GEOMETRIC THEORY OF THE NATURAL OPTICAL ACTIVITY IN NONCENTROSYMMETRIC METALS

by

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ABSTRACT

Ignited by the chiral anomaly of recently discovered Weyl (semi-)metals, we study the chiral magnetic effect and the natural optical activity of noncentrosymmetric metals. Both phenomena are related to the linear-in-$q$ spatial dispersion of the optical conductivity tensor, and can be calculated within the formalism of the semiclassical kinetic equation. Therefore, we calculate the dispersion of optical conductivity up to the linear order of the wave vector, in the low frequency regime, with both the semiclassical Boltzmann equation and the Kubo formula. The two different methods of calculation provide us the same result. In this result, the static and dynamic chiral magnetic effects are revealed to have different origin: one comes from topology, related to Berry monopoles, and the other has a geometric origin, which is determined by the orbital magnetic moment. The Faraday rotation of the polarization of light transmitted through a slab of the sample provides us the most direct way to measure the magnitude of dynamic chiral magnetic effect. We develop an effective medium theory for electromagnetic wave propagating through gapless nonuniform systems, to calculate macroscopic sample inhomogeneities induced corrections to the chiral magnetic conductivity. We show that, in metals with low carrier density, the way in which macroscopic fluctuations of the local conductivity affect the frequency dependent of the measured optical polarization rotation angle: by creating a sharp feature near the plasma edge, which can be detected by experiments. Then we narrow down our research a bit further to the current induced magnetization.

In this thesis, I start with an introduction of some fundamental concepts and semiclassical transport theory which has been used throughout this thesis. Then, I give a brief review of the recent development of Weyl semimetal, in which I show the purpose and concentration of our research. Chapter 3 and chapter 5 are the main parts of our research, which are published papers. Chapter 4 is, generally speaking, a glance of our current work. The appendices present Kubo formula derivations.
I would like to dedicate this thesis to my parents, who always give me absolute understanding and support during my life. I also want to dedicate this thesis to all my friends. Life would be miserable without you guys.
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### NOTATION AND SYMBOLS

| Symbol | Description |
|--------|-------------|
| $\alpha$ | fine-structure (dimensionless) constant, approximately $1/137$ |
| $c$ | speed of light |
| $C$ | Chern number |
| $\delta(x)$ | Dirac’s famous function |
| $\nabla$ | nabla operator, a vector differential operator |
| $e$ | the charge of an electron, $e \approx -1.6 \times 10^{-19}$ coulombs |
| $\varepsilon_0$ | vacuum permittivity, $\varepsilon_0 \approx 8.85 \times 10^{-12} \text{ F/m}$ |
| $f(r, k, t)$ | electron distribution function |
| $g_{ab}$ | gyrotropic tensor |
| $\gamma(\omega)$ or $\eta(\omega)$ | chiral magnetic conductivity |
| $\gamma_n$ | Berry phase |
| $A_n$ | Berry connection |
| $\Omega_n$ | Berry curvature |
| $h$ | reduced Planck’s constant, with a value of $\sim 6.58 \times 10^{16} \text{ eV} \cdot \text{s/rad}$ |
| $\hbar$ | Planck’s constant, equals $2\pi \hbar$ |
| $T$ | inversion symmetry |
| $\mathcal{T}$ | time reversal symmetry |
| $m$ | magnetic moment |
| $\mu$ | chemical potential |
| $\mu_0$ | vacuum permeability, $\mu_0 = 4\pi \times 10^{-7} \text{ H/m}$ |
| $\sigma_{ij}$ | conductivity tensor |
| $\sigma$ | a triplet of Pauli matrices: $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ |
| $\omega_c$ | cyclotron frequency, $\omega_c = qB/m$ |
| $\Phi_0$ | the quantum of flux, $\Phi_0 = h/e$ |
| $Q$ | chirality |
| $\tau$ | relaxation time |
| $\text{Tr}$ | trace |
| $v_F$ | Fermi velocity |
| $p_F$ | Fermi momentum |
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CHAPTER 1

INTRODUCTION: BASIC CONCEPTS IN GEOMETRIC BAND THEORY
The last decade has witnessed the flourishing in condensed matter field, especially in the study of systems with unconventional band structures, which are topologically protected, like graphene and topological insulator, or the recent Weyl semimetal. To study the transport properties of these materials, the most common way is applying some electromagnetic field on them. Theoretically, the most common method used is the semi-classical transport theory based on the Boltzmann transport equations. This chapter will start with Berry phase, the most basic and important concept of geometric band theory. After that, I will introduce the basic idea of semi-classical transport theory. In general, this chapter is a detailed introduction of some basic concepts and methods used in studying those topological band systems.

1.1 Berry phase, Berry connection and Berry curvature

Berry phase or Pancharatnam-Berry phase (named after S. Pancharatnam and Sir Michael Berry, as it was first discovered by S. Pancharatnam in 1956 [1], then rediscovered by M. V. Berry in 1984[2]) is the most important concept in geometric band theory. However, its discovery was not specifically related to Bloch-periodic system, but to the general idea of quantum adiabatic transport. It is the geometric phase difference gained through a path of a cycle when a system is under a cyclic adiabatic process, which results from the geometrical properties of the parameter space of the Hamiltonian of the system. The so-called “Berry connection” and “Berry curvature” are local gauge potential and gauge field associated with the Berry phase.

1.1.1 General Formalism of Berry Phase

In quantum mechanics, the Berry phase emerges in a cyclic adiabatic evolution. The adiabatic theorem, introduced by Max Born and Vladimir Fock in 1928[3], states that a physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian’s spectrum. We consider such system with a Hamiltonian \( H(\mathbf{R}) \) that depends on time through a vector parameter \( \mathbf{R} = (R_1, R_2, R_3, \ldots) \). Here \( R_i = R_i(t) \) are slowly varying parameters, which can be anything, such as electric field, magnetic field, strains and so on. By slowly varying, we mean that \( \mathbf{R} \) changes slightly during the period of
motion $T$: $T \frac{dR}{dt} \ll R[4]$. Denote an instantaneous orthonormal basis of the instantaneous eigenstates as $|n(R)\rangle$:

$$H(R)|n(R)\rangle = E_n(R)|n(R)\rangle.$$ (1.1)

This equation determines the eigenfunction $|n(R)\rangle$ up to a phase. We want to study the phase of the wave function of a system that starts from an initial pure state $|n(R(0))\rangle$ as we move $R(t)$ along the path $C$.

Assuming that the eigenstates $E_n(R)$ is non-degenerate everywhere along $C$, then according to the adiabatic theorem, as $R(t)$ varies slowly along $C$, $|n(R(0))\rangle$ evolves with $H(R)$, and hence $|n(R(t))\rangle$ stays as an instantaneous eigenstate of $H(R(t))$ during the whole process. Still, there can be arbitrary phases which may evolve with $R$ as well. Let’s assume an eigenstate $|\psi_n(t)\rangle$ which differs from $|n(R(t))\rangle$ only by a phase factor $\theta(t)$:

$$|\psi_n(t)\rangle = e^{-i\theta(t)}|n(R(t))\rangle.$$ Applying $H(R(t))$ on it, we have

$$H(R(t))|\psi_n(t)\rangle = i \frac{\partial}{\partial t} |\psi_n(t)\rangle,$$ (1.2)

which gives

$$E_n(R(t))e^{-i\theta(t)}|n(R(t))\rangle = i \frac{\partial}{\partial t} (e^{-i\theta(t)}|n(R(t))\rangle) = e^{-i\theta(t)}\frac{\partial \theta(t)}{\partial t} |n(R(t))\rangle + i e^{-i\theta(t)} \frac{\partial}{\partial t} |n(R(t))\rangle.$$ (1.3)

Here one may have noticed that I use the so-called natural unit system, and hence take $\hbar \rightarrow 1$.

Multiplying $\langle \psi_n(t) \rangle = \langle n(R(t)) | e^{i\theta(t)} \rangle$ on both sides, we end up with

$$\frac{\partial \theta(t)}{\partial t} = E_n(R(t)) - i \langle n(R(t)) | \frac{\partial}{\partial t} |n(R(t))\rangle,$$ (1.4)

since $|n(R(t))\rangle$ is normalized: $\langle n(R(t)) | n(R(t)) \rangle = 1$. Integrate from 0 to $t$, we get

$$\theta(t) = \int_0^t E_n(R(t'))dt' - i \int_0^t \langle n(R(t')) | \frac{\partial}{\partial t'} |n(R(t'))\rangle dt'.$$ (1.5)

Therefore, regarding the phase, the state at time $t$ can be written as

$$|\psi_n(t)\rangle = e^{i\gamma_n} e^{-i \int_0^t E_n(R(t'))dt'} |n(R(t))\rangle.$$ (1.6)

The second exponential term $e^{-i \int_0^t E_n(R(t'))dt'}$ is the “dynamic phase factor”, while the first phase term is the famous Berry phase:

$$\gamma_n = i \int_0^t \langle n(R(t')) | \frac{\partial}{\partial t'} |n(R(t'))\rangle dt'.$$ (1.7)
Time can be removed explicitly from this formula:

\[
\gamma_n = i \int_{t_{\text{end cycle}}}^{t_{\text{end}}} \langle n(R(t')) | \partial_{\partial t'} | n(R(t')) \rangle \frac{\partial R}{\partial t'} dt' = i \int_C \langle n(R) | \nabla_R | n(R) \rangle dR,
\]

indicating that the Berry phase only depends on the path in the parameter space, and has nothing to do with the rate at which the path is traversed. It is a geometric phase. We also notice that the Berry phase \(\gamma_n\) is real (it’s Berry phase, not Berry decay), since \(\langle n(R) | \nabla_R | n(R) \rangle\) is purely imaginary: \(\langle n(R) | n(R) \rangle = 1 \Rightarrow \langle n(R) | \nabla_R | n(R) \rangle = -\langle n(R) | \nabla_R | n(R) \rangle^*\). Therefore, the Berry phase can also be written as

\[
\gamma_n = -\text{Im} \int_C \langle n(R) | \nabla_R | n(R) \rangle dR.
\]

### 1.1.2 From Aharonov-Bohm effect to Berry connection and Berry curvature

The first geometric phase studied and observed was Aharonov-Bohm effect, which is an effect happened in real space, unlike the Berry phase, which is a geometric phase in momentum space. Aharonov-Bohm effect is a phenomenon in which a charged particle is affected by vector potential \(A\), despite being confined to a region in which both the magnetic field \(B\) and electric field \(E\) are zero. Before the discovery of Aharonov-Bohm effect, people believe that the vector potential \(A\) was introduced into physics only as a mathematical crutch, as there was no magnetic monopole discovered: \(\nabla \cdot B = \rho_M = 0 \Rightarrow B = \nabla \times A\). It was widely believed that vector potential \(A\) should not have any physical meaning or any physical effect, as said by the distinguished nineteenth-century physicist Heaviside: “Physics should be purged of such rubbish as the scalar and vector potentials; only the fields \(E\) and \(B\) are physical.”

The Aharonov-Bohm effect was brought out in 1959[5]. The idea is: Considering an electron passing by an infinite solenoid which has a magnetic field \(B\) confined in it, see Fig.1.1. The electromagnetic theory implies that by traveling along a path, the electron acquires a phase \(\varphi = e \int_P \mathbf{A} \cdot d\mathbf{x}\). Thus, when calculate the probability for the propagation, there will be an interference between the contributions from path 1 and path 2

\[
(e^{ie \int_{P_1} \mathbf{A} \cdot d\mathbf{x}})(e^{ie \int_{P_2} \mathbf{A} \cdot d\mathbf{x}})^* = e^{ie \int B d\mathbf{S}} = e^{ie \Phi_B}.
\]

The electron feels the magnetic potential in the region where the magnetic field is zero. Therefore, the vector potential is essential in physics.
**Figure 1.1.** Magnetic solenoid effect. Confined magnetic field in the infinite solenoid affects the phase of the electrons traveling beside it.

Similarly, we can define a “vector potential” for Berry phase, which is called Berry connection:

\[
\mathcal{A}_n(R) = i\langle n(R) | \nabla_R | n(R) \rangle, \quad \gamma_n = \int_C dR \cdot \mathcal{A}_n(R). \tag{1.11}
\]

Just like the vector potential \(A\), the Berry connection \(\mathcal{A}_n\) is gauge dependent. Under a gauge transformation \(|n(R)\rangle \rightarrow e^{i\zeta(R)}|n(R)\rangle\), where \(\zeta(R)\) is a smooth, single-valued function. The Berry connection transforms in the usual way:

\[
\mathcal{A}_n(R) \rightarrow \mathcal{A}_n(R) - \frac{\partial}{\partial R} \zeta(R), \tag{1.12}
\]

so that the Berry phase is changed by

\[
\gamma_n \rightarrow \gamma_n - \int_C \frac{\partial}{\partial R} \zeta(R) = \gamma_n - \zeta(R_f) + \zeta(R_i). \tag{1.13}
\]

Here \(R_i\) and \(R_f\) stand for the initial and final \(R\) respectively when moving along path \(C\). One may doubt whether we will always be able to cancel the Berry phase by a smart choice of the gauge factor \(\zeta(R)\). The answer is no. We can consider a closed path \(C\), \(R_f = R_i\), hence \(|n(R_f)\rangle = |n(R_i)\rangle\). Gauge transformation must maintain this property \(e^{i\zeta(R)}|n(R_i)\rangle = e^{i\zeta(R)}|n(R_f)\rangle = e^{i\zeta(R_f)}|n(R_f)\rangle\). Therefore, \(\zeta(R_f) - \zeta(R_i) = 2\pi m\), where \(m\) stands for any integer. That is to say, under a closed path, the Berry phase cannot be canceled unless it is equal to \(2\pi\) times an integer. Therefore, Berry phase is not trivial.[6]

Considering only closed paths, with Stoke’s theorem, the “field”, Berry curvature is obtained as:

\[
\Omega_n(R) = \nabla_R \times \mathcal{A}_n = i \langle \nabla_R n(R) | \times | \nabla_R n(R) \rangle, \tag{1.14}
\]

\[
\gamma_n = \int_C dR \cdot \mathcal{A}_n(R) = i \int_S dS \cdot (\nabla \times \langle n(R) | \nabla_R | n(R) \rangle)
\]

\[
= i \int_S dS \epsilon_{ijk} \nabla_j \langle n(R) | \nabla_k | n(R) \rangle) = \int_S dS \cdot \Omega_n(R). \tag{1.15}
\]
Here I need to add a comment: The discovery of Aharonov-Bohm effect does not confirm that the magnetic monopole should not exist.[7] In other words, the existence of magnetic monopole does not conflict the reality of vector potential $\mathbf{A}$, even though the magnetic monopole can be written as the divergency of the magnetic field, $\nabla \cdot \mathbf{B} = \nabla \cdot (\nabla \times \mathbf{A})$, and the divergence of the curl of a vector field is zero. $\nabla \cdot (\nabla \times \mathbf{A}) = 0$ is actually the “Bianchi identity”($dd = 0$) in electromagnetism: acting differential operation $d$ on any form twice gives zero[8]. ($A = A_\mu dx^\mu$ is the potential 1-form, with $A_\mu$ denoting the electromagnetic 4-potential. $F = (1/2!)F_{\mu \nu} dx^\mu \wedge dx^\nu$ is the field 2-form, with $F_{\mu \nu}$ denoting the electromagnetic tensor. Of course $F = dA$). The Poincaré lemma states that a closed form is locally exact. (A $p$-form $\alpha$ is said to be closed when $d\alpha = 0$, and it is exact if there exists a $(p-1)$-form $\beta$ such that $\alpha = d\beta$). Thus, if the curl of a vector field vanishes, the vector field is locally the gradient of some scalar field; if the divergence of a vector field vanishes, the vector field is locally the curl of some vector field. However, a closed form does not need to be globally exact, while only globally exact form ensure a trivial result after integrating over the whole manifold. Just think about a sphere surrounding a magnetic monopole with magnetic charge $g$. The magnetic 2-form is $F = (g/2\pi)d \cos \theta d\phi$. Then we find that the potential 1-form $A$ is well-defined everywhere except for that on the south pole or north pole of the sphere, and that is essentially how we end up with a possible nonzero magnetic monopole. Similar to this, we may have Berry monopoles in reciprocal space which gives nonzero Chern number.

### 1.1.3 Berry phase in Bloch band theory

As mentioned at the very beginning, the Berry phase was studied since 1959, but those works around it were mainly on quantum adiabatic transport. It had not been related to the Bloch-periodic system until 1984, a Japanese guy Mahito Kohmoto[9], as well as a group of people from University of Washington, Qian Liu, D. J. Thouless and Yong-Shi Wu[10], build a relation between the Berry curvature and the Hall conductivity, making the Berry phase a significant concept in topological band theory. In Bloch band theory, because of the periodic structure of lattices, the Hamiltonian eigenstates are expressed as

$$
\psi_{\nu k} = e^{ik \cdot r} u_{\nu k}(r),
$$

(1.16)
where \( n \) is a band index, \( \mathbf{k} \) is a wave vector in the reciprocal-space (Brillouin zone), and \( u_{n\mathbf{k}}(\mathbf{r}) \) is a periodic function of \( \mathbf{r} \). Letting \( \mathbf{k} \) play the role of the parameter \( \mathbf{R} \), one can define Berry connections, and Berry curvatures in the reciprocal space:

\[
\mathcal{A}_n(\mathbf{k}) = i \langle n(\mathbf{k})|\nabla_{\mathbf{k}}|n(\mathbf{k})\rangle, \quad (1.17)
\]

\[
\Omega_n(\mathbf{k}) = i \langle \nabla_{\mathbf{k}} n(\mathbf{k})| \times |\nabla_{\mathbf{k}} n(\mathbf{k})\rangle. \quad (1.18)
\]

The Berry phase across the Brillouin zone is called Zak’s phase

\[
\gamma_n = \oint d\mathbf{k} \cdot \langle n(\mathbf{k})|\nabla_{\mathbf{k}}|n(\mathbf{k})\rangle = \oint d\mathbf{k} \cdot \mathcal{A}_n(\mathbf{k}) = \oint_{BZ} d\mathbf{k} \cdot \Omega_n(\mathbf{k}) = 2\pi C, \quad (1.19)
\]

where \( C \) is the Chern number.

For a two-dimensional band insulator, the Hall conductivity of it is given by

\[
\sigma_{xy} = \frac{e^2}{\hbar} \int_{BZ} \frac{d^2k}{(2\pi)^2} \Omega_{k_x,k_y}. \quad (1.20)
\]

Here, the \( \hbar \) is restored, and this expression is in CGS.

### 1.1.3.1 Position operator

We know that without lattice, the momentum operator \( \mathbf{p} = -i\hbar \nabla_{\mathbf{r}} \) and the position operator \( \mathbf{r} = i\hbar \nabla_{\mathbf{p}} \), which can be straightly forward obtained by plane wave expansion:

\[
\Psi(\mathbf{k}) = \int d\mathbf{r} \Psi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}, \quad (1.21)
\]

\[
\Psi(\mathbf{r}) = \int d\mathbf{k} \Psi(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (1.22)
\]

\[
\mathbf{k} \Psi(\mathbf{r}) = \int d\mathbf{k} \mathbf{k} \Psi(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} = \int d\mathbf{k} \Psi(\mathbf{k})(-i\partial_{\mathbf{k}}) e^{i\mathbf{k}\cdot\mathbf{r}} = -i \nabla_{\mathbf{r}} \Psi(\mathbf{r}), \quad (1.23)
\]

\[
\mathbf{r} \Psi(\mathbf{k}) = \int d\mathbf{r} \mathbf{r} \Psi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} = \int d\mathbf{r} \Psi(\mathbf{r})(i\partial_{\mathbf{k}}) e^{-i\mathbf{k}\cdot\mathbf{r}} = i \nabla_{\mathbf{k}} \Psi(\mathbf{k}). \quad (1.24)
\]

By restoring \( \hbar \) (or \( \mathbf{p} = \hbar \mathbf{k} \)), we get the operators which we are familiar with. Also, but less straight forward we can get the position operator in momentum space by

\[
\mathbf{r} \Psi(\mathbf{r}) = \int d\mathbf{k} (\mathbf{r} \Psi(\mathbf{k})) e^{i\mathbf{k}\cdot\mathbf{r}} = \int d\mathbf{k} \mathbf{r} \Psi(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} = \int d\mathbf{k} \Psi(\mathbf{k})(-i\partial_{\mathbf{k}}) e^{i\mathbf{k}\cdot\mathbf{r}} = \int d\mathbf{k} (i \nabla_{\mathbf{k}} \Psi(\mathbf{k})) e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (1.25)
\]

Here, we use \( \mathbf{r} \) to denote the operator and distinguish with the vector \( \mathbf{r} \). What happens if we have a lattice?
Similarly, any wave function can be written as a superposition of the Bloch waves, in the case of lattice:

\[ \Psi(r) = \sum_n \int dk \Psi_n^*(k) u_{nk}(r) e^{ik \cdot r}. \] (1.26)

To obtain the position operator \( r \) in momentum space, we need to do the same thing as what we did in Eq.(1.25):

\[
\begin{align*}
\begin{align*}
\hat{r}\Psi(r) &= \sum_n \int dk (\hat{r}\Psi_n^*(k)) u_{nk}(r) e^{ik \cdot r} = \sum_n \int dk \Psi_n^*(k) u_{nk}(r) (\frac{\partial}{\partial \mathbf{r}}) e^{ik \cdot r} \\
&= \sum_n \int dk \left\{ (i\mathbf{\nabla}_k \Psi_n(k)) u_{nk}(r) e^{ik \cdot r} + \Psi_n(k) \left( \frac{\partial}{\partial \mathbf{r}} \right) u_{nk}(r) e^{ik \cdot r} \right\} \\
&= \sum_n \int dk \left\{ (i\mathbf{\nabla}_k \Psi_n(k)) u_{nk}(r) e^{ik \cdot r} + \Psi_n(k) \left( \int dr' \delta(r - r') i\partial_{\mathbf{r}} u_{nk}(r') \right) e^{ik \cdot r} \right\} \\
&= \sum_n \int dk \left\{ (i\mathbf{\nabla}_k \Psi_n(k)) u_{nk}(r) e^{ik \cdot r} + \Psi_n(k) \sum_{m} \int dr' u_{mk}^*(r') i\partial_{\mathbf{r}} u_{nk}(r') \right\} e^{ik \cdot r} \\
&= \sum_n \int dk \left\{ (i\mathbf{\nabla}_k \Psi_n(k)) u_{nk}(r) e^{ik \cdot r} + \Psi_n(k) \sum_{m} \mathcal{A}_{mn}(k) u_{mk}(r) e^{ik \cdot r} \right\} \\
&= \sum_n \int dk \left\{ \sum_{m} (i\mathbf{\nabla}_k \delta_{mn} + \mathcal{A}_{mn}(k)) \Psi_n(k) \right\} u_{nk}(r) e^{ik \cdot r} \\
&= \sum_n \int dk \left\{ \sum_{m} (i\mathbf{\nabla}_k \delta_{mn} + \mathcal{A}_{mn}(k)) \Psi_m(k) \right\} u_{nk}(r) e^{ik \cdot r}. \tag{1.27}\end{align*} \end{align*}
\]

Therefore, we have

\[ \hat{r}\Psi_n(k) = \sum_{m} (i\mathbf{\nabla}_k \delta_{mn} + \mathcal{A}(k)) \Psi_m(k), \] (1.28)

thus, the position operator in reciprocal lattice (here I took the tilde off, since there is no need to make distinction) is

\[ \mathbf{r}_{mn} = \sum_{m} i\mathbf{\nabla}_k \delta_{mn} + \mathcal{A}_{mn}. \] (1.29)

For single band \( n \), we have

\[ \mathbf{r} = i\nabla_k + \mathcal{A}_n. \] (1.30)

This result can be compared to the momentum operator for a charged particle:

\[ \mathbf{p} = -i\nabla + e\mathbf{A}. \] (1.31)
1.1.3.2 Equations of motion

It is well known that the equation of motion for a particle with charge $e$ under the electromagnetic field is

$$\dot{p} = F = eE + e\dot{r} \times B = -e\nabla\phi + e\dot{r} \times (\nabla \times A), \quad (1.32)$$

which is just Lorentz force. The dual equation is easily guessed out, as shown previously that $p$ and $r$ are conjugate variables, and $A$ acts just like $A$, $\Omega_n$ acts just like $B$ in the momentum space: (Also, this equation can be carefully derived, see the reference [11])

$$\dot{r} = \frac{e_{np}}{\partial p} - \dot{p} \times (\nabla_p \times A_n) = v_{np} - \dot{p} \times \Omega_{np}. \quad (1.33)$$

These two equations are tangled with each other. We want to separate $\dot{r}$ and $\dot{p}$ out. Taking the Lorentz force equation into the velocity equation, we have

$$\dot{r} = v_{np} - eE \times \Omega_{np} - e\dot{r} \times B \times \Omega_{np} = v_{np} - eE \times \Omega_{np} + e\dot{r}(\Omega_{np} \cdot B) - eB(\Omega_{np} \cdot \dot{r}). \quad (1.34)$$

Take the third term on the right hand side to the left hand side:

$$(1 - eB \cdot \Omega_{np})\dot{r} = v_{np} - eE \times \Omega_{np} - eB(\Omega_{np} \cdot \dot{r}). \quad (1.35)$$

Take dot product with $\Omega_{np}$ on both sides of the equation:

$$(1 - eB \cdot \Omega_{np})\dot{r} \cdot \Omega_{np} = v_{np} \cdot \Omega_{np} - e(B \cdot \Omega_{np})(\Omega_{np} \cdot \dot{r}). \quad (1.36)$$

$$\Rightarrow \dot{r} \cdot \Omega_{np} = v_{np} \cdot \Omega_{np}. \quad (1.37)$$

Substitute it into Eq.(1.35). Finally, we get

$$\dot{r} = \frac{1}{1 - eB \cdot \Omega_{np}} [v_{np} - eE \times \Omega_{np} - eB(v_{np} \cdot \Omega_{np})]. \quad (1.38)$$

The first term is the normal group velocity; the second term is the anomalous velocity appeared due to the interband coherence effects induced by the electric part of Lorentz force; the third term is interband coherence effects induced by the magnetic part of Lorentz force.

Same way, we obtain

$$\dot{p} = \frac{1}{1 - eB \cdot \Omega_{np}} [eE + ev_{np} \times B - e^2(E \cdot B)\Omega_{np}]. \quad (1.39)$$

The first and second terms represent Lorentz force, and the third term is the origin of chiral anomaly.
1.1.4 Time reversal symmetry and inversion symmetry

In this section, I am going to talk about the time-reversal symmetric $\mathcal{T}$ and inversion symmetric $\mathcal{I}$ properties of Berry curvature and Chern number.

Time reversal symmetry $\mathcal{T}$ can be represented by

$$ T = UK, \quad (1.40) $$

where $U$ is a unitary matrix and $K$ is complex conjugation. It changes $k$ to $-k$, $i$ to $-i$, and the periodic part of the Bloch wave function this way:

$$ \mathcal{T} u_n(k)(r) = u_n^*(r), \quad (1.41) $$

Act time reversal symmetry on Berry connection $A_n(k) = i \langle u_n^{[k]} | \nabla_k | u_n^{[k]} \rangle$:

$$ \mathcal{T} A_n(k) = -i \langle \mathcal{T} u_n | -\nabla_k | \mathcal{T} u_n \rangle = -i \int d\mathbf{r} u_{n,-k}^*(\mathbf{r}) \partial_k u_{n,-k}^*(\mathbf{r}) = -i \int d\mathbf{r} u_{n,-k}^*(\mathbf{r}) \partial_k u_{n,-k}^*(\mathbf{r}) = A_n(-k). \quad (1.42) $$

If a system has time reversal symmetry,

$$ \mathcal{T} A_n(k) = A_n(k) + \nabla_k \zeta(k) \Rightarrow A_n(-k) = A_n(k) + \nabla_k \zeta(k), \quad (1.43) $$

$A_n(-k)$ and $A_n(k)$ differ only by a gauge transformation $\nabla_k \zeta(k)$.

Under time reversal symmetry, the Berry curvature $\Omega_n(k) = i \epsilon_{ijl} \langle \partial_i u_n^{[k]} | \partial_l u_n^{[k]} \rangle$ changes:

$$ \mathcal{T} \Omega_n(k) = \Omega_n(k), \quad (1.44) $$

Thus, the Berry curvature $\Omega_n(k)$ is an odd function of $k$. Since the Chern number is the total integral of Berry curvature over the whole Brillouin Zone, it must vanish when Berry curvature is an odd function. Therefore, a system with time reversal symmetry always has zero Chern number.
The inversion $\mathcal{I}$ changes $k$ to $-k$, and the periodic part of Bloch wave function this way:

$$\mathcal{I}u_{nk}(r) = u_{n,-k}(-r). \quad (1.46)$$

Act on the Berry connection:

$$\mathcal{I}\mathcal{A}_n(k) = i\langle\mathcal{I}u_{nk}| -\nabla_k|\mathcal{I}u_{nk}\rangle = \mathcal{A}_n(-k). \quad (1.47)$$

Therefore, if a system has inversion symmetry,

$$\mathcal{I}\mathcal{A}_n(k) = \mathcal{A}_n(k) + \nabla_k \zeta(k) \Rightarrow \mathcal{A}_n(-k) = \mathcal{A}_n(k) + \nabla_k \zeta(k), \quad (1.48)$$

$\mathcal{A}_n(-k)$ and $\mathcal{A}_n(k)$ differs only by a gauge transformation $\nabla_k \zeta(k)$.

Act inversion on Berry curvature:

$$\mathcal{I}\Omega_n(k) = \Omega_n(-k). \quad (1.49)$$

If a system is invariant under $\mathcal{I}$:

$$\Omega_n(-k) = \Omega_n(k). \quad (1.50)$$

Berry curvature should be an even function over $k$.

If a system has both time reversal symmetry and inversion symmetry, the Berry curvature is both odd and even over $k$, thus vanish everywhere in the Brillouin zone. That is essentially the reason why we need to break one of these two symmetries in order to get a topological nontrivial Weyl semi-metal.

### 1.2 Semi-classical transport: Wave packet and Boltzmann equation

Semi-classical theory is a theory in which one part is described with quantum mechanism while the other part is described classically. Transport properties of electrons in crystals are usually studied by semi-classical transport theory. In the free electron theory, electrons move between two collisions according to the classical equations of motion, while the collisions obey the quantum mechanical Fermi-Golden rule. Therefore, semi-classical models are natural choices. Taking the periodic structure of crystal structure into account, the free electron models have to be extended by the Bloch’s theory, in which the electrons
are described by Bloch’s wave functions. How could the motion between two collisions being classical? Thus, we need the concept of wave packet.

Essentially, electron transport in the crystal is a complicated quantum mechanical many-body problem: we’ve taken the periodic structure of the crystal into the Hamiltonian to get the Bloch’s wave function, but we still need to consider the impurities, crystal defects, and thermal vibrations of the irons, which is electron-phonon interaction. Even if we are lucky enough to find a solution, which must be rather complicated, it would be hard to extract transport properties from the solution. Therefore, a semi-classical theory is preferred, and a statistical treatment is required. Since we are working with statistical mechanism, we need to get the distribution function of the electrons, and that is why Boltzmann equation lies at the heart of the transport theory.

In this part, I will give a short introduction to the wave packet construction, which is the basis for the semi-classical theories, and the Boltzmann equation, which plays a key role in the transport mechanism.

1.2.1 Wave packet construction and its orbital moment

From the quantum mechanical point of view, the equations of motion of electrons in periodic potential describe the behavior of wave packets constructed by the superposition of single free electron eigenstates. Therefore, a semi-classical theory works only when the electron position is measured with an accuracy of the wave packet width. Just like what we did to obtain the position operator in the reciprocal lattice in the Berry phase part of this paper, the plane waves are replaced by Bloch’s wave, considering the electrons in crystal. The wave packet we construct with the Bloch functions

\[ \psi_{nk} = e^{ik \cdot r} u_{nk}(r) \]

from the \( n \)th band:

\[ |W_0 \rangle = \int d\mathbf{k} \ \omega(\mathbf{k}, t) |\psi_{nk} \rangle \]  \hspace{1cm} (1.51)

\( \omega(\mathbf{k}, t) \) must have sharp distribution, such that the wave vector of \( \mathbf{k}_0 \) of the the wave packet makes sense:

\[ \mathbf{k}_0 = \int d\mathbf{k} \ \mathbf{k} |\omega(\mathbf{k}, t)|^2, \]  \hspace{1cm} (1.52)

\[ f(\mathbf{k}_0) = \int d\mathbf{k} \ f(\mathbf{k}) |\omega(\mathbf{k}, t)|^2 \]  \hspace{1cm} (1.53)
What is the criterion for the “sharpness”? Since we are working in crystal, a natural choice is the Brillouin zone dimension: The width of the wave packet $\delta k$ should be much smaller than the Brillouin zone dimensions, which are of the order of the inverse lattice constant $1/a$. It follows that $\Delta R = 1/\Delta k$ must be larger than $a$. Thus, a wave packet of Bloch levels with a wave vector that is well-defined on the scale of the Brillouin zone must be spread in the real space over many primitive cells. The semi-classical model describes the response of the electrons to externally applied electron and magnetic fields that vary slowly over the dimension of such a wave packet (a few primitive cells).

Unlike a classical point particle, a wave packet has a finite spread around its center of mass, denoted by $r_c$, in real space:

\[
\begin{align*}
\mathbf{r}_c &= \langle W_0 | \mathbf{r} | W_0 \rangle \\
&= \int d\mathbf{k}'d\mathbf{k} \omega^*(\mathbf{k}')\omega(\mathbf{k})\langle \psi_{nk'} | (-i \frac{\partial}{\partial \mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}) | u_{nk} \rangle \\
&= \int d\mathbf{k}'d\mathbf{k} \omega^*(\mathbf{k}')\omega(\mathbf{k}) \left[ (-i \frac{\partial}{\partial \mathbf{k}}) \delta(\mathbf{k} - \mathbf{k}') + \delta(\mathbf{k} - \mathbf{k}') \langle u_{nk} | i \frac{\partial}{\partial \mathbf{k}} | u_{nk} \rangle \right] \\
&= \int d\mathbf{k} \left[ i \left( \frac{\partial}{\partial \mathbf{k}} \omega^*(\mathbf{k}) \right) \omega(\mathbf{k}) + |\omega(\mathbf{k})|^2 A_n(\mathbf{k}) \right], (1.54)
\end{align*}
\]

where $A_n(\mathbf{k}) = i \langle u_{nk} | \frac{\partial}{\partial \mathbf{k}} | u_{nk} \rangle$ is the Berry connection. We have already known that the Berry connection involved with the position operator in the reciprocal lattice from Eq.(1.29) and Eq.(1.30), so this $r_c$ formula we get here looks alright. Because of its finite spread in the real space, it may possess a self-rotation around its center of mass, which leads to an orbital magnetic moment [12]:

\[
\begin{align*}
\mathbf{r}_c &= \langle W_0 | \mathbf{r} | W_0 \rangle \\
&= \int d\mathbf{k}'d\mathbf{k} \omega^*(\mathbf{k}')\omega(\mathbf{k})\langle \psi_{nk'} | (-i \frac{\partial}{\partial \mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}) | u_{nk} \rangle \\
&= \int d\mathbf{k}'d\mathbf{k} \omega^*(\mathbf{k}')\omega(\mathbf{k}) \left[ (-i \frac{\partial}{\partial \mathbf{k}}) \delta(\mathbf{k} - \mathbf{k}') + \delta(\mathbf{k} - \mathbf{k}') \langle u_{nk} | i \frac{\partial}{\partial \mathbf{k}} | u_{nk} \rangle \right] \\
&= \int d\mathbf{k} \left[ i \left( \frac{\partial}{\partial \mathbf{k}} \omega^*(\mathbf{k}) \right) \omega(\mathbf{k}) + |\omega(\mathbf{k})|^2 A_n(\mathbf{k}) \right], (1.54)
\end{align*}
\]
\textbf{m}(k_0) = \frac{1}{2}\langle \mathcal{W}_0 | (r - r_c) \times j | \mathcal{W}_0 \rangle

= \frac{e}{2m} \langle \mathcal{W}_0 | (r - r_c) \times \mathcal{P} | \mathcal{W}_0 \rangle

= \frac{e}{2m} \int dk' \int dk \; \omega^*(k') \omega(k) \langle \psi_{nk'} | (r - r_c) \times \mathcal{P} | \psi_{nk} \rangle

= \frac{e}{2m} \int dk' \int dk \; \omega^*(k') \omega(k) \langle u_{nk'} | e^{i(r \cdot (k - k'))} (r - r_c) \times \mathcal{P} | u_{nk} \rangle

= \frac{e}{2m} \int dk' \int dk \; \tilde{\omega}^*(k') \tilde{\omega}(k) \langle u_{nk'} | e^{i(k - k') \cdot (r - r_c)} (r - r_c) \times \mathcal{P} | u_{nk} \rangle

= \frac{e}{2m} \sum n' \int dk' \int dk \; \tilde{\omega}^*(k') \tilde{\omega}(k) \langle u_{nk'} | i \frac{\partial}{\partial k'} e^{i(k - k') \cdot (r - r_c)} | u_{nk} \rangle \langle u_{n'k'} | \mathcal{P} | u_{nk} \rangle

= \frac{e}{2m} \sum n' \int dk' \int dk \; \tilde{\omega}^*(k') \tilde{\omega}(k) [i \frac{\partial}{\partial k'} \delta_{n, n'} \delta(k - k')

- \langle i \frac{\partial}{\partial k'} u_{nk'} | e^{i(k - k') \cdot (r - r_c)} | u_{n'k'} \rangle \langle u_{n'k'} | \times \mathcal{P} | u_{nk} \rangle

= \frac{e}{2m} \sum n' \int dk' \int dk \; \tilde{\omega}^*(k') \tilde{\omega}(k) [i \frac{\partial}{\partial k'} \delta_{n, n'} \delta(k - k')

- \delta(k - k') \langle i \frac{\partial}{\partial k'} u_{nk'} | u_{n'k'} \rangle \langle u_{n'k'} | \times \mathcal{P} | u_{nk} \rangle

= -i \frac{e}{2m} \int dk \left[ \frac{\partial}{\partial k} \tilde{\omega}^*(k) | \tilde{\omega}(k) \times \mathcal{P} | u_{nk} \right] - i \frac{e}{2m} \int dk | \tilde{\omega}(k) |^2 \langle \frac{\partial}{\partial k} u_{nk} | \times \mathcal{P} | u_{nk} \rangle

= -i \frac{e}{2m} \int dk \left[ \frac{\partial}{\partial k} \tilde{\omega}^*(k) | \tilde{\omega}(k) \times \langle \mathcal{P} | u_{nk} \rangle - i \frac{e}{2m} \int dk | \tilde{\omega}(k) |^2 \langle \frac{\partial}{\partial k} u_{nk} | \times \mathcal{P} | u_{nk} \rangle. \quad (1.55)

\mathbf{P} = m \frac{\partial H(k)}{\partial k} \text{ is the mechanical momentum operator, hence } (r - r_c) \times \mathbf{P} \text{ is the mechanical angular momentum operator. Also we defined } \tilde{\omega}(k) = e^{i(k - k') \cdot \omega(k)} \text{ to meet the requirement of calculation. The integrant part of the second term can be written as:}

\langle \frac{\partial}{\partial k} u_{nk} | \times \mathcal{P} | u_{nk} \rangle = \frac{m}{\hbar} \langle \frac{\partial}{\partial k_1} u_{nk} | \frac{\partial H}{\partial k_2} | u_{nk} \rangle - (k_1 \leftrightarrow k_2)

= \frac{m}{\hbar} \frac{\partial}{\partial k_2} \langle \partial_{k_1} u_{nk} | H | u_{nk} \rangle - \frac{m}{\hbar} \langle \partial_{k_1} u_{nk} | H | \partial_{k_2} u_{nk} \rangle - (k_1 \leftrightarrow k_2)

= \frac{m}{\hbar} \langle \partial_{k_1} u_{nk} | u_{nk} \rangle \frac{\partial \epsilon_n}{\partial k_2} + \frac{m}{\hbar} \langle \partial_{k_1} u_{nk} | \partial_{k_2} u_{nk} \rangle \epsilon_n - \frac{m}{\hbar} \langle \partial_{k_1} u_{nk} | H | \partial_{k_2} u_{nk} \rangle

- (k_1 \leftrightarrow k_2)

= \langle \partial_{k} u_{nk} | u_{nk} \rangle \times \langle \mathcal{P} | u_{nk} \rangle + \frac{m}{\hbar} \langle \partial_{k} u_{nk} | \times (\epsilon_n - H) | \partial_{k} u_{nk} \rangle. \quad (1.56)

Therefore, the formula of orbital magnetic moment becomes
\[ m(k_0) = -\frac{i e}{2m} \int dk \left[ \frac{\partial}{\partial k} \omega^*(k) \right]\omega(k) \times \langle P \rangle_n - i \frac{e}{2m} \int dk \left| \omega(k) \right|^2 \langle \partial_k u_{nk} | u_{nk} \rangle \times \langle P \rangle_n \]
\[ -i \frac{e}{2\hbar} \int dk \left| \omega(k) \right|^2 \langle \partial_k u_{nk} | \times (\epsilon_n - H) \right| \partial_k u_{nk} \rangle \]
\[ = -\frac{e}{2m} \int dk \left\{ i \frac{\partial}{\partial k} \omega^*(k) \right\} \omega(k) + \left| \omega(k) \right|^2 A_n(k) \} \times \langle P \rangle_n \]
\[ -i \frac{e}{2\hbar} \int dk \left| \omega(k) \right|^2 \langle \partial_k u_{nk} | \times (\epsilon_n - H) \right| \partial_k u_{nk} \rangle \]
\[ = -\frac{e}{2\hbar} \int d\mathbf{k} \left| \omega(k) \right|^2 \mathbf{r} \times \frac{\partial \epsilon_{nk}}{\partial k} - i \frac{e}{2\hbar} \int d\mathbf{k} \left| \omega(k) \right|^2 \langle \partial_k u_{nk} | \times (\epsilon_n - H) \right| \partial_k u_{nk} \rangle \]
\[ = i \frac{e}{2\hbar} \langle \nabla_{k_0} u \rangle \times [H(k_0) - \epsilon(k_0)] | \nabla_{k_0} u \rangle. \quad (1.57) \]

Here I used Eq.(1.54) and Eq.(1.53) to get the first two terms vanish.

Finally we obtain the orbital magnetic moment
\[ m(k) = i \frac{e}{2\hbar} \langle \nabla_k u \rangle \times [H(k) - \epsilon(k)] | \nabla_k u \rangle, \quad (1.58) \]

which does not depend on the actual shape and size of the wave packet but only on the Bloch functions. It does not depend on the way the wave packet was constructed as well, since there is no \( \omega(k) \) dependence in the final formula. The orbital moment transforms exactly like the Berry curvature under discrete symmetry operations. Therefore, it vanishes if both time reversal symmetry and inversion symmetry are protected. This intrinsic orbital moment act exactly like electron spin: By applying a magnetic field, it couples to the field through a Zeeman term \(-m(k) \cdot \mathbf{B}\).

### 1.2.2 Boltzmann equation

The Boltzmann equation is used to describe the statistical behavior of a thermodynamic system, which is not in a state of equilibrium. To be exact, it describes the time evolution of the electron distribution function \( f(\mathbf{r}, \mathbf{k}, t) \). Its physical interpretation is that \( f(\mathbf{r}, \mathbf{k}, t) d\mathbf{r}d\mathbf{k} \) is the number of electrons at point \( \mathbf{r} \) with wave vector \( \mathbf{k} \) (or wave packets with mean position \( \mathbf{r} \) and mean momentum \( \mathbf{k} \)), in the phase space volume \( d\mathbf{r}d\mathbf{k} \). Thus, the total integral of \( f(\mathbf{r}, \mathbf{k}, t) \) over the whole phase space gives the number of electrons. The time variation of it comes from three effects: diffusion, drift and collision. Diffusion is caused by any nontrivial gradient in the electron concentration, \( \nabla_r f(\mathbf{r}, \mathbf{k}, t) \) (or \( \partial_r f(\mathbf{r}, \mathbf{k}, t) \)). Drift is caused by external forces, which can be deemed as diffusion in \( k \) space, \( \nabla_k f(\mathbf{r}, \mathbf{k}, t) \) (or \( \partial_k f(\mathbf{r}, \mathbf{k}, t) \)), since
\[ \frac{d}{dt} f(\mathbf{r}, \mathbf{k}, t) = \frac{\partial}{\partial t} f(\mathbf{r}, \mathbf{k}, t) + \mathbf{r} \frac{\partial}{\partial \mathbf{r}} f(\mathbf{r}, \mathbf{k}, t) + \mathbf{k} \frac{\partial}{\partial k} f(\mathbf{r}, \mathbf{k}, t), \quad (1.59) \]
and $\dot{k}$ is apparently a force term given by Newton’s second law. The third term (drift term) can be deemed as the dual of the second term (diffusion term) in $k$ space.

If without collision, $\frac{df}{dt}(r, k, t) = 0$, given by Liouville’s theorem, which can be proven by continuity equation:

$$\frac{\partial}{\partial t} f + \frac{\partial(f \dot{r})}{\partial r} + \frac{\partial(f \dot{k})}{\partial k} = 0,$$

(1.60)

where $(f, f \dot{r}, f \dot{k})$ is a conserved current in $r$-$k$ space.[13]

According to Bloch’s theory, an electron in a perfect lattice should experience no collision at all. However, real lattices are not prefect: they have impurities and crystal defects, which scatter the electrons. What is more, the ions that form the lattices are not fixed: they have thermal vibrations, which is usually described as phonons in quantum mechanics. The phonon-electron interaction usually dominates the collision term in room temperature, while at low temperature, the impurity and defect scatterings dominate, since the vibration of the ions declined with the temperature drop.

The distribution function changed by all kinds of collisions is denoted as $(\frac{df}{dt})_{coll}$. If it is positive, it means that the collisions lead to an increasing number of electrons at $(r, k, t)$, and negative means decrease. Obviously, we get

$$\left(\frac{df(r, k, t)}{dt}\right)_{coll} = \frac{\partial}{\partial t} f(r, k, t) + \dot{r} \frac{\partial}{\partial r} f(r, k, t) + \dot{k} \frac{\partial}{\partial k} f(r, k, t).$$

(1.61)

This is the famous Boltzmann equation. $\dot{r}$ and $\dot{k}$ are obtained by solving equation of motion, which is done in the previous Berry phase part.

Now, I am going to deal with the collision part. First, let me introduce the scattering probability $W_{k,k'}$, which is defined this way: assume an electron with wave vector $k$ is scattered into any one of the group of levels (with the same spin) contained in the infinitesimal $k$-space volume $dk'$ around $k'$. (Suppose all these levels are unoccupied, hence not forbidden by the exclusion principle). The probability for this scattering to happen, in an infinitesimal time interval $dt$, is

$$W_{k,k'} dt dk' = \frac{2\pi}{(2\pi)^3}.$$

(1.62)

$W_{k,k'}$ is usually obtained by Fermi’s Golden Rule:

$$W_{k,k'} = \frac{2\pi}{\hbar} n_i \delta(\epsilon(k) - \epsilon(k')) |\langle k' | U | k \rangle|^2,$$

(1.63)
where \( n_i \) is the impurity density, and \( U \) describes the interaction between the impurity and the electron. Here, we assume a low temperature case with sufficiently dilute impurities, and the interaction is sufficiently weak. More general cases are studied in Many Body Quantum Field Theory, where loop graphs and Green’s functions based on different approximations for different circumstances were used to get the scattering amplitude. We use \( U(r) = U_0 \delta(r) \) to represent short range disorders, while for long range disorders we use correlation functions such as \( \langle U(r_1)U(r_2) \rangle = W^2 \) with \( \langle U(r) \rangle = 0 \).

Because of the exclusive principle, only unoccupied \( k' \) states are not forbidden, so the total probability for any electron with wave vector \( k \) scattered into states with wave vector \( k' \) per unit time is given by

\[
\frac{1}{\tau(k)} = \int dk' W_{k,k'} [1 - f(k')].
\]

(1.64)

\( \tau(k) \) is the relaxation time. By integrate over \( dk \), I mean integrating over \( \frac{d^3k}{(2\pi)^3} \). Usually, I neglect \( (2\pi)^3 \) when performing the formulas, but during the calculations, we know that it has to be there. To make the collision happen, we need not only \( k' \) states unoccupied but also \( k \) states occupied. Therefore, the change of the distribution function per unit time, because of electrons that have wave vector \( k \) scattering out, is

\[
\left( \frac{df(k)}{dt} \right)_{\text{out}} = -\frac{f(k)}{\tau(k)} = -f(k) \int dk' W_{k,k'} [1 - f(k')].
\]

(1.65)

Similarly, we can get the change of distribution function per unit time, that comes from “scattering in” collisions (electrons that was not in \( k \) states get their wave vector changed to \( k \) after scattering):

\[
\left( \frac{df(k)}{dt} \right)_{\text{in}} = [1 - f(k)] \int dk' W_{k',k} f(k').
\]

(1.66)

Therefore, the total contribution from collision is

\[
\left( \frac{df(k)}{dt} \right)_{\text{coll}} = -\int dk' \{ W_{k,k'} f(k) [1 - f(k')] - W_{k',k} f(k') [1 - f(k)] \}.
\]

(1.67)

In the relaxation-time approximation this is simplified to

\[
\left( \frac{df(k)}{dt} \right)_{\text{coll}} = -\frac{f(k) - f_0(k)}{\tau(k)},
\]

(1.68)

where \( f_0(k) \) is the equilibrium distribution function, which is just Fermi-Dirac distribution function for electrons.
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CHAPTER 2

AN OVERVIEW OF WEYL SEMIMETAL PHASE
In the last century, or even in a more distant past, physics is mostly centered on symmetries, which are intimately related to conservation laws by Noether’s theorem\[1\]. One of the most important examples of symmetry in physics is that the speed of light is the same in any coordinate system, which is indicated by mathematicians as “Poincaré group”, the symmetry group of the special relativity. Another important example is the invariance of the form of physical laws under arbitrary differentiable coordinate transformations, which is a representative idea in general relativity. Also last century witnessed the prosperity of high energy physics not only the discovery of all those fundamental particles but also when quantum electrodynamics, Glashow-Weinberg-Salam theory of electroweak processes, quantum chromodynamics come together, forming the so called standard model, while from the symmetry point of view, an $\text{SU}(3) \times \text{SU}(2) \times \text{U}(1)$ group.

Our current century is believed to be a century of topology. In mathematics, topology is a concept concerned with the properties of space that are preserved under continuous deformations, such as stretching, bending and crumpling, but not tearing or gluing. Since the study into the topological insulators at very the beginning of our century\[2, 3, 4\], the study of electron structure topology of crystalline material has been an extremely important subject in the modern condensed matter physics. These topological phases have some property to which an integer can be assigned (Chern number, as introduced in chapter 1), which is robust and only depends on global properties: they cannot be destroyed by local perturbations such as disorder and scattering, as long as the bulk gap is not closed, and that is why we call them “topological”. In 2016, David J. Thouless, F. Duncan M. Haldane, and J. Michael Kosterlitz won Nobel Prize in Physics for “theoretical discoveries of topological phase transitions and topological phases of matter”. Recently, the enthusiasm on this theme shifted to topological semimetals or metals, due to the theoretical prediction of topological Weyl semimetals\[5, 6, 7, 8, 9\] and Dirac semimetals\[10, 11, 12\], followed by experimental realizations of them: Dirac semimetal\[13, 14, 15\] and topological Weyl semimetal\[16, 17, 18\].

### 2.1 From Graphene to Weyl semimetal

The Nobel prize in physics for 2010 was awarded to Andre Geim and Konstantin Novoselov “for groundbreaking experiments regarding the two-dimensional material gra-
Graphene is a single sheet of carbon atoms arranged in a honeycomb lattice. Electrons moving around the carbon atoms interact with the periodic potential of the honeycomb lattice, which give rise to a Fermi surface with six double cones where the valence and conductance bands touch each other. The dispersion relation is linear near the band touching point, which brings about relativistic Dirac fermions as quasi-particles, where the speed of light is replaced by the Fermi velocity and the spins are replaced by pseudo-spins associated with the sublattices. The general Hamiltonian is usually expressed as

\[ H = v_F (\sigma_x p_x + \sigma_y p_y) \]  \hspace{1cm} (2.1)

Clearly, it can be easily gapped out by perturbations (mass terms) proportional to \( \sigma_z \). The stability of graphene comes from the extra symmetries under time-reversal and spatial inversion, which enforce the vanishing of terms proportional to \( \sigma_z \), ensuring that no gap is induced, when perturbations do not break time-reversal and inversion symmetry.

It is possible to generalize this model into 3D, and we can have Hamiltonian looks like this:

\[ H = \begin{bmatrix} 0 & v_F \sigma \cdot p \\ v_F \sigma \cdot p & 0 \end{bmatrix} \]  \hspace{1cm} (2.2)

Here \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) is a triplet of Pauli matrices. This is the simplest model for Dirac semimetal. It is still easily gapped out by \( 4 \times 4 \) diagonal matrices, and need crystal symmetries to protect it. However, it is possible to split the degeneracy of the Dirac node in momentum space by breaking either time-reversal or inversion symmetry. This generates two Weyl nodes with opposite chiralities (or helicities), of which dispersion is given by the massless Weyl Hamiltonian.

The robustness Weyl nodes is obvious: the Hamiltonian of Weyl semimetal is written with \( 2 \times 2 \) Pauli matrices, and we have used all three of them, so it is hard to gap it out. From topological point of view, Weyl points with opposite nonzero Chern number, associated with the 2D Fermi surface sheet, are separated, so they are topologically protected: a Gauss surface surround a Weyl node detect the chirality of it, preventing it from disappear unless another Weyl node with opposite chirality enter in the surface. One might be familiar with the Gauss-Bonnet theorem, which is a theorem on 2D manifold. The origin for 2D topological insulators to be “topological” is that their completely filled bands leave the first Brillouin Zone a perfect torus in momentum space, where Gauss-Bonnet theorem
applies. Weyl semimetal has a 3D Brillouin Zone, so we must choose a closed 2D manifold around the Weyl points, within the 3D bulk Brillouin Zone. The Chern number is defined as

$$C = \frac{1}{2\pi} \int_{S} \Omega(k) dS, \quad (2.3)$$

where $S$ denotes a closed 2D manifold in the Brillouin Zone, compared to the 2D topological insulator case, which is integral over the whole Brillouin Zone. Apparently, the Chern number only depends on the number of Weyl nodes or monopoles contained in the closed manifold, and that is why it is a topological property. Since for metals, everything interesting happens around the Fermi surface, we require Weyl nodes being located near the Fermi surface, to make it a Weyl (semi-)metal. Those with Weyl nodes located exactly at the Fermi level are called “Weyl semimetals”, and those with Weyl nodes around the Fermi energy are named as “Weyl metals”. I may not distinguish them if not necessary to.

In the vicinity of Weyl points, the Berry curvature takes a general form (similar to the assumed magnetic monopole formula):

$$\Omega(k) = \pm \frac{k}{2k^3}, \quad (2.4)$$

which leads to a Chern number $C = \pm 1$, indicating a sink or source enclosed by the 2D surface we chose. A nonzero Chern number, or topological number, is the reason why Weyl semimetal is called “topological Weyl semimetal”, compared to Dirac semimetal, where all bands are doubly-degenerated due to the Kramers theorem, and Berry curvature is zero everywhere.

Near the Weyl points, the Hamiltonian takes a universal form as well:

$$H = \pm v_F \sigma \cdot k. \quad (2.5)$$

This Hamiltonian is identical to the Hamiltonian of free Weyl fermions proposed by Hermann Weyl in 1929, if one replace $v_F$ with the speed of light $c$. The $\pm$ sign, which indicates the opposite Chern numbers, now corresponds to Left- and Right-handed Weyl fermions. In 1929, Hermann Weyl had noticed that the Dirac equation could be separated into two Weyl spinors with opposite chirality. However, as the lightest neutrinos turned out to have nonzero mass, it seemed hopeless to find a natural particle which is a Weyl fermion. Now we know that, in condensed matter field, it is accomplishable to get quasi-particles
with every property a Weyl fermion supposed to have. Weyl semimetals might be able to provide us a platform for testing theories about Weyl fermions, with a lower “speed of light”.

Remark : How to gap a Weyl (semi-)metal out, as it is topologically stable? Since the total Chern number in the entire Brillouin zone has to be zero, known as the “Nielsen-Ninomiya theorem”[19], we cannot gap out a single Weyl point. Instead, we have to move two Weyl points with opposite chirality on top of each other to annihilate them. Then further perturbation might gap out the system. If we go beyond band theory, superconductivity might be able to gap the system by breaking U(1) symmetry. In addition, charge density wave (CDW) and disorders may gap the Weyl points out by breaking translational symmetries. Weyl (semi-)metals are protected by U(1) charge symmetry and translational symmetries[20].

2.2 Theoretical model and special surface states

To provide a more intuitive idea about Weyl semimetal, let me at least adopt a theoretical model[21]:

\[
\hat{h}(\mathbf{k}) = a(\mathbf{k})\sigma_x + b(\mathbf{k})\sigma_y + c(\mathbf{k})\sigma_z, \quad H = \sum_{\mathbf{k}} \hat{h}(\mathbf{k}) \\
a(\mathbf{k}) = -2t_x (\cos k_x - \cos k_0) + m(2 - \cos k_y - \cos k_z), \\
b(\mathbf{k}) = 2t_y \sin k_y, \quad c(\mathbf{k}) = 2t_z \sin k_z.
\] (2.6)

Obviously, it has two nodes at \( \mathbf{k} = \pm k_0 \mathbf{e} \). Denote \( \mathbf{p}^\pm = (\pm k_x \mp k_0, k_y, k_z) \), and expand the Hamiltonian around the nodes, we get:

\[
H^\pm = 2t_x \sin k_0 p_x^\pm \sigma_x + 2t_y p_y^\pm \sigma_y + 2t_z p_z^\pm \sigma_z,
\] (2.7)

which is an anisotropic version of \( H = \pm v_F \sigma \cdot \mathbf{k} \). It is okay to have different Fermi velocity in different directions, since we are in the lattice, where Lorentz invariance is not required. The fact that the Lorentz invariance need not exist is also the origin of a new type of Weyl semimetal: the Type II Weyl semimetal[22]. We are not going to give a further introduction to the Type II Weyl semimetal, since it is not the points of focus of this thesis.

With this model, we can calculate the eigenstates:
\[ \psi_+ = \frac{1}{\sqrt{2d(d + 2t_z p_z)}} \left[ \begin{array}{c} 2t_z p_z + d \\ 2t_x p_x + 2it_y p_y \end{array} \right], \]

\[ \psi_- = \frac{1}{\sqrt{2d(d - 2t_z p_z)}} \left[ \begin{array}{c} 2t_z p_z - d \\ 2t_x p_x + 2it_y p_y \end{array} \right], \]

\[ d = \sqrt{(2t_x p_x)^2 + (2t_y p_y)^2 + (2t_z p_z)^2}, \tag{2.8} \]

and the Berry connection

\[ A_i(k) = i \langle \psi_- | \partial_k | \psi_- \rangle = \frac{1}{d(d - 2t_z p_z)} \{ 2t_y p_y \partial_i(t_x p_x) - 2t_x p_x \partial_i(t_y p_y) \}, \tag{2.9} \]

and the Berry curvature

\[ \Omega_i = \frac{1}{2d^3} \epsilon_{ijk} \epsilon_{abc} (2t_a p_a) \partial_j (2t_b p_b) \partial_k (2t_c p_c). \tag{2.10} \]

When integrating over the base manifold, we can find that the Chern number is always an integer, \( \pm 1 \).

Now we look into the surface states of this model. The first nontrivial question to ask is: how can surface states be protected from hybridizing with bulk states in a gapless system? The answer lies in the translational symmetry: the translational symmetry in the lattice guarantees the conservation of momentum of surface states, so the surface states at the Fermi level are stable at any momenta where there are no bulk states at the same energy, since they cannot decay into bulk states. For Weyl semimetals, which have Fermi energy strictly located at the Weyl nodes, the bulk states at Fermi level are just at the projections of the Weyl nodes to the surface Brillouin zone, and all other surface states at the Fermi energy are stable and well-defined. This leads to unique, non-closed surface states at the Fermi energy: the Fermi arcs.

Think the momentum space of the 3D Weyl system as a stack of 2D slices as shown in Fig.(2.1). Certainly, for slices that do not contain a Weyl node, they are totally gapped 2D systems, and we can calculate the Chern number by integrating the Berry curvature over the 2D surface. Those slices with 0 Chern number are just 2D normal insulators. The slices between two Weyl points are Chern insulators with Chern number \( C=1 \). We know that Chern insulators have a chiral edge state. The Fermi arc is nothing special, but a stacking of chiral edge states of Chern insulators.
Figure 2.1. Surface states of a Weyl semimetal. (a) C=0 slices correspond to 2D normal insulators (NI), and C=1 slices correspond to Chern insulators with Chern number C=1. Fermi arc is formed by adding all edge states of 2D Chern insulators. (b) A graph of the dispersion relation of surface states (the pink plane) and bulk states (blue and red cone). We can see how the surface state joins to the bulk states here. These two graphs are from the paper “Beyond Band Insulators: Topology of Semi-metals and Interacting Phases” by Ari M. Turner and Ashvin Vishwanath[21]. Permission has been received from the authors.

Fermi arcs have been observed by ARPES measurements in monophosphides TaAs class Weyl semimetals [16, 18, 23, 24]. However, to be exact the Fermi arcs detected in TaAs is not disjoint arcs but closed contours, dubbed as Fermi kinks. What is a Fermi kink? Why can it be a proof of the existence of the Weyl nodes? We know that the two ends of a Fermi arc are the projection of a pair of Weyl points on the surface Brillouin zone. What if there are more than one Weyl point projecting on the same point of the surface Brillouin zone? Yes, we will have more than one Fermi arcs start and end at the same Weyl points projection. If the number of pairs of Weyl points sharing same projection points on the surface is an even number, we have closed contours. That is the case for TaAs. However, closed contours does not mean that we will miss the signal of Weyl points,
because generally speaking, those Fermi arcs attach to same Weyl projection points with different slopes, which leads to a kink in the contour. Therefore, either odd number of Fermi arcs or Fermi kinks being observed can stand as the evidence of the existence of Weyl points.

2.3 Where to find Weyl things?

In this section, I will first try to recover the most famous attempts that physicists took to search possible materials and realize Weyl (semi-)metals in the past decade. Followed by this, I will talk about experimental breakthroughs in this area.

2.3.1 Search for possible materials

Let us give a guess first: where to start if one is seeking for Weyl material? There is a hint lying in the last section where we introduce Fermi arcs by viewing Weyl system as a stack of 2D normal insulators and Chern insulators. We might be able to find Weyl (semi-)metals at some quantum phase transition point. That is an idea proposed by Shuichi Murakami in 2007[25]. Murakami suggests that a gapless phase (Weyl points) appears between the quantum spin Hall (QSH) phase and the insulator phase in 3D inversion symmetry broken systems. In order to get Weyl (semi-)metals, three necessary conditions are required: either breaking inversion symmetry or time reversal symmetry to avoid double degeneracy, gapless points as Weyl nodes which are sinks and sources of Berry flux and Fermi energy located at/near the Weyl points. We might be able to find Weyl nodes at some phase transition point in a magnetic system (time reversal symmetry broken) or an inversion-symmetry-break system. How to make the Fermi energy locate at the Weyl points? Luttinger’s theorem, which is obtained directly from Pauli exclusion principle, states that the volume enclosed by a Fermi surface of a material is directly proportional to its electron density. Therefore, the Fermi level is only determined by the electron density. This suggests that, at least theoretically, one way to get Weyl (semi-)metals is to find an insulator with time reversal symmetry or inversion symmetry broken, and then close a gap. This will lead the Fermi level being pinned to the band touching point. Followed by this intuition, in 2011, A. A. Burkov and Leon Balents proposed the idea of realizing Weyl semimetal in a magnetic topological insulator(TI) multilayer, which consists of
identical thin films of a magnetically doped (to break time reversal symmetry of course) 3D topological insulator, separated by ordinary insulator layers[26]. They used a simple tight-binding model which showed that their multilayer exhibit a quantum Hall plateau transition from $\sigma_{xy} = 0$ (normal insulator) to $\sigma_{xy} = e^2/h$ (quantum Hall insulator) when varying the tunneling between the top and bottom surface of the TI layer, or the exchange spin-splitting (raised by the magnetic impurities). Weyl nodes appear as an intermediate phase in this quantum phase transition. This model is still to be realized in experiments.

Historically, somehow, nearly all attempts of seeking and prediction of Weyl materials were concentrated on time reversal symmetry breaking Weyl semimetals at the very beginning. The first material candidate for Weyl semimetals was a family of magnetic pyrochlore iridates, $R_2\text{Ir}_2\text{O}_7$, where $R$ is a rare earth element. It was suggested by Wan et al. in 2011[7]. Theoretical study shows that $R_2\text{Ir}_2\text{O}_7$ exhibits a transition from an ordinary magnetic metal to a Mott insulator, with the increasing of the on-site Coulomb interaction, and a Weyl semimetal sits in between. They also studied the possible Fermi arcs in this system. Their calculation results brought a fever in Weyl material seeking projects. However, attempts to realize a Weyl semimetal in $R_2\text{Ir}_2\text{O}_7$ encountered unprecedented difficulties. The metal-insulator phase transition was observed and transport behaviors were roughly the way it should be for a semimetal, but the overall results were not persuasive enough, not to say that ARPES measurements were lacking. (ARPES stands for angle-resolved photoemission spectroscopy. It is a technique provide direct observation of bulk and surface states. Intuitively, it works by shedding light on material and measuring energy, momentum, and spin of the photoelectrons.) After $R_2\text{Ir}_2\text{O}_7$, there are also some other proposals about time reversal symmetry breaking Weyl material, like $\text{Hg}_{1-x-y}\text{Cd}_x\text{Mn}_y\text{Te}$[27], and magnetic doping of Dirac semimetals, but none of them got a successful ARPES measurement. They all faced same difficulties such, that it is hard to grow high quality magnetically dopped crystals with a useful magnetic order, as disorder from doping degrades the sample quality, while the spin splitting from magnetic doping might be too small to produce Weyl points.

Since there are many problems involved with magnetic doping for time reversal symmetry broken Weyl semimetals, people started to think, that it might be easier to realize inversion symmetry broken Weyl material. Since inversion symmetry broken is a prop-
property of crystal structure, which can be detected by X-ray diffraction, the research into the inversion symmetry broken Weyl material benefits a lot from those databases provided by X-ray diffraction experiments in the past century. Inversion symmetry breaking adds no complications to ab initio calculation, compared to those magnetic materials. In 2012, Halasz and Balents proposed HgTe/CdTe heterostructure as possible inversion symmetry broken Weyl material [28]. They state a Weyl semimetal phase between the normal insulator and the topological insulator phases in this system, which is similar to the time reversal symmetry broken topological multilayer. This proposal is still not realized, as it requires topological insulator and normal insulator with matching lattice structures that can both be grown by a thin film technique. In 2014, with first principle calculation, Jianpeng Liu and David Vanderbilt suggested there was a robust Weyl-semimetal phase exists in the solid solutions LaBi$_{1-x}$Sb$_x$Te$_3$ and LuBi$_{1-x}$Sb$_x$Te$_3$ for $x \sim 38\% - 41.9\%$ and $x \sim 40.5\% - 45\%$, which remains unrealized[29]. There are also a lot of other unrealized proposals for inversion symmetry broken Weyl materials, like tellurium or selenium crystals under pressure. For further reading, see the review paper by M. Zahid Hasan et al[30].

In 2015, two groups of people independently predict Weyl semimetal phase in noncentrosymmetric transition-metal monophosphides, TaAs class with first principles calculations[8, 31]. The TaAs family are natural Weyl semimetals, with 12 pairs of Weyl points for each of them. They are experimentally detected to have Weyl points in the bulk, as well as Fermi arcs on the surface shortly after the theoretical prediction[16, 18].

### 2.3.2 Milestones in experiments

In 2015, both Weyl points in bulk states and Fermi arcs in surface states were directly observed by ARPES measurements in TaAs by Zahid Hasan’s group in Princeton University[18] and Hong Ding’s group in Beijing National Laboratory for Condensed Matter Physics[16]. Soon after the identification of TaAs, experiments on other TaAs family Weyl semimetals, like NbAs[23] and TaP[24] also got prominent results.

Meanwhile, Marin Soljačić’s group from MIT, and Lixin Ran’s group from Zhejiang University observed Weyl states in a photonic crystal, which is a material with a periodic pattern of holes that only transmits light with certain frequencies[17]. They carved arrays of holes into ceramic layers with a computer controlled milling machine, and then stacked...
them to make a 3D inversion symmetry broken photonic crystal.

TaAs has a body-centered tetragonal lattice, with a space group I4_1md (#109). Its structure lacks an inversion symmetry. A non-zero Chern number of Weyl points in TaAs was directly measured from an ARPES measurement [32], which again verifies that it is a Weyl semimetal. As we mentioned in the previous section, that Fermi arcs do not always appear as disjoint arcs in Weyl semimetals. In TaAs, the Fermi arcs appear in pairs which together form a closed contour, a surface state kink.

2.4 Landau levels, Chiral anomaly and magnetotransport properties

Perhaps the most significant consequence of a nontrivial electronic band topology is that it may bring unique transport phenomena or response to external probing, such as quantum hall effect. In this section, we will present the most famous consequence of having a nontrivial Weyl points topology – chiral anomaly, followed by the negative longitudinal magnetoresistance induced by it, and an inverse process called chiral magnetic effect. To explain the mechanism of chiral anomaly in condensed matter, we have to start with Landau levels.

2.4.1 Landau levels basics

Landau levels in quantum mechanics are the result of quantization of the cyclotron orbits of charged particles in magnetic fields [33]. You might be familiar with it, but let’s give a brief review before coming to the Landau levels of system with linear dispersion relationship.

Assume a 2D system of non-interacting electrons with charge denoted as $e$ (in my notation, $e \approx -1.6 \times 10^{-19} \text{C}$ is the charge of electron, not the positive elementary charge), confined in an area $L_x L_y$. Applying a uniform magnetic field $\mathbf{B} = B\hat{e}_z$, the Hamiltonian of this system can be written as

$$H = \frac{1}{2m} \left[ \hat{p}_x^2 + (\hat{p}_y - eB\hat{x})^2 \right],$$

(2.11)

when we choose the Landau gauge: $\mathbf{A} = (0, Bx, 0)$.

Since the Hamiltonian is independent of $y$, it commutes with $\hat{p}_y$: $[H, \hat{p}_y] = 0$. Therefore, the eigenstates of $H$ are simultaneously eigenstates of $\hat{p}_y$: 
\[ H |\Psi\rangle = \epsilon |\Psi\rangle, \]  
(2.12)

\[ \hat{p}_y |\Psi\rangle = \hbar k_y |\Psi\rangle. \]  
(2.13)

We may simply replace \( \hat{p}_y \) in the \( H \) with \( \hbar k_y \). With a cyclotron frequency defined as \( \omega_c = qB/m \), we reach the simplified Hamiltonian:

\[
H = \frac{\hat{p}_x^2}{2m} + \frac{1}{2} m \omega_c^2 (\hat{x} - \frac{\hbar k_y}{m \omega_c})^2,
\]  
(2.14)

which is exactly the Hamiltonian of the quantum harmonic oscillation. The energy of this system is

\[
\epsilon_n = \hbar \omega_c (n + \frac{1}{2}),
\]  
(2.15)

\( n \geq 0 \) is the energy level. \( \epsilon_n \) is independent of \( k_y \), so it is degenerate.

Since \( \hat{p}_y \) commutes with \( H \), the wavefunctions can be written as

\[
|\Psi(x, y)\rangle = e^{ik_y y} \psi_n (x - x_0),
\]  
(2.16)

with \( x_0 = \frac{\hbar k_y}{m \omega_c} \). Each set of wave functions with the same value of \( n \) is known as a Landau level, where \( k_y = \frac{2\pi N}{L_y} \), and \( N \) is the degeneracy of the Landau level (without considering the spin degeneracy). Remember that the system is confined in an area \( A = L_x L_y \), so 

\[
0 \leq x_0 \leq L_x.
\]

Since \( x_0 = \frac{\hbar k_y}{m \omega_c} = \frac{2\pi \hbar N}{m \omega_c L_y} \), we can easily get

\[
0 \leq N \leq \frac{m \omega_c L_x L_y}{2\pi \hbar} = \frac{\Phi}{\Phi_0},
\]  
(2.17)

where \( \Phi = BA \) is the magnetic flux, and \( \Phi_0 = \hbar/e \) is the quantum of flux. We also need to consider the spin degeneracy, so \( N \) is twice in case of electron. For particle with charge \( q = Ze \) and spin \( s \), the upper limit is \( Z(2s + 1)\Phi/\Phi_0 \).

### 2.4.2 Landau quantization in Weyl metals

Chiral anomaly is found as a consequence of the Landau quantization in system with linear dispersion relation[34]. Therefore, lets study the Landau quantization of that kind of system first. Instead of the quadratic momentum Hamiltonian we used above, we need to use a simplest Weyl metal model:

\[
H = \pm v \sigma \cdot \textbf{p},
\]  
(2.18)

where \( \pm \) represents different chirality of two Weyl points, \( v \) is the band speed, \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) are Pauli matrices. Still, we choose \( \textbf{A} = (0, Bx, 0) \). Because of the magnetic field in z-direction, \( \hat{p}_y \) in the original Hamiltonian should be replaced by \( \hat{p}_y - eB \hat{x} \), and it commutes
with the Hamiltonian, $[\hat{p}_y, H] = 0$. Therefore, $\hat{p}_y$ in the Hamiltonian can be replaced by $\hbar k_y$. In the same way, $\hat{p}_z$ can be replaced by $\hbar k_z$.

\begin{equation}
\pm v \begin{pmatrix}
\hat{p}_z \\
\hat{p}_x + i(\hat{p}_y - eB\hat{x})
\end{pmatrix}
\begin{pmatrix}
\psi_1 \\
\psi_2
\end{pmatrix} = \epsilon \begin{pmatrix}
\psi_1 \\
\psi_2
\end{pmatrix}
\end{equation}

\begin{align}
\Rightarrow \{ & (\hat{p}_z - \frac{e}{\pm 0})\psi_1 + (\hat{p}_x - i(\hat{p}_y - eB\hat{x}))\psi_2 = 0 \\
& (\hat{p}_x + i(\hat{p}_y - eB\hat{x}))\psi_1 - (\hat{p}_z + \frac{e}{\pm 0})\psi_2 = 0
\end{align}

\begin{equation}
\Rightarrow \{ \hat{p}_z^2 - (\frac{e}{\pm 0})^2 + \hat{p}_x^2 + (\hat{p}_y - eBx)^2 + eB_i[\hat{x}, \hat{p}_x] \psi_{1,2} = 0
\end{equation}

\begin{equation}
\Rightarrow \frac{1}{2m} [\hat{p}_x^2 + (\hbar k_y - eBx)^2 + (\hbar k_z)^2 - e\hbar B] \psi_{1,2} = \frac{1}{2m} (\frac{e}{v})^2 \psi_{1,2}
\end{equation}

We may define a new “Hamiltonian” $H' = \frac{\hat{p}_z^2}{2m} + \frac{1}{2} m \omega_c (x - \frac{\hbar k_y}{m \omega_c})^2 + (\frac{\hbar k_z}{2m})^2 - \frac{1}{2} \hbar \omega_c$, which is again a harmonic oscillator, but with a free motion in $z$-direction. Therefore, its eigenvalue is:

\begin{equation}
\frac{1}{2m} (\frac{e_n}{v})^2 = \hbar \omega_c (n + \frac{1}{2}) + (\frac{\hbar k_z}{2m})^2 - \frac{1}{2} \hbar \omega_c = n \hbar \omega_c + (\frac{\hbar k_z}{2m})^2,
\end{equation}

where $n \geq 0$ is the energy level of harmonic oscillation, but since $H'$ is a fake Hamiltonian, the real one $H$ is not a harmonic oscillator, so there is no reason for $n$ to be positive for $H$. Thus, we replace $n$ here with $|n|$, and allow the new $n$ to be negative. Actually, here the positive $n$ stands for conducting bands, while negative $n$ stands for valence bands.

Then we get the eigenvalue of the previous Hamiltonian $H$:

\begin{equation}
\epsilon_n = \pm v \sqrt{2eB \hbar |n| + \hbar^2 k_z^2}.
\end{equation}

Since we want positive $n$ to be conducting bands and negative $n$ to be valence bands, we can write the above result for $n \neq 0$ this way:

\begin{equation}
\epsilon_n = \text{sgn}(n) v \sqrt{2eB \hbar |n| + \hbar^2 k_z^2}.
\end{equation}

The zeroth Landau level has a linear dispersion relation:

\begin{equation}
\epsilon_0 = \pm v \hbar k_z = \pm v p_z.
\end{equation}

Here the ± stand for right and left moving Weyl fermions.
2.4.3 Chiral anomaly

The Adler-Bell-Jackiw (ABJ) axial anomaly [35][36] or chiral anomaly is the anomalous non-conservation of the chiral current. It was introduced to condensed matter field by Nielson and Ninomiya[34] in 1983. The idea is: Followed by the above section, we have strong magnetic field applied on the Weyl metal system to get Landau levels, and at the zeroth Landau level we get right and left moving Weyl fermions. Now apply a uniform electric field $E = E\hat{e}_z$ parallel to the magnetic field. The equation of motion has been obtained as Eq.(1.38) and Eq.(1.39) (we consider the zeroth band only, therefore no $n$ is needed here):

$$
\dot{r} = \frac{1}{1 - eB \cdot \Omega_p} [v - eE \times \Omega_p - eB (v \cdot \Omega_p)],
$$

$$
\dot{p} = \frac{1}{1 - eB \cdot \Omega_p} [eE + ev \times B - e^2 (E \cdot B) \Omega_p].
$$

Substituting them into the Boltzmann equation

$$
\left( \frac{df(r, p, t)}{dt} \right)_{coll} = \frac{\partial}{\partial t} f(r, p, t) + \dot{r} \frac{\partial}{\partial r} f(r, p, t) + \dot{p} \frac{\partial}{\partial p} f(r, p, t),
$$

with relaxation time approximation Eq.(1.68), we get

$$
- \frac{\delta f^i(r, p, t)}{\tau} = \frac{\partial}{\partial t} f^i(r, p, t) + \frac{1}{1 - eB \cdot \Omega_p} \{[v - eE \times \Omega_p - eB (v \cdot \Omega_p)] \frac{\partial}{\partial r} f^i(r, p, t) \\
+ [eE + ev \times B - e^2 (E \cdot B) \Omega_p] \frac{\partial}{\partial p} f^i(r, p, t) \}.
$$

where $i$ stands for different valleys. $\tau$ is the relaxation time, which contain both intravalley scattering contribution $\tau_{intr}$ and intervalley scattering $\tau_v$ contribution. We assume $\tau_{intr} \ll \tau_v$, the anisotropy of the distribution function within each valley can be neglected, and the latter depends only on the energy $f^i(p) = f^i(\epsilon)$. Denote the density of states[37]

$$
\rho^i(\epsilon) = \int \frac{d\mathbf{p}}{(2\pi \hbar)^3} (1 - eB \cdot \Omega_p^i) \delta(\epsilon_p - \epsilon).
$$

In the homogeneous case ($\frac{\partial}{\partial r} f^i(r, p, t) = 0$, average of the direction of $p$ makes first two force terms vanish), and we get the Boltzmann equation:

$$
\frac{\partial}{\partial t} f^i(\epsilon) - \frac{k^i}{\rho^i(\epsilon) 4\pi^2 \hbar^2 (E \cdot B)} \frac{e^2}{\epsilon^2} \frac{\partial^2 f^i(\epsilon)}{\partial \epsilon^2} = - \frac{\delta f^i(\epsilon)}{\tau_v}
$$

where

$$
k^i = \frac{1}{2\pi \hbar} \int d\mathbf{S} \cdot \Omega_p^i = 0, \pm 1, ...
$$
for right and left valley, its just ±1. The electron density in each valley is given by

$$N^i = \int d\epsilon \rho^i(\epsilon) f^i(\epsilon).$$  \hspace{1cm} (2.34)

Integrating Eq.(2.32) over $\rho^i(\epsilon)\, d\epsilon$ we get

$$\frac{\partial N^i}{\partial t} = k^i \frac{e^2}{4\pi^2\hbar^2} (\mathbf{E} \cdot \mathbf{B}) - \frac{\delta(N^i)}{\tau_v}.$$  \hspace{1cm} (2.35)

The number of electrons in each valley is not conserved even when $\tau_v \to \infty$. Finally, we get

$$\frac{\partial N^R}{\partial t} - \frac{\partial N^L}{\partial t} = \frac{e^2}{2\pi^2\hbar^2} (\mathbf{E} \cdot \mathbf{B}) - \frac{N^R - N^L}{\tau_v}.$$  \hspace{1cm} (2.36)

Electrons are bumped from left valley to the right one, thus a deviation from the thermodynamic equilibrium appears, which can be expressed by different chemical potential $\mu_R$ and $\mu_L$, see Fig.(2.2)[38].

**Figure 2.2.** Chiral Anomaly. Applying $\mathbf{E}$ and $\mathbf{B}$ both in $z$-direction, electron in left valley are bumped into electrons in right valley, which lead to an imbalance of the chemical potential which can be and has been detected.

### 2.4.4 Negative longitudinal magnetoresistance

The existence of chiral anomaly in Weyl semimetals results in a negative longitudinal magnetoresistance, which has been detected in TaAs family Weyl semimetals[39, 40, 41,
It does not seem unique to Weyl semimetals, since this phenomenon is also observed in Dirac semimetals\cite{46, 47, 48}. However, in Dirac semimetals, the magnetic field not only produces a chiral anomaly but also works in splitting a Dirac cone into a pair of Weyl cones of opposite chirality by time reversal symmetry break. Therefore, the mechanism is deemed as similar to the chiral anomaly induced negative magnetoresistance in Weyl semimetals. (Remark: A Dirac cone split into two Weyl cones is one explanation for the observation of the negative magnetoresistance phenomenon in Dirac semimetals, but it is not a fully convincing explanation. For instance, it cannot explain the negative magnetoresistance in ZrTe$_5$\cite{49}, when photoemission and STM experiments\cite{50, 51} show that the robust electronic ground state of ZrTe$_5$ has a small gap ($\sim$ 50 meV), not a Dirac cone to be split into Weyl cones. The theoretical explanation of it is still under investigation.)

Now let’s talk about the mechanism of chiral anomaly induced negative longitudinal magnetoresistance. Magnetoresistance refers to the increase of resistance (decrease of conductivity) when applying a magnetic field in the same direction of the current. The ordinary magnetoresistance was first discovered by William Thomson in 1856\cite{52}. After that, other related effects, such as negative magnetoresistance, giant magnetoresistance, tunnel magnetoresistance, colossal magnetoresistance, and extraordinary magnetoresistance are studied. Negative magnetoresistance means an increasing of conductivity with parallel magnetic field applied. In order to verify that it is the case for Weyl semimetal because of the chiral anomaly, we need to get the conductivity for our previous model of a pair of Weyl nodes in parallel electric and magnetic field, shown in Fig.(2.2). To calculate the chiral anomaly related distribution of the conductivity, we can use the Boltzmann equations\cite{53}, and keep the second order term of electromagnetic field, but the calculation will be very complicated. Son and Spivak used an easier way to calculate it in their paper\cite{37}, by estimating the rate of entropy production $\dot{S}$ in the presence of an electric field, and use the relation $\dot{S} = \sigma E^2 / T$ to get $\sigma$ tensor. The chiral anomaly term enters the equation of conductivity through the electron density difference between the right valley and left valley, which affects the rate of entropy $\dot{S}$. By keeping only the chiral anomaly $\mathbf{E} \cdot \mathbf{B}$ related term, the conductivity tensor has only one nonzero component, which is

$$\sigma_{zz} = \frac{e^2}{4\pi^2 \hbar c} \frac{u (eB)^2 v^2}{\mu^2 \tau}, \quad (2.37)$$
where $z$ is the direction of electric field as well as the magnetic field. This result indicates that the longitudinal conductivity increases with an increasing magnetic field, which is dubbed as negative magnetoresistance.

There are a number of other effects which also lead to a negative magnetoresistance in metals, and some of them appear just like chiral anomaly induced negative magnetoresistance: they are prominent only when electric and magnetic fields are parallel[54] and the presence of magnetoresistance does not depend on the direction of the electric field with respect to the crystalline axis. The uniqueness of the chiral anomaly induced negative magnetoresistance is that the magnitude of it have an inverse dependence on the square of the chemical potential $1/\mu^2$[40].

2.4.5 The chiral magnetic effect: the inverse of the chiral anomaly

Previously, we had parallel magnetic and electric fields applied to Weyl semimetal, which bump electrons in the zeroth Landau level from one valley to the other, leading to an imbalance of the chemical potential. Think about an inverse process: If we have an imbalance of the chemical potential in two valleys of a Weyl metal, say $\mu_R > \mu_L$, and then we apply a (static) magnetic field on it, what will happen? There will be a current produced along the magnetic field:[55]

$$j^{CME}_{\omega=0} = \frac{e^2(\mu_R - \mu_L)}{4\pi^2} B,$$

which can be easily obtained by calculating conductivity tensor (or gyrotropic tensor) and keeping up to the linear order of the electromagnetic field. Details about calculations and theoretical analysis can be found in chapter 3 (part III.B).

This effect is dubbed as chiral magnetic effect (CME). Just like chiral anomaly, chiral magnetic effect was firstly studied in QED and QCD[55, 56, 57], then because of the recent study of chiral anomaly in Weyl metals, it was brought into condensed matter field, to be exact, into the study of Weyl metals[58, 59, 60, 61, 62, 63].

Chiral magnetic effect can be detected via nonlocal transport experiments as suggested by my advisor Dima Pesin and his co-workers in 2013[64], when the chiral anomaly stimulates the imbalance of the chemical potential, $\mu_R \neq \mu_L$, and then a probe magnetic field converts this imbalance into a measurable voltage drop far from source and drain, indicated by the mechanism of CME. The basic idea is shown in Fig.(2.3).
From Eq.(2.38), we see that in equilibrium case, where $\mu_R = \mu_L$, there is no chiral magnetic current at all, which is quite reasonable: nobody would expect a current induced by a static magnetic field in equilibrium system. However, if we have a slowly vibrating magnetic field, that is $\omega \neq 0$, there might be a current, even when system is in equilibrium $\mu_R = \mu_L$. The phenomenon of nontrivial current response to slowly oscillating magnetic field is named as dynamic chiral magnetic effect (dCME). We will show that it happens in equilibrium Weyl metal system when a pair of Weyl nodes have different energies, $E_L \neq E_R$, which could happen in nature. Further discussions are in chapter 3.

### 2.5 Our motivation: to learn the optical and transport properties of Weyl metals

For high energy physicists, the exciting part of the new phase of Weyl semimetal is that it provides us a plateau to test theories about 3D massless Dirac fermions, although these Weyl fermions are quasi-particles, not real particles. For condensed matter physicists, the
most interesting part is the new phase itself: will it bring any new phenomena, or will it response differently to external probe? Therefore, our concentration would be on the topic of revealing possibly unique optical and transport properties.

In the last section, we have already had a quick glance about the chiral anomaly related negative longitudinal magnetoresistance and the chiral magnetic effect, which were thought to be candidates of unique phenomena associated with Weyl (semi-)metal. Chapter 3 will be a deep research into the mechanism and properties of chiral magnetic effect (CME) and optical activity in (Weyl) metals, in which we will find that the dynamic CME-like response, originated from local geometry of electronic bands (not topology), is actually not unique to Weyl metals only: it might happen even without Berry monopoles. Followed by this is a natural question: how to measure the dynamic chiral magnetic conductivity? The answer is Faraday rotation, as the Faraday rotation angle is directly proportional to the chiral magnetic conductivity, which gives a most direct way to measuring it. Based on that insight, chapter 4 gives a prediction about the chiral magnetic conductivity measured with Faraday rotation experiment. However, when studying optical and transport phenomena in a Weyl metal, or more generally speaking, a gapless topological system, the challenge is: in principle, with a gapless bulk, it manifests all responses similar to a normal metal with the same symmetries. In order to distinguish them, in chapter 4, we studied the omnipresent disorder effects: how macroscopic sample inhomogeneities affect the dynamic chiral magnetic conductivity to be measured by Faraday rotation experiment. We pushed our study a bit further to the current induced magnetization in chapter 5. One thing has to be pointed out is that, our research was ignited by Weyl semimetals, but all our results have a wider application.

2.6 References

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CHAPTER 3

CHIRAL MAGNETIC EFFECT AND NATURAL OPTICAL ACTIVITY IN (WEYL) METALS

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Chiral magnetic effect and natural optical activity in metals with or without Weyl points

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We consider the phenomenon of natural optical activity, and related chiral magnetic effect in metals with low carrier concentration. To reveal the correspondence between the two phenomena, we compute the optical conductivity of a noncentrosymmetric metal to linear order in the wave vector of the light wave, specializing to low carrier concentration. We show that it is the orbital magnetic moment of quasiparticles that is responsible for the natural optical activity, and thus the chiral magnetic effect. While for purely static magnetic fields the chiral magnetic effect is known to have a topological origin and to be related to the presence of Berry curvature monopoles (Weyl points) in the band structure, we show that the existence of Berry monopoles is not required for the dynamic chiral magnetic effect to appear; the latter is thus not unique to Weyl metals. The magnitude of the dynamic chiral magnetic effect in a material is related to the trace of its gyrotropic tensor. We discuss the conditions under which this trace is nonzero; in noncentrosymmetric Weyl metals it is found to be proportional to the space-energy dipole moment of Berry curvature monopoles. The calculations are done within both the semiclassical kinetic equation, and Kubo linear-response formalisms, with coincident results.

I. INTRODUCTION

The phenomenon of natural optical activity was discovered by Arago in 1811, while observing passage of polarized light through crystals of quartz. This was the first example of a general family of phenomena related to optical activity, which is characterized by a material’s different response to right- and left-handedly polarized light. Since then natural optical activity has become one of the most studied optical phenomena in molecules and crystals, with a wide spectrum of biomedical applications, ranging from determining sugar concentration in biological fluids, to studies of RNA and DNA molecules.

From a modern perspective, natural optical activity in time-reversal invariant systems appears due to a linear in wave vector of the light wave spatial dispersion of the conductivity (or, equivalently, dielectric) tensor \( \sigma_{ab}^{\omega, \mathbf{q}} \) [1]:

\[
\sigma_{ab}^{\omega, \mathbf{q}} = \sigma_{ab}^{\omega} + \lambda_{abc}^{\omega} \mathbf{q}_c.
\]

Since the third-rank tensor \( \lambda_{abc} \) changes sign under inversion, the latter cannot be a symmetry of a material showing natural optical activity. The lack of an inversion center is a necessary, but not sufficient, condition for natural optical activity [2]. Noncentrosymmetric (lacking an inversion center) optically active materials are called gyrotropic.

This work considers natural optical activity in metallic systems, since mechanisms of natural optical activity/gyrotropy in molecules and insulating crystals are well understood [3,4]. Our motivation comes from the observation that the so-called “chiral magnetic effect” (CME) [5–9], in particular discussed [10–15] in the context of Weyl (semi)metals [16–19], is nothing but a particular case of optical activity.

Indeed, CME is defined as the existence of a current \( j^{\omega, \mathbf{q}} \) flowing in response to a magnetic field \( \mathbf{B} \) along the latter; in Fourier components, such a relation is written as

\[
j^{\omega, \mathbf{q}} = \eta^{\omega, \mathbf{q}} \mathbf{B}(\omega, \mathbf{q}).
\]

Since this response exists only at finite frequencies in an equilibrium crystal [13–15], the Faraday’s law \( \mathbf{B} = \mathbf{q} \times \mathbf{E}/\omega \) (\( c = 1 \) throughout this paper) allows us to rewrite this relation as a particular case of spatial dispersion part of Eq. (1):

\[
\lambda_{abc}^{\text{metal}}(\omega) = -\frac{\eta^{\omega, \mathbf{q}}}{\omega} \epsilon_{abc},
\]

where \( \epsilon_{abc} \) is the fully antisymmetric Levi-Civita tensor. At small frequencies (the precise condition is to be discussed below) \( \eta^{\omega, \mathbf{q}} \approx \text{const} \), and thus dependence on a frequency of \( \lambda_{abc}^{\text{metal}}(\omega) \propto 1/\omega \) is markedly different from \( \lambda_{abc}^{\text{insulator}}(\omega) \propto \omega \) in the insulating case. The latter fact is expected, since in an insulator \( \lambda_{abc}^{\text{insulator}}(\omega) \) should be an analytic function of \( \omega \), and can be established on general grounds within band theory [20,21]. At high frequencies, the metallic and insulating cases cannot be distinguished by the frequency dependencies of respective \( \lambda_{abc} \), hence we limit ourselves to the low-frequency regime in what follows.

In this work we extend the understanding of natural optical activity in metals in the following ways: (i) We obtain an expression for tensor \( \lambda_{abc} \) that determines the spatial dispersion of conductivity, Eq. (1), which is valid for arbitrary band structures at low frequencies, both from semiclassical kinetic equation, and from Kubo formalism. In general, we find that there are many conflicting results regarding this tensor in the literature. In particular, our results differ from those of Refs. [22–25]. (ii) Using the obtained results, we show that as far as Weyl metals are concerned, only the static limit of the CME has a topological origin and a universal magnitude, which universally vanishes in an equilibrium crystal. In the dynamic limit, the CME, being a particular part of current due to natural optical activity of the material, does exist, but is not universal: the tensorial structure of \( \lambda_{abc} \) is more complicated than that of Eq. (3), and the magnitude of dynamic CME depends on the peculiarities of band structure (like its curvature). For the ideal case of a Weyl metal represented by a collection of particle-hole symmetric Weyl points, we show in full generality that the magnitude of the CME is determined by the energy-space dipole moment of Berry monopoles that correspond to these Weyl points. (iii) Finally, we show that the possibility of CME-like response is not restricted to Weyl semimetals: In fact, the existence of Berry monopoles, and thus...
chiral anomaly, is not necessary for nonzero dynamic CME at all. The rest of the paper is organized as follows: In Sec. II we obtain a description of natural optical activity in metals based on the semiclassical kinetic equation. This section also contains a discussion of the relation between the results of this paper, and other works. In Sec. III we consider several specific examples of model Hamiltonians that illustrate the results we obtained. In Sec. IV we summarize our main results. Finally, in the Appendixes we discuss the static CME within the semiclassical kinetic equation formalism, and present a derivation of the results from Sec. II based on the Kubo formalism.

II. SEMICLASSICAL THEORY OF NATURAL OPTICAL ACTIVITY IN METALS

In this section we describe the response of a time-reversal invariant metal to an electromagnetic field that varies slowly in time and space, at the linear-response level. The main results of this section are Eq. (18) for the gyrotropic current, Eqs. (19) and (20) for tensor \( \lambda_{ab} \) that determines the spatial dispersion of conductivity, and Eqs. (24) and (25) for the gyrotropic tensor and its trace.

The formalism is borrowed from the Berry phase theory of semiclassical transport [26]. Since we are interested in the leading effects of spatial dispersion of conductivity, we concentrate on current contributions that are proportional to the leading effects of spatial dispersion of conductivity, and Eqs. (4) for the gyrotropic current, Eqs. (8) for the gyrotropic tensor, and Eqs. (24) and (25) for the gyrotropic tensor and its trace.

In order to calculate the current response to electromagnetic fields in the semiclassical regime, we need to express the electric current through the distribution function of electrons, and formulate a kinetic equation for the latter. We thus briefly recall known facts about semiclassical theory of electrons in crystals.

In what follows, we will denote the \( p \)-space Hamiltonian, the energy spectrum of the crystal, and the periodic parts of the corresponding Bloch wave functions in the absence of external fields with \( \hbar_p, \epsilon_p, \) and \( |u_p \rangle \), respectively. The gradient in the quasimomentum space is denoted with \( \partial_p \), and the derivative with respect to the \( n \)-th component of \( \mathbf{p} \) with \( \partial_n \). The operator of gradient in real space is denoted with \( \partial_s \). For brevity, we set \( \hbar = c = 1 \) throughout the paper.

At the semiclassical level, the dependence of periodic parts of Bloch functions on quasimomentum leads to the appearance of two objects [26], central for our discussion: The first is the Berry curvature of band \( n \), \( \Omega_{np} \):

\[
\Omega_{np} = i \langle \partial_p u_{np} \rangle \times |\partial_p u_{np}|; \tag{4}
\]

the other one is the orbital magnetic moment of quasiparticles, \( \mathbf{m}_{np} \):

\[
\mathbf{m}_{np} = \frac{i e}{2} \langle \partial_p u_{np} \rangle \times (\hbar_p - \epsilon_p)(\partial_p u_{np}). \tag{5}
\]

By choosing appropriate band, we obtain a description of natural optical activity in metals.

Finally, we have to establish the expression for the electric current. It contains two contributions: one, \( \mathbf{j}_p \), that comes from the wave packet velocity of Eq. (8), and the other coming from the curl of quasiparticle orbital magnetization, \( \mathbf{j}_m \). The former can be obtained from the continuity equation for the electric charge implied by kinetic equation (9) [9,29]; the latter

Denoting the renormalized band velocity with \( \mathbf{v}_{np} = \partial_p \epsilon_{np} - \partial_p (\mathbf{m}_n \mathbf{B}) \), the semiclassical equations of motion for band \( n \) can be written as [26]

\[
\dot{\mathbf{r}} = \mathbf{v}_{np} - \mathbf{p} \times \Omega_{np}, \tag{6}
\]

\[
\dot{\mathbf{p}} = e \mathbf{E} + e \mathbf{v}_{np} \times \mathbf{B}. \tag{7}
\]

These equations yield

\[
\dot{\mathbf{r}} = \frac{1}{D_B} [\mathbf{v}_{np} - e \mathbf{E} \times \Omega_{np} - e (\mathbf{v}_{np} \cdot \Omega_{np}) \mathbf{B}],
\]

\[
\dot{\mathbf{p}} = \frac{1}{D_B} [e \mathbf{E} + e \mathbf{v}_{np} \times \mathbf{B} - e^2 (\mathbf{E} \cdot \mathbf{B}) \Omega_{np}],
\]

\[
D_B = 1 - e \mathbf{B} \Omega_{np}.
\]

In the equation for \( \dot{\mathbf{r}} \), the first term on the right-hand side is the usual group velocity, including the effect of energy renormalization, Eq. (6); the second one is the anomalous velocity [26], associated with interband coherence effects induced by the electric part of the Lorentz force; the last contribution is the velocity that appears due to the interband coherence effects induced by the magnetic part of the Lorentz force, and is commonly associated with the static CME [5–9,13]. The equation for \( \mathbf{p} \), besides the usual Lorentz force, contains an “\( \mathbf{E} \cdot \mathbf{B} \)” term, which is a manifestation of chiral anomaly at the quasiclassical level [29,30]. We note that the signs of the terms in the right-hand sides of Eqs. (8) vary between different works, which is related to the Berry curvature definition, and whether \( e \) is taken to be positive or negative. We chose \( e < 0 \) and \( \Omega_{np} \) given by Eq. (4). In accord with our plan to limit ourselves to linear response in \( \mathbf{E} \) and \( \mathbf{B} \) fields, in what follows we will disregard terms in Eqs. (8) that are nonlinear in electromagnetic fields. In particular, the chiral anomaly will play no role in our discussion.

Equations (8) allow us to write down the semiclassical kinetic equation. We concentrate on the collisionless regime, \( \hbar \tau \to \infty \), where \( \tau \) is the shortest relaxation time, since it is sufficient to bring out the points we would like to make. Later we will introduce a finite \( \tau \) phenomenologically to discuss dissipative phenomena. The kinetic equation has the following form:

\[
\partial_s f_{np} + \mathbf{r} \partial_s f_{np} + \mathbf{p} \partial_p f_{np} = 0. \tag{9}
\]
is given by
\[ j_m = \partial_r \sum_n \int (d\mathbf{p}) |\mathbf{m}_n| f_{n\mathbf{p}}, \]  
where \((d\mathbf{p}) \equiv d^3p/(2\pi)^3\). This expression is expected on physical grounds, and can be formally obtained from a more low-level semiclassical kinetic equation for the full density matrix, by considering interband coherences established by gradients of the intraband distribution function \[9,30–32\].

To find \(j_{n\mathbf{p}}\), we note that the density of electric charge is given by \[\rho = e \int (d\mathbf{p}) D_{n\mathbf{p}} f_{n\mathbf{p}},\] (11) and must satisfy \[\partial_t \rho + \partial_r j_{n\mathbf{p}} = 0.\] (12)

(We neglected the chiral anomaly as a nonlinear effect, hence no anomalous divergence in this equation. Alternatively, we could have noticed that \(\mathbf{E} \cdot \mathbf{B} = 0\) for an electromagnetic wave.) Multiplying the kinetic equation by \(D_{n\mathbf{p}}\), observing that \(D_{n\mathbf{p}} \partial_t f_{n\mathbf{p}} = \partial_t (D_{n\mathbf{p}} f_{n\mathbf{p}}) - f_{n\mathbf{p}} \partial_t D_{n\mathbf{p}}\), and that according to the Faraday’s law \(\partial_t \mathbf{B} = -\partial_r \times \mathbf{E}\), after simple manipulations we obtain that \(j_{n\mathbf{p}}\) is given by
\[ j_{n\mathbf{p}} = e \sum_n \int (d\mathbf{p}) [\partial_\mathbf{p} \epsilon_n - \partial_\mathbf{p} (\mathbf{m}_n \cdot \mathbf{B}) - e\mathbf{E}] \times \Omega_{n\mathbf{p}} - e (\partial_\mathbf{p} \epsilon_n \cdot \Omega_{n\mathbf{p}}) B f_{n\mathbf{p}}.\] (13)

Combining Eqs. (10) and (13), we obtain the final expression for the electric current:
\[ j = e \sum_n \int (d\mathbf{p}) [\partial_\mathbf{p} \epsilon_n - \partial_\mathbf{p} (\mathbf{m}_n \cdot \mathbf{B}) - e\mathbf{E} \times \Omega_{n\mathbf{p}} - \partial_r \sum_n \int (d\mathbf{p}) |\mathbf{m}_n| f_{n\mathbf{p}} f_{n\mathbf{p}}].\] (14)

For our purpose of finding a linear response to the fields, the distribution function \(f_{n\mathbf{p}}\) should be replaced with the equilibrium one whenever it is multiplied by \(\mathbf{E}\) or \(\mathbf{B}\) in Eq. (14).

Since we are interested in linear response to electromagnetic fields, we can simplify the kinetic equation (9) further. The kinetic equation for band \(n\), in which we keep only the terms linear in \(\mathbf{E}\) or \(\mathbf{B}\) (such are time and space derivatives of the distribution function), has the usual form:
\[ \partial_t f_{n\mathbf{p}} + \partial_\mathbf{p} \epsilon_n \partial_\mathbf{p} f_{n\mathbf{p}} + e\mathbf{E} \partial_\mathbf{p} f_{n\mathbf{p}0} = 0.\] (15)

Here \(f_{n\mathbf{p}0}\) is the equilibrium distribution function, and only the electric part of the Lorentz force enters, since \(\mathbf{v} \times \mathbf{B} \cdot \partial_\mathbf{p} f_{n\mathbf{p}0} = 0\). This simplicity has a price: The usual galvanomagnetic phenomena \[33\], as well as the effects related to the chiral anomaly, are then beyond the scope of the present treatment. Nonetheless, Eqs. (14) and (15) are sufficient to describe linear electric current response to \(\mathbf{E}\) and \(\mathbf{B}\) fields that vary slowly in space and time.

\section{Gyrotropic current}

We now calculate the response at finite frequency and wave vector, satisfying \(\omega \gg v q\), where \(v\) is the relevant speed of electrons in the crystal. We thus restrict ourselves to linear order in the wave vector \(q\). We will see that it is the orbital magnetic moment of quasiparticles that is responsible for low-frequency chiral magnetic effect in clean metals, as well as the spatial dispersion of their optical conductivity.

For harmonic perturbations, the solution of the kinetic equation (15) for the nonequilibrium part of the distribution function is trivially found by switching to Fourier space:
\[ \delta f_{n\mathbf{p}} = \frac{1}{i(\omega - \mathbf{q} \cdot \mathbf{v}_p) + e\mathbf{E} \partial_\mathbf{p} f_{n\mathbf{p}0}. \] (16)

We emphasize that since we are considering response at frequencies that are high compared to inverse relaxation times of the system, the equilibrium distribution function is given by \(f_{n\mathbf{p}}(\epsilon_p)\), not by \(f_{n\mathbf{p}}(\epsilon_p)\) with total quasiparticle energy \(6\). The quasiparticle velocity is still given by \(\mathbf{p}\)-space gradient of Eq. (6), since the variation of magnetic field in time is slow on quantum-mechanical time scales.

The current is obtained from Eq. (14), keeping in mind that the terms with \(\mathbf{E}\) or \(\mathbf{B}\) fields present must contain the equilibrium distribution function. \(f_{n\mathbf{p}0} = f_{n\mathbf{p}}(\epsilon_p)\). Those without the fields have \(\delta f_{n\mathbf{p}}\) from Eq. (16) entering, since they are nullified by \(f_{n\mathbf{p}}(\epsilon_p)\).

Keeping only nonzero terms up to the linear order in \(\mathbf{E}/\omega\) or \(\mathbf{B}\), and taking into account that the anomalous Hall effect current coming from the anomalous velocity vanishes in a time-reversal invariant system, we obtain
\[ j(q, \omega) = \sum_n \int (d\mathbf{p}) \left( e^2 \frac{\partial_\mathbf{p} \epsilon_n}{i\omega} (\mathbf{E} \partial_\mathbf{p} f_{n\mathbf{p}}) - e^2 (\partial_\mathbf{p} \epsilon_n \cdot \Omega_{n\mathbf{p}}) f_{n\mathbf{p}} \times \mathbf{B} - e \partial_\mathbf{p} (\mathbf{m}_n \cdot \mathbf{B}) f_{n\mathbf{p}} + \frac{e}{\omega} (\mathbf{q} \times \mathbf{m}_n) (\mathbf{E} \partial_\mathbf{p} f_{n\mathbf{p}}) \right). \] (17)

This expression for the gyrotropic current is one of the central results of our work. All terms in Eq. (17) have clear physical meaning: the first term is the reactive current that exists in any metal in the collisionless regime; the second term represents the static chiral magnetic effect \[34\], discussed in Appendix B; the third and fourth contributions appear due to the presence of orbital magnetic moment of quasiparticles, the former being due to the corresponding energy renormalization, Eq. (6), and the latter representing the current due to nonequilibrium orbital magnetization. The current due to the velocity renormalization does not vanish because one has to use \(f_{n\mathbf{p}}(\epsilon_p)\) as the unperturbed distribution function, as explained above. It does vanish if response to a purely static magnetic field is sought (thus in the absence of electric field), where a truly equilibrium distribution function \(f_{n\mathbf{p}}(\epsilon_p)\) is established, see Appendix B.

The last three terms in Eq. (17) represent the leading contributions to the gyrotropic current \(j_E\) in a metal. Using integration by parts to rewrite all terms as contributions from the Fermi surface, we obtain
\[ j_E(q, \omega) = \sum_n \int (d\mathbf{p}) \left( e^2 \frac{\partial_\mathbf{p} \epsilon_n}{i\omega} (\partial_\mathbf{p} f_{n\mathbf{p}} \cdot \Omega_{n\mathbf{p}}) \mathbf{B} + e (\mathbf{m}_n \cdot \mathbf{B}) \partial_\mathbf{p} f_{n\mathbf{p}} \right. \]
\[ + \left. \frac{e}{\omega} (\mathbf{q} \times \mathbf{m}_n) (\mathbf{E} \partial_\mathbf{p} f_{n\mathbf{p}}) \right). \] (18)
Having the expression for the gyrotropic current, we can write down the expression for tensor $\lambda_{abc}$ that determines the spatial dispersion of conductivity, Eq. (1):

$$\lambda_{abc} = -\frac{e^2}{\omega} \sum_n \int (dp) \left( \epsilon_{np}(\partial_p f_{sp} \cdot \Omega_{np}) \epsilon_{abc} + \frac{1}{e} \delta_{np} \delta_{a} \sum_m \epsilon_{mp} f_{mp} \epsilon_{bdc} + \frac{1}{e} \delta_{np} \delta_{b} \sum_m \epsilon_{mp} f_{mp} \epsilon_{adc} \right).$$  \hspace{1cm} (19)

where $\epsilon_{abc}$ is the Levi-Civita tensor, $m_{nd}$ is the $d$th Cartesian component of $m_{np}$ and summation over repeated indices is implied.

Equation (19) is useful when one is interested in a contribution to the conductivity made by a particular region of quasimomentum space, e.g., close to a particular Weyl point. If only the total contribution is sought, the first term on the right-hand side of Eