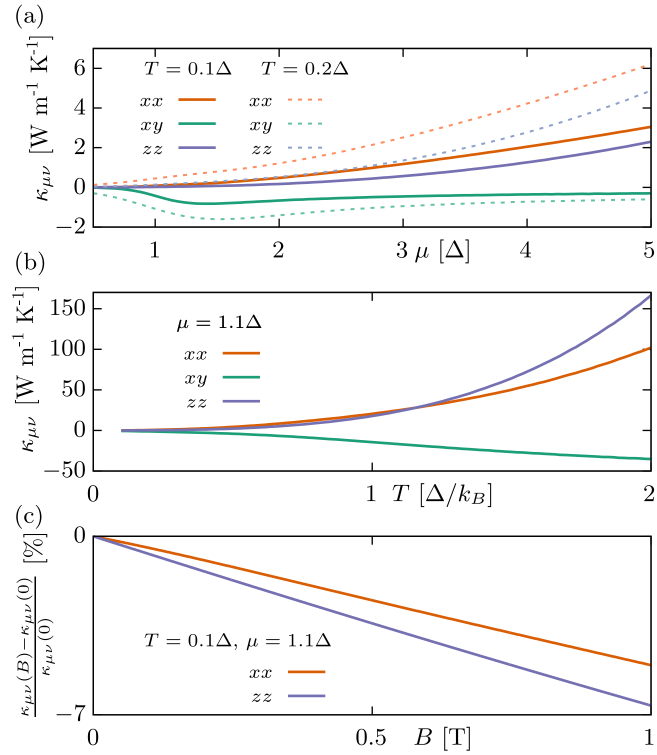

FIG. 6. Different components of the thermal conductivity tensor of (42) up to linear order in the magnetic field. The panels and parameters are the same as in Fig. 4.

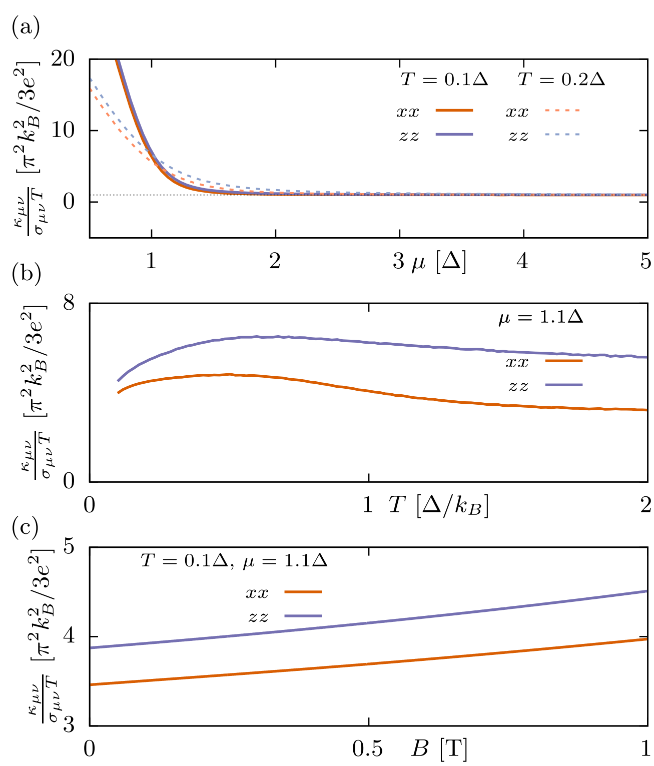

FIG. 7. The Lorenz number in the x and z directions of (42) up to linear order in the magnetic field. The panels and parameters are the same as in Fig. 4.

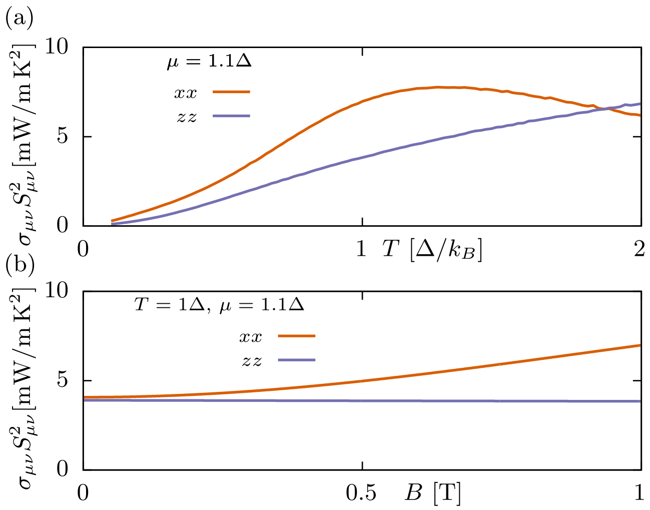

FIG. 8. Power factor of (42) up to linear order in the magnetic field. The panels and parameters are the same as in Fig. 4.

These are experimentally relevant quantities characterizing good thermoelectric materials. A high figure of merit means more efficient conversion of heat energy into electrical energy. The results for the power factor and figure of merit show a strong enhancement as a function of the magnetic field in the x direction. However, note that the contribution of phonons to the thermal conductivity κ is not taken into account, so the figure of merit in Fig. 9 is generally suppressed by the presence of the phonon thermal conductivity.

VI. CONCLUSION AND DISCUSSION

In this paper we presented an analytic formalism to calculate thermoelectric coefficients in the presence of a low magnetic field up to linear order in the magnetic field. The formulas are based on linear response theory and are taken in the limit of small scattering rates. The resulting expression for the transport coefficients in Eq. (17) is general and can be applied to any system described by a single-particle Bloch Hamiltonian or effective Bloch Hamiltonian.

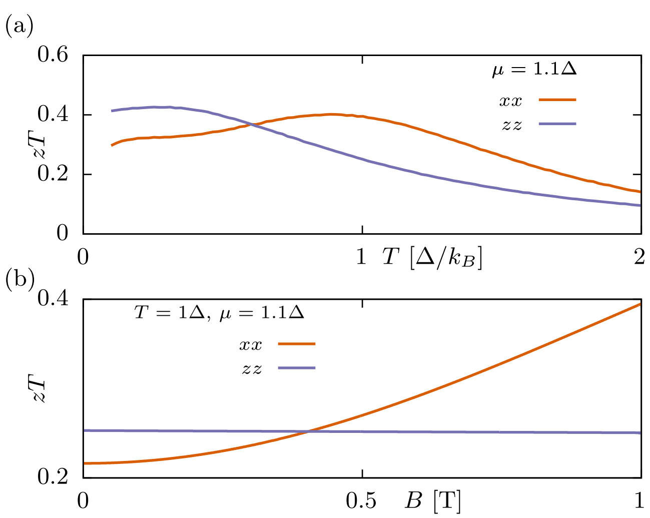

FIG. 9. Figure of merit zT of (42) up to linear order in the magnetic field. The panels and parameters are the same as in Fig. 4.

In order to showcase the nontrivial effects that can be studied with our formalism we computed different magnetothermoelectric observable quantities for a simple model of an insulator with broken time-reversal symmetry. This effect is a linear longitudinal magnetothermopower related to the presence of nonvanishing Berry curvature and orbital magnetic moment.

The formalism presented in this paper is a fully microscopic description that can be used to validate the semiclassical approaches used in the literature [7–13,16,18,20–22]. The microscopic formulas in the limit of small scattering rates can be compared with explicit results using the semiclassical Boltzmann theory found in the literature. In the case of the Hall conductivity σ_{xy} [18] the terms proportional to Γ^{-2} match perfectly after partial integrations, meaning that the semiclassical Boltzmann theory without anomalous velocity gives the correct result for the lowest order approximation in the scattering rate.

The terms proportional to Γ^{-1} containing the Berry curvature and orbital magnetic moment are harder to compare. Often, the orbital magnetic moment appears through a Zeeman shift of the energy and does not explicitly appear in formulas. Explicit results include σ_{xy} in Ref. [18] and σ_{zz} in Ref. [7]. They match perfectly with our results, except for the term that is proportional to the orbital magnetic moment $2(\partial_\mu \partial_\nu) M_{xy}$ in Eq. (17). That term is missing from the semiclassical calculations. The disadvantage of semiclassical methods is that we cannot check whether we included all relevant terms. This further strengthens our claim that using a fully microscopic approach like in the present paper is necessary to verify that we take into account all terms.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: CURRENT AND HEAT CURRENT OPERATORS IN THE PRESENCE OF MAGNETIC FIELD

In the presence of a magnetic field, we use the Hamiltonian

$$\begin{aligned} H(\boldsymbol{r}) = &\frac{1}{2m}[\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{r})]^2 + V(\boldsymbol{r}) + \frac{\hbar^2}{8m^2c^2}\nabla^2 V(\boldsymbol{r}) \\ &- \frac{e\hbar}{2m}\boldsymbol{\sigma}\cdot\{\boldsymbol{b}(\boldsymbol{r}) + \boldsymbol{B}(\boldsymbol{r})\} + \frac{\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot\nabla V \\ &\times [\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{r})], \end{aligned} \tag{A1}$$

with $\boldsymbol{B}(\boldsymbol{r}) = \mathrm{rot}\,\boldsymbol{A}(\boldsymbol{r})$, which is an extension of Eq. (2).

We derive the current operator using the continuity equation (5). The time derivative of the charge density is

$$\frac{d}{dt}e\rho(\boldsymbol{r}) = -\frac{ie}{\hbar}[\rho(\boldsymbol{r}), \mathcal{H}] = -\frac{ie}{\hbar}\psi^\dagger(\boldsymbol{r})\{H(\boldsymbol{r}) - \overleftarrow{H}(\boldsymbol{r})\}\psi(\boldsymbol{r}). \tag{A2}$$

Then, we can show that

$$H(\boldsymbol{r}) - \overleftarrow{H}(\boldsymbol{r}) = (\boldsymbol{p} - \overleftarrow{\boldsymbol{p}})\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r}) = -i\hbar(\nabla + \overleftarrow{\nabla})\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r}), \tag{A3}$$

where $\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r})$ is defined as

$$\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r}) = \frac{1}{2m}(-i\hbar\nabla + i\hbar\overleftarrow{\nabla} - 2e\boldsymbol{A}) + \frac{\hbar}{4m^2c^2}\boldsymbol{\sigma}\times\nabla V. \tag{A4}$$

Therefore, we obtain

$$\frac{d}{dt}e\rho(\boldsymbol{r}) = -e\nabla[\psi^\dagger(\boldsymbol{r})\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r})\psi(\boldsymbol{r})], \tag{A5}$$

which leads to the current density operator

$$\boldsymbol{j}(\boldsymbol{r}) = e\psi^\dagger(\boldsymbol{r})\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r})\psi(\boldsymbol{r}). \tag{A6}$$

The contribution proportional to the vector potential $\boldsymbol{A}$ is the diamagnetic current. When $\boldsymbol{A} = \boldsymbol{0}$, this current density operator becomes the one in Eq. (6).

Similarly, the time derivative of the energy density is

$$\begin{aligned}\frac{d}{dt}h(\boldsymbol{r}) &= -\frac{i}{\hbar}[h(\boldsymbol{r}), \mathcal{H}]\\ &= -\frac{i}{2\hbar}\psi^\dagger(\boldsymbol{r})[\{H(\boldsymbol{r}) - \overleftarrow{H}(\boldsymbol{r})\}H(\boldsymbol{r})\\ &\quad + \overleftarrow{H}(\boldsymbol{r})\{H(\boldsymbol{r}) - \overleftarrow{H}(\boldsymbol{r})\}]\psi(\boldsymbol{r}).\end{aligned} \tag{A7}$$

Again using Eq. (A3), we obtain

$$\frac{d}{dt}h(\boldsymbol{r}) = -\nabla\left[\frac{1}{2}\psi^\dagger(\boldsymbol{r})\{\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r})H(\boldsymbol{r}) + \overleftarrow{H}(\boldsymbol{r})\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r})\}\psi(\boldsymbol{r})\right], \tag{A8}$$

which leads to the energy current operator

$$\boldsymbol{j}_E(\boldsymbol{r}) = \tfrac{1}{2}\psi^\dagger(\boldsymbol{r})\{\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r})H(\boldsymbol{r}) + \overleftarrow{H}(\boldsymbol{r})\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r})\}\psi(\boldsymbol{r}). \tag{A9}$$

Finally, let us derive the relationship between the current and heat current operator in Eq. (9). Using the imaginary time interaction representation, we obtain

$$\begin{aligned}\frac{1}{2e}\left(\frac{\partial}{\partial\tau} - \frac{\partial}{\partial\tau'}\right)\boldsymbol{j}(\boldsymbol{r},\tau,\tau') &= \frac{1}{2}\{[\mathcal{H} - \mu N, \psi^\dagger(\boldsymbol{r},\tau)]\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r})\psi(\boldsymbol{r},\tau') - \psi^\dagger(\boldsymbol{r})\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r},\tau)[\mathcal{H} - \mu N, \psi(\boldsymbol{r},\tau')]\}\\ &= \frac{1}{2}\{\psi^\dagger(\boldsymbol{r},\tau)[\overleftarrow{H}(\boldsymbol{r}) - \mu]\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r})\psi(\boldsymbol{r},\tau') + \psi^\dagger(\boldsymbol{r})\overleftrightarrow{\boldsymbol{j}}_{0A}(\boldsymbol{r},\tau)[H(\boldsymbol{r}) - \mu]\psi(\boldsymbol{r},\tau')\}\\ &= \boldsymbol{j}_E(\boldsymbol{r},\tau,\tau') - \mu\boldsymbol{j}(\boldsymbol{r},\tau,\tau')/e.\end{aligned} \tag{A10}$$

APPENDIX B: GENERALIZATION OF FUKUYAMA'S FORMULA OF HALL CONDUCTIVITY

Fukuyama [41] used the Luttinger-Kohn representation of the Bloch wave functions and obtained the current-current correlation function $\Phi_{xy}(i\omega_\lambda)$ at the first order in the magnetic field. That formula can be generalized for cases with other components ($\mu, \nu = x, y, z$) as follows:

$$\begin{aligned}\Phi^{11}_{\mu\nu}(i\omega_\lambda) &= \frac{k_BT}{V}\sum_{n,\boldsymbol{k}}\frac{i|e|^3B}{2m\hbar}\mathrm{Tr}[-\delta_{\nu y}(\gamma_\mu\mathcal{G}_+\mathcal{G}\gamma_x\mathcal{G} - \gamma_\mu\mathcal{G}_+\gamma_x\mathcal{G}_+\mathcal{G})\\ &\quad + \delta_{\nu x}(\gamma_\mu\mathcal{G}_+\mathcal{G}\gamma_y\mathcal{G} - \gamma_\mu\mathcal{G}_+\gamma_y\mathcal{G}_+\mathcal{G})] + \frac{k_BT}{V}\sum_{n,\boldsymbol{k}}\frac{i|e|^3B}{2\hbar^3}\mathrm{Tr}\,[\gamma_\mu\mathcal{G}_+\gamma_x\mathcal{G}_+\gamma_\nu\mathcal{G}\gamma_y\mathcal{G} - \gamma_\mu\mathcal{G}_+\gamma_y\mathcal{G}_+\gamma_\nu\mathcal{G}\gamma_x\mathcal{G}\\ &\quad + \gamma_\mu\mathcal{G}_+\gamma_\nu\mathcal{G}\gamma_x\mathcal{G}\gamma_y\mathcal{G} - \gamma_\mu\mathcal{G}_+\gamma_\nu\mathcal{G}\gamma_y\mathcal{G}\gamma_x\mathcal{G} + \gamma_\mu\mathcal{G}_+\gamma_x\mathcal{G}_+\gamma_y\mathcal{G}_+\gamma_\nu\mathcal{G} - \gamma_\mu\mathcal{G}_+\gamma_y\mathcal{G}_+\gamma_x\mathcal{G}_+\gamma_\nu\mathcal{G}],\end{aligned} \tag{B1}$$

where the magnetic field is parallel to the z axis. In the Luttinger-Kohn representation, the relations

$$\frac{\partial}{\partial k_\mu}\mathcal{G} = \mathcal{G}\gamma_\mu\mathcal{G}, \quad \frac{\partial}{\partial k_\nu}\gamma_\mu = \frac{\hbar^2}{m}\mathbf{1}\delta_{\mu\nu} \tag{B2}$$

hold, where $\mathbf{1}$ represents the unit matrix. Therefore, using these relations and integration by parts, we can rewrite the first term in the second summation in Eq. (B1) as

$$\begin{aligned}\sum_{\boldsymbol{k}}\gamma_\mu\mathcal{G}_+\gamma_x\mathcal{G}_+\gamma_\nu\mathcal{G}\gamma_y\mathcal{G} &= \sum_{\boldsymbol{k}}\gamma_\mu\mathcal{G}_+\gamma_x\mathcal{G}_+\gamma_\nu\frac{\partial}{\partial k_y}\mathcal{G}\\ &= -\sum_{\boldsymbol{k}}\frac{\hbar^2}{m}\{\delta_{\mu y}\mathcal{G}_+\gamma_x\mathcal{G}_+\gamma_\nu\mathcal{G} + \delta_{\nu y}\gamma_\mu\mathcal{G}_+\gamma_x\mathcal{G}_+\mathcal{G}\} - \sum_{\boldsymbol{k}}\{\gamma_\mu\mathcal{G}_+\gamma_y\mathcal{G}_+\gamma_x\mathcal{G}_+\gamma_\nu\mathcal{G} + \gamma_\mu\mathcal{G}_+\gamma_x\mathcal{G}_+\gamma_y\mathcal{G}_+\gamma_\nu\mathcal{G}\}\end{aligned} \tag{B3}$$

for any μ and ν. A similar integration by parts for the second term in the second summation in Eq. (B1),

$$-\sum_{\boldsymbol{k}} \gamma_\mu \mathcal{G}_+ \gamma_y \mathcal{G}_+ \gamma_\nu \mathcal{G} \gamma_x \mathcal{G} = -\sum_{\boldsymbol{k}} \gamma_\mu \left(\frac{\partial}{\partial k_y} \mathcal{G}_+ \right) \gamma_\nu \mathcal{G} \gamma_x \mathcal{G}, \tag{B4}$$

can also be used. As a result, we obtain Eq. (21). We used a similar relation in our previous paper [15].

APPENDIX C: EXPLICIT FORMS OF $C^{(\ell)}_{abc}$ AND $D^{(\ell)}_{abcd}$

The summation over the Matsubara frequency in Eq. (27) can be carried out using complex integration (for details see the Supplemental Material of Ref. [15]). For example,

$$\begin{aligned}
-k_{\mathrm{B}}T \sum_n \left(i\varepsilon_n + \frac{i\omega_\lambda}{2} \right)^\ell (\mathcal{G}_+)_a (\mathcal{G})_b (\mathcal{G})_c &= \int \frac{dz}{2\pi i} F(z) \left(z + \frac{i\omega_\lambda}{2} \right)^\ell \mathcal{G}_a(z + i\omega_\lambda) \mathcal{G}_b(z) \mathcal{G}_c(z) \\
&= \int \frac{d\varepsilon}{2\pi i} f(\varepsilon) \Bigg[\left(\varepsilon - \mu + \frac{i\omega_\lambda}{2} \right)^\ell G^{\mathrm{R}}_a(\varepsilon + i\omega_\lambda) \{ G^{\mathrm{R}}_b(\varepsilon) G^{\mathrm{R}}_c(\varepsilon) - G^{\mathrm{A}}_b(\varepsilon) G^{\mathrm{A}}_c(\varepsilon) \} \\
&\quad + \left(\varepsilon - \mu - \frac{i\omega_\lambda}{2} \right)^\ell \{ G^{\mathrm{R}}_a(\varepsilon) - G^{\mathrm{A}}_a(\varepsilon) \} G^{\mathrm{A}}_b(\varepsilon - i\omega_\lambda) G^{\mathrm{A}}_c(\varepsilon - i\omega_\lambda) \Bigg],
\end{aligned} \tag{C1}$$

where $\boldsymbol{k}$ in the thermal Green's functions is not shown, $F(z) = 1/(e^{\beta z} + 1)$, and $f(\varepsilon)$ is the Fermi distribution function with chemical potential μ, $f(\varepsilon) = 1/(e^{\beta(\varepsilon - \mu)} + 1)$. The retarded and advanced Green's functions G^{R}_a and G^{A}_a are defined as

$$G^{\mathrm{R}}_a = \frac{1}{\varepsilon - \varepsilon_a(\boldsymbol{k}) + i\Gamma}, \quad G^{\mathrm{A}}_a = [G^{\mathrm{R}}_a]^*, \tag{C2}$$

respectively. After the analytic continuation of $i\omega_\lambda \to \hbar(\omega + i\delta)$, we can take the linear order with respect to ω, which yields

$$\begin{aligned}
C^{(\ell)}_{abc} = \int \frac{d\varepsilon}{2\pi i} f(\varepsilon) \Bigg[(\varepsilon - \mu)^\ell \left\{ \frac{\partial G^{\mathrm{R}}_a(\varepsilon)}{\partial \varepsilon} [G^{\mathrm{R}}_b(\varepsilon) G^{\mathrm{R}}_c(\varepsilon) - G^{\mathrm{A}}_b(\varepsilon) G^{\mathrm{A}}_c(\varepsilon)] - [G^{\mathrm{R}}_a(\varepsilon) - G^{\mathrm{A}}_a(\varepsilon)] \frac{\partial G^{\mathrm{A}}_b(\varepsilon) G^{\mathrm{A}}_c(\varepsilon)}{\partial \varepsilon} \right\} \\
+ \frac{\ell}{2} (\varepsilon - \mu)^{\ell - 1} \{ G^{\mathrm{R}}_a(\varepsilon) [G^{\mathrm{R}}_b(\varepsilon) G^{\mathrm{R}}_c(\varepsilon) - G^{\mathrm{A}}_b(\varepsilon) G^{\mathrm{A}}_c(\varepsilon)] - [G^{\mathrm{R}}_a(\varepsilon) - G^{\mathrm{A}}_a(\varepsilon)] G^{\mathrm{A}}_b(\varepsilon) G^{\mathrm{A}}_c(\varepsilon) \} \Bigg].
\end{aligned} \tag{C3}$$

Using the same method, we obtain $\tilde{C}^{(\ell)}_{abc} = -[C^{(\ell)}_{cba}]^*$.

The quantity $D^{(\ell)}_{abcd}$ can be calculated in a similar way, which gives

$$\begin{aligned}
D^{(\ell)}_{abcd} = \int \frac{d\varepsilon}{2\pi i} f(\varepsilon) \Bigg[(\varepsilon - \mu)^\ell \Bigg\{ \frac{\partial G^{\mathrm{R}}_a(\varepsilon)}{\partial \varepsilon} [G^{\mathrm{R}}_b(\varepsilon) G^{\mathrm{R}}_c(\varepsilon) G^{\mathrm{R}}_d(\varepsilon) - G^{\mathrm{A}}_b(\varepsilon) G^{\mathrm{A}}_c(\varepsilon) G^{\mathrm{A}}_d(\varepsilon)] \\
- [G^{\mathrm{R}}_a(\varepsilon) - G^{\mathrm{A}}_a(\varepsilon)] \frac{\partial G^{\mathrm{A}}_b(\varepsilon) G^{\mathrm{A}}_c(\varepsilon) G^{\mathrm{A}}_d(\varepsilon)}{\partial \varepsilon} \Bigg\} + \frac{\ell}{2} (\varepsilon - \mu)^{\ell - 1} \{ G^{\mathrm{R}}_a(\varepsilon) [G^{\mathrm{R}}_b(\varepsilon) G^{\mathrm{R}}_c(\varepsilon) G^{\mathrm{R}}_d(\varepsilon) \\
- G^{\mathrm{A}}_b(\varepsilon) G^{\mathrm{A}}_c(\varepsilon) G^{\mathrm{A}}_d(\varepsilon)] - [G^{\mathrm{R}}_a(\varepsilon) - G^{\mathrm{A}}_a(\varepsilon)] G^{\mathrm{A}}_b(\varepsilon) G^{\mathrm{A}}_c(\varepsilon) G^{\mathrm{A}}_d(\varepsilon) \} \Bigg].
\end{aligned} \tag{C4}$$

Similarly, we obtain $\tilde{D}^{(\ell)}_{abcd} = -[D^{(\ell)}_{dcba}]^*$.

APPENDIX D: SMALL Γ EXPANSION OF THE ENERGY INTEGRALS AND DETAILED EXPRESSIONS FOR THE ELECTRIC AND THERMOELECTRIC CONDUCTIVITY TENSORS

We evaluate the energy integral in Eq. (C3) in powers of Γ^ℓ in the small Γ region. We always have integrals of the form

$$\int \frac{d\varepsilon}{2\pi i} f(\varepsilon) (\varepsilon - \mu)^\ell F(G^{\mathrm{R}}_{a'}, G^{\mathrm{A}}_{a'}, \ldots) (G^{\mathrm{R}}_a \cdots G^{\mathrm{R}}_b - G^{\mathrm{A}}_a \cdots G^{\mathrm{A}}_b). \tag{D1}$$

We calculate these kinds of integrals using the contour integrals of complex functions. The case with $\ell = 0$ was discussed before in Ref. [15], and here, we extend the previous results to $\ell = 1, 2$.

First, there are poles at $\varepsilon = \mu + i(2n + 1)k_{\mathrm{B}}T$ in $f(\varepsilon)$, with n being an integer. However, the residues of these poles vanish as $\Gamma \to 0$ since the factor $G^{\mathrm{R}}_a \cdots G^{\mathrm{R}}_b - G^{\mathrm{A}}_a \cdots G^{\mathrm{A}}_b$ in (D1) approaches zero as $\Gamma \to 0$. This means that these residues are of order Γ^1. Second, the factor $(\varepsilon - \mu)^\ell$ does not have singular points. Third, the contribution containing only the retarded Green's functions does not give any terms with Γ^{-1} or Γ^{-2} because even if the two Green's functions have the same energy ε_a, they give only higher-order derivatives of $f(\varepsilon)$. Therefore, the contributions that give Γ^{-1} or Γ^{-2} are those that contain at least one G^{R}_a and one G^{A}_a, which have the same energy ε_a but have different imaginary parts, $\pm i\Gamma$.

Accounting for this prescription, Eq. (C3) can be evaluated as

$$C^{(\ell)}_{abc} = \int \frac{d\varepsilon}{2\pi i} f'(\varepsilon)(\varepsilon-\mu)^\ell G^{\mathrm{R}}_a(\varepsilon)G^{\mathrm{A}}_b(\varepsilon)G^{\mathrm{A}}_c(\varepsilon) + O(\Gamma^0), \tag{D2}$$

where we have used integration by parts. Then, if we make the contour integral in the lower half of the complex plane, only the pole of G^{R}_a contributes to the integral, which gives

$$C^{(\ell)}_{abc} = -\frac{f'(\varepsilon_a - i\Gamma)(\varepsilon_a-\mu-i\Gamma)^\ell}{(\varepsilon_a-\varepsilon_b-2i\Gamma)(\varepsilon_a-\varepsilon_c-2i\Gamma)} + O(\Gamma^0). \tag{D3}$$

For example, we obtain

$$\begin{aligned} C^{(0)}_{aaa} &= -\frac{f'(\varepsilon_a - i\Gamma)}{(-2i\Gamma)^2} + O(\Gamma^0) \\ &= \frac{f'(\varepsilon_a)}{4\Gamma^2} - i\frac{f''(\varepsilon_a)}{4\Gamma} + O(\Gamma^0). \end{aligned} \tag{D4}$$

Note that, in this case, we have used the Γ expansion of the function $f(\varepsilon_a - i\Gamma)$. This treatment of the Fermi distribution function is unusual, but here, we regard $f(\varepsilon)$ just as a mathematical complex function. Furthermore, note that, if we make the contour integral in the upper half of the complex plane for

$$C^{(0)}_{aaa} = \int \frac{d\varepsilon}{2\pi i} f'(\varepsilon)G^{\mathrm{R}}_a(\varepsilon)\big[G^{\mathrm{A}}_a(\varepsilon)\big]^2 + O(\Gamma^0) \tag{D5}$$

and take the residue of $[G^{\mathrm{A}}_a(\varepsilon)]^2$, we obtain the same result as in Eq. (D4).

In a similar way, we obtain

$$\begin{aligned} C^{(1)}_{aaa} &= (\varepsilon_a-\mu)\left\{\frac{f'(\varepsilon_a)}{4\Gamma^2} - i\frac{f''(\varepsilon_a)}{4\Gamma}\right\} - i\frac{f'(\varepsilon_a)}{4\Gamma} + O(\Gamma^0), \\ C^{(2)}_{aaa} &= (\varepsilon_a-\mu)^2\left\{\frac{f'(\varepsilon_a)}{4\Gamma^2} - i\frac{f''(\varepsilon_a)}{4\Gamma}\right\} - i(\varepsilon_a-\mu)\frac{f'(\varepsilon_a)}{2\Gamma} + O(\Gamma^0). \end{aligned} \tag{D6}$$

We can rewrite the above results as

$$C^{(\ell)}_{aaa} = \frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{4\Gamma^2} - i\frac{\frac{\partial}{\partial\varepsilon_a}[(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)]}{4\Gamma} + O(\Gamma^0) \tag{D7}$$

for $\ell = 0, 1, 2$. Similarly, $C^{(\ell)}_{aab}$ and $C^{(\ell)}_{aba}$ can be calculated as

$$C^{(\ell)}_{aab} = C^{(\ell)}_{aba} = -i\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{2\Gamma(\varepsilon_a-\varepsilon_b)} + O(\Gamma^0). \tag{D8}$$

From Eq. (D3), we can see that all the others, such as $C^{(\ell)}_{abb}$ and $C^{(\ell)}_{abc}$, are at least $O(\Gamma^0)$.

In a very similar way, $D^{(\ell)}_{abcd}$ can be evaluated from

$$D^{(\ell)}_{abcd} = -\frac{f'(\varepsilon_a - i\Gamma)(\varepsilon_a-\mu-i\Gamma)^\ell}{(\varepsilon_a-\varepsilon_b-2i\Gamma)(\varepsilon_a-\varepsilon_c-2i\Gamma)(\varepsilon_a-\varepsilon_d-2i\Gamma)} + O(\Gamma^0). \tag{D9}$$

From this expression, we obtain

$$\begin{aligned} D^{(\ell)}_{aaaa} &= (\varepsilon_a-\mu)^\ell\left\{i\frac{f'(\varepsilon_a)}{8\Gamma^3} + \frac{f''(\varepsilon_a)}{8\Gamma^2} - i\frac{f'''(\varepsilon_a)}{16\Gamma}\right\} + \ell(\varepsilon_a-\mu)^{\ell-1}\left\{\frac{f'(\varepsilon_a)}{8\Gamma^2} - i\frac{f''(\varepsilon_a)}{8\Gamma}\right\} - i\frac{f'(\varepsilon_a)}{8\Gamma}\delta_{\ell,2} + O(\Gamma^0) \\ &= i\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{8\Gamma^3} + \frac{\frac{\partial}{\partial\varepsilon_a}[(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)]}{8\Gamma^2} - i\frac{\frac{\partial^2}{\partial\varepsilon_a^2}[(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)]}{16\Gamma} + O(\Gamma^0), \\ D^{(\ell)}_{\mathrm{aaab}} &= D^{(\ell)}_{aaba} = D^{(\ell)}_{\mathrm{abaa}} = \frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{4\Gamma^2(\varepsilon_a-\varepsilon_b)} - i\frac{\frac{\partial}{\partial\varepsilon_a}[(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)]}{4\Gamma(\varepsilon_a-\varepsilon_b)} + i\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{2\Gamma(\varepsilon_a-\varepsilon_b)^2} + O(\Gamma^0), \\ D^{(\ell)}_{\mathrm{aabb}} &= D^{(\ell)}_{abba} = D^{(\ell)}_{\mathrm{abab}} = -i\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{2\Gamma(\varepsilon_a-\varepsilon_b)^2} + O(\Gamma^0), \\ D^{(\ell)}_{\mathrm{aabc}} &= D^{(\ell)}_{abac} = D^{(\ell)}_{\mathrm{abca}} = -i\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{2\Gamma(\varepsilon_a-\varepsilon_b)(\varepsilon_a-\varepsilon_c)} + O(\Gamma^0), \end{aligned} \tag{D10}$$

and all the other $D^{(\ell)}_{abcd}$ are $O(\Gamma^0)$.

Using the above expansions and substituting the matrix elements in Eq. (11) for γ_μ and γ_ν, the electric and thermoelectric conductivity tensors are given as in Eq. (29). Each contribution in Eq. (29) is as follows:

$$L_{\mu\nu}^{(\ell)C,1} = \frac{e^{3-\ell}B}{mV}\sum_{\boldsymbol{k},a}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{4\Gamma^2}(\delta_{\mu y}\partial_\nu\varepsilon_a\partial_x\varepsilon_a+\delta_{\nu x}\partial_\mu\varepsilon_a\partial_y\varepsilon_a), \tag{D11}$$

$$L_{\mu\nu}^{(\ell)C,2} = \frac{e^{3-\ell}B}{mV}\sum_{\boldsymbol{k},a,b(a\neq b)}\mathrm{Im}\left[\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{2\Gamma(\varepsilon_a-\varepsilon_b)}\big(\delta_{\mu y}p_{ab,\nu}p_{ba,x}+\delta_{\nu x}p_{ba,\mu}p_{ab,y}\big)\right], \tag{D12}$$

$$L_{\mu\nu}^{(\ell),1} = \frac{e^{3-\ell}B}{\hbar^2V}\sum_{\boldsymbol{k},a}\frac{\frac{\partial}{\partial\varepsilon}[(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)]}{4\Gamma^2}\partial_\mu\varepsilon_a\partial_\nu\varepsilon_a\partial_x\varepsilon_a\partial_y\varepsilon_a, \tag{D13}$$

$$L_{\mu\nu}^{(\ell),2} = \frac{e^{3-\ell}B}{\hbar^2V}\sum_{\boldsymbol{k},a,b(a\neq b)}\mathrm{Re}\left[\left\{\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{2\Gamma^2(\varepsilon_a-\varepsilon_b)}-i\frac{\frac{\partial}{\partial\varepsilon_a}[(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)]}{2\Gamma(\varepsilon_a-\varepsilon_b)}+i\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{\Gamma(\varepsilon_a-\varepsilon_b)^2}\right\}\right.$$
$$\left.\times\,(\partial_\mu\varepsilon_a p_{ab,\nu}p_{ba,x}\partial_y\varepsilon_a+\partial_\mu\varepsilon_a\partial_\nu\varepsilon_a p_{ab,x}p_{ba,y}+p_{ba,\mu}\partial_\nu\varepsilon_a\partial_x\varepsilon_a p_{ab,y})\right], \tag{D14}$$

$$L_{\mu\nu}^{(\ell),3} = \frac{e^{3-\ell}B}{\hbar^2V}\sum_{\boldsymbol{k},a,b(a\neq b)}\mathrm{Im}\left[\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{\Gamma(\varepsilon_a-\varepsilon_b)^2}(\partial_\mu\varepsilon_a p_{ab,\nu}\partial_x\varepsilon_b p_{ba,y}+p_{ba,\mu}\partial_\nu\varepsilon_a p_{ab,x}\partial_y\varepsilon_b)\right], \tag{D15}$$

$$L_{\mu\nu}^{(\ell),4} = \frac{e^{3-\ell}B}{\hbar^2V}\sum_{\boldsymbol{k},a,b,c}{}^{'}\,\mathrm{Im}\left[\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{\Gamma(\varepsilon_a-\varepsilon_b)(\varepsilon_a-\varepsilon_c)}(\partial_\mu\varepsilon_a p_{ab,\nu}p_{bc,x}p_{ca,y}+p_{ca,\mu}\partial_\nu\varepsilon_a p_{ab,x}p_{bc,y})\right], \tag{D16}$$

$$L_{\mu\nu}^{(\ell),5} = \frac{e^{3-\ell}B}{\hbar^2V}\sum_{\boldsymbol{k},a,b(a\neq b)}\mathrm{Im}\left[\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{\Gamma(\varepsilon_a-\varepsilon_b)^2}p_{ba,\mu}p_{ab,\nu}p_{ba,x}p_{ab,y}\right], \tag{D17}$$

$$L_{\mu\nu}^{(\ell),6} = \frac{e^{3-\ell}B}{\hbar^2V}\sum_{\boldsymbol{k},a,b,c}{}^{'}\,\mathrm{Im}\left[\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{\Gamma(\varepsilon_a-\varepsilon_b)(\varepsilon_a-\varepsilon_c)}p_{ca,\mu}p_{ab,\nu}p_{ba,x}p_{ac,y}\right], \tag{D18}$$

where the summation with the prime, $\sum'$, means that all the band indices (a, b, c or a, b, c, d) are different from each other. A schematic representation of the contributions to $L_{\mu\nu}^{(\ell),1}$–$L_{\mu\nu}^{(\ell),6}$ is shown in Fig. 1.

APPENDIX E: THE DERIVATION OF THE GENERALIZED f-SUM RULES

In this Appendix, we derive the generalized f-sum rules in Eqs. (34) and (38). Using the definition of $p_{ab,\mu}$ in Eq. (11), we have

$$\sum_{b,(b\neq a)}\frac{p_{ab,\mu}p_{ba,\nu}}{\varepsilon_a-\varepsilon_b} = -\sum_{b,(b\neq a)}(\varepsilon_a-\varepsilon_b)\langle a|\partial_\mu b\rangle\langle b|\partial_\nu a\rangle. \tag{E1}$$

Since the term with $b = a$ is equal to zero on the right-hand side, we can add the $b = a$ term, resulting in the complete summation over b. Then, using the relation $\langle a|\partial_\mu b\rangle = -\langle\partial_\mu a|b\rangle$, since $\langle a|b\rangle = \delta_{ab}$, we can obtain

$$\begin{aligned}\sum_{b,(b\neq a)}\frac{p_{ab,\mu}p_{ba,\nu}}{\varepsilon_a-\varepsilon_b} &= \sum_b\langle\partial_\mu a|b\rangle(\varepsilon_a-\varepsilon_b)\langle b|\partial_\nu a\rangle\\ &= \langle\partial_\mu a|(\varepsilon_a-H_{\boldsymbol{k}})|\partial_\nu a\rangle.\end{aligned} \tag{E2}$$

Now, it is apparent that the imaginary part of the right-hand side is $iM_{\mu\nu}^a$. The real part of the right-hand side is obtained as follows. Taking the k_μ and k_ν derivative of $(\varepsilon_a - H_{\boldsymbol{k}})|a\rangle = 0$, we have

$$\left(\partial_\mu\partial_\nu\varepsilon_a-\frac{\hbar^2}{m}\delta_{\mu\nu}\right)|a\rangle+(\partial_\mu\varepsilon_a-\partial_\mu H_{\boldsymbol{k}})|\partial_\nu a\rangle+(\partial_\nu\varepsilon_a-\partial_\nu H_{\boldsymbol{k}})|\partial_\mu a\rangle+(\varepsilon_a-H_{\boldsymbol{k}})|\partial_\mu\partial_\nu a\rangle = 0. \tag{E3}$$

When we take the inner product using $\langle a|$, we obtain

$$\begin{aligned}\partial_\mu\partial_\nu\varepsilon_a-\frac{\hbar^2}{m}\delta_{\mu\nu} &= -\langle a|(\partial_\mu\varepsilon_a-\partial_\mu H_{\boldsymbol{k}})|\partial_\nu a\rangle-\langle a|(\partial_\nu\varepsilon_a-\partial_\nu H_{\boldsymbol{k}})|\partial_\mu a\rangle\\ &= \langle\partial_\mu a|(\varepsilon_a-H_{\boldsymbol{k}})|\partial_\nu a\rangle+\langle\partial_\nu a|(\varepsilon_a-H_{\boldsymbol{k}})|\partial_\mu a\rangle\\ &= 2\mathrm{Re}\langle\partial_\mu a|(\varepsilon_a-H_{\boldsymbol{k}})|\partial_\nu a\rangle,\end{aligned} \tag{E4}$$

where we have used the relation

$$(\partial_\mu \varepsilon_a - \partial_\mu H_{\boldsymbol{k}})|a\rangle = -(\varepsilon_a - H_{\boldsymbol{k}})|\partial_\mu a\rangle. \tag{E5}$$

Combining these, we obtain the generalized f-sum rule in Eq. (34).

Next, we show the other type of f-sum rule in Eq. (38). Similarly, using the definition of $p_{ab,\mu}$ in Eq. (11), we obtain

$$\sum_{b,(b\neq a)} \frac{p_{ab,\mu}p_{ba,\nu}}{(\varepsilon_a - \varepsilon_b)^2} = -\sum_{b,(b\neq a)} \langle a|\partial_\mu b\rangle\langle b|\partial_\nu a\rangle. \tag{E6}$$

Then, the term with $b = a$ in the summation is added to use the complete set of b, and it is subtracted as follows:

$$\begin{aligned}\sum_{b,(b\neq a)} \frac{p_{ab,\mu}p_{ba,\nu}}{(\varepsilon_a - \varepsilon_b)^2} &= \langle \partial_\mu a|\partial_\nu a\rangle - \langle \partial_\mu a|a\rangle\langle a|\partial_\nu a\rangle \\ &= \mathrm{Re}\langle \partial_\mu a|\partial_\nu a\rangle - \langle \partial_\mu a|a\rangle\langle a|\partial_\nu a\rangle - \frac{i}{2}\,\Omega^a_{\mu\nu},\end{aligned} \tag{E7}$$

where we have divided $\langle \partial_\mu a|\partial_\nu a\rangle$ into its real part and imaginary part.

APPENDIX F: DETAILED CALCULATIONS FOR OBTAINING THE FINAL RESULTS IN EQUATION (17)

The remaining contributions are calculated as follows. Using the generalized f-sum rule, we obtain

$$L^{(\ell)C,2}_{\mu\nu} = \frac{e^{3-\ell}B}{mV}\sum_{\boldsymbol{k},a}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{2\Gamma}\left(\delta_{\mu y}M^a_{\nu x} + \delta_{\nu x}M^a_{\mu y}\right) \tag{F1}$$

and

$$L^{(\ell),5}_{\mu\nu} + L^{(\ell),6}_{\mu\nu} = \frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{2\Gamma}\left[\left(\partial_\mu\partial_y\varepsilon_a - \frac{\hbar^2}{m}\delta_{\mu y}\right)M^a_{\nu x} + \left(\partial_\nu\partial_x\varepsilon_a - \frac{\hbar^2}{m}\delta_{\nu x}\right)M^a_{y\mu}\right]. \tag{F2}$$

Here, the Kronecker's δ functions in $L^{(\ell),5}_{\mu\nu} + L^{(\ell),6}_{\mu\nu}$ exactly cancel with $L^{(\ell)C,2}_{\mu\nu}$. Noting that the summation over c in $L^{(\ell)C,4}_{\mu\nu}$ does not contain the terms with $c = a$ and $c = b$, we obtain

$$\begin{aligned}L^{(\ell),4}_{\mu\nu} &= -\frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a,b,c}{}^{'}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{\Gamma}\mathrm{Im}[\partial_\mu\varepsilon_a(\varepsilon_c-\varepsilon_b)\langle a|\partial_\nu b\rangle\langle b|\partial_x c\rangle\langle c|\partial_y a\rangle + (\text{2nd term})] \\ &= \frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a,b(b\neq a),c(c\neq a)}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{\Gamma}\mathrm{Im}[\partial_\mu\varepsilon_a\langle a|\partial_\nu b\rangle\langle \partial_x b|c\rangle(H_{\boldsymbol{k}}-\varepsilon_b)\langle c|\partial_y a\rangle + (\text{2nd term})] \\ &= \frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a,b(b\neq a)}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{\Gamma}\mathrm{Im}[\partial_\mu\varepsilon_a\langle a|\partial_\nu b\rangle\{\langle \partial_x b|(H_{\boldsymbol{k}}-\varepsilon_b)|\partial_y a\rangle - \langle \partial_x b|a\rangle(\varepsilon_a-\varepsilon_b)\langle a|\partial_y a\rangle\} + (\text{2nd term})] \\ &= \frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a,b(b\neq a)}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{\Gamma}\mathrm{Im}[\partial_\mu\varepsilon_a\langle a|\partial_\nu b\rangle\{\langle b|(\partial_x\varepsilon_b-\partial_x H_{\boldsymbol{k}})|\partial_y a\rangle - \langle \partial_x b|a\rangle(\varepsilon_a-\varepsilon_b)\langle a|\partial_y a\rangle\} + (\text{2nd term})],\end{aligned} \tag{F3}$$

where "(2nd term)" means the contribution in which the variables (μ, ν, x, y) in the first term are replaced by (ν, x, y, μ). We can see that the term containing $\partial_x\varepsilon_b$ in the last line exactly cancels with that in $L^{(\ell),3}_{\mu\nu}$. Therefore, we can take the summation over b in the total of $L^{(\ell),3}_{\mu\nu}$ and $L^{(\ell),4}_{\mu\nu}$ as follows:

$$\begin{aligned}L^{(\ell),3}_{\mu\nu} + L^{(\ell),4}_{\mu\nu} = \frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{\Gamma}&\mathrm{Im}[\partial_\mu\varepsilon_a\{\langle \partial_\nu a|\partial_x H_{\boldsymbol{k}}|\partial_y a\rangle - \langle \partial_\nu a|a\rangle\langle a|\partial_x H_{\boldsymbol{k}}|\partial_y a\rangle - \langle \partial_\nu a|(\varepsilon_a - H_{\boldsymbol{k}})|\partial_x a\rangle\langle a|\partial_y a\rangle\} \\ &+ (\text{2nd term})].\end{aligned} \tag{F4}$$

Considering that $\langle a|\partial_\mu a\rangle$ is purely imaginary and using the relation in Eq. (E4), we can see

$$\begin{aligned}L^{(\ell),3}_{\mu\nu} + L^{(\ell),4}_{\mu\nu} = \frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{\Gamma}\mathrm{Im}\Bigg[&\partial_\mu\varepsilon_a\Bigg\{\langle \partial_\nu a|\partial_x H_{\boldsymbol{k}}|\partial_y a\rangle - \frac{1}{2}\partial_x\partial_y\varepsilon_a\langle \partial_\nu a|a\rangle \\ &- \frac{1}{2}\left(\partial_\nu\partial_x\varepsilon_a - \frac{\hbar^2}{m}\delta_{\nu x}\right)\langle a|\partial_y a\rangle\Bigg\} + \partial_\nu\varepsilon_a\Bigg\{\langle \partial_x a|\partial_y H_{\boldsymbol{k}}|\partial_\mu a\rangle - \frac{1}{2}\left(\partial_\mu\partial_y\varepsilon_a - \frac{\hbar^2}{m}\delta_{\mu y}\right)\langle \partial_x a|a\rangle - \frac{1}{2}\partial_x\partial_y\varepsilon_a\langle a|\partial_\mu a\rangle\Bigg\}\Bigg],\end{aligned} \tag{F5}$$

where we have used the relation

$$\mathrm{Re}\langle a|\partial_\mu H_{\boldsymbol{k}}|\partial_\nu a\rangle = \mathrm{Re}\langle a|(\partial_\mu H_{\boldsymbol{k}} - \partial_\mu\varepsilon_a)|\partial_\nu a\rangle = \mathrm{Re}\langle\partial_\mu a|(\varepsilon_a - H_{\boldsymbol{k}})|\partial_\nu a\rangle = \frac{1}{2}\left(\partial_\mu\partial_\nu\varepsilon_a - \frac{\hbar^2}{m}\delta_{\mu\nu}\right). \tag{F6}$$

The final form of Eq. (F5) can be rewritten in a compact form using the following relation. Taking the inner product of Eq. (E3) with $\langle\partial_\tau a|$, we obtain

$$\begin{aligned}0 &= \left(\partial_\mu\partial_\nu\varepsilon_a - \frac{\hbar^2}{m}\delta_{\mu\nu}\right)\langle\partial_\tau a|a\rangle + \langle\partial_\tau a|(\partial_\mu\varepsilon_a - \partial_\mu H_{\boldsymbol{k}})|\partial_\nu a\rangle + \langle\partial_\tau a|(\partial_\nu\varepsilon_a - \partial_\nu H_{\boldsymbol{k}})|\partial_\mu a\rangle + \langle\partial_\tau a|(\varepsilon_a - H_{\boldsymbol{k}})|\partial_\mu\partial_\nu a\rangle \\ &= \left(\partial_\mu\partial_\nu\varepsilon_a - \frac{\hbar^2}{m}\delta_{\mu\nu}\right)\langle\partial_\tau a|a\rangle + \partial_\mu[\langle\partial_\tau a|(\varepsilon_a - H_{\boldsymbol{k}})|\partial_\nu a\rangle] - \langle\partial_\tau\partial_\mu a|(\varepsilon_a - H_{\boldsymbol{k}})|\partial_\nu a\rangle + \langle\partial_\tau a|(\partial_\nu\varepsilon_a - \partial_\nu H_{\boldsymbol{k}})|\partial_\mu a\rangle.\end{aligned} \tag{F7}$$

By subtracting the same equation with μ and τ exchanged and taking the imaginary part, we obtain

$$0 = \left(\partial_\mu\partial_\nu\varepsilon_a - \frac{\hbar^2}{m}\delta_{\mu\nu}\right)\mathrm{Im}\langle\partial_\tau a|a\rangle - \left(\partial_\tau\partial_\nu\varepsilon_a - \frac{\hbar^2}{m}\delta_{\tau\nu}\right)\mathrm{Im}\langle\partial_\mu a|a\rangle + \partial_\mu M^a_{\tau\nu} - \partial_\tau M^a_{\mu\nu} - \partial_\nu\varepsilon_a\Omega^a_{\tau\mu} - 2\mathrm{Im}\langle\partial_\tau a|\partial_\nu H_{\boldsymbol{k}}|\partial_\mu a\rangle. \tag{F8}$$

When we apply this equation to Eq. (F5), we obtain

$$L^{(\ell),3}_{\mu\nu} + L^{(\ell),4}_{\mu\nu} = \frac{e^{3-\ell}B}{\hbar^2 V}\sum_{\boldsymbol{k},a}\frac{(\varepsilon_a-\mu)^\ell f'(\varepsilon_a)}{2\Gamma}\left\{\partial_\mu\varepsilon_a\left(\partial_y M^a_{\nu x} - \partial_\nu M^a_{yx} - \partial_x\varepsilon_a\Omega^a_{\nu y}\right) + \partial_\nu\varepsilon_a\left(\partial_\mu M^a_{xy} - \partial_x M^a_{\mu y} - \partial_y\varepsilon_a\Omega^a_{x\mu}\right)\right\}. \tag{F9}$$

When we sum all the terms and carry out the integration by parts, we obtain Eq. (17).

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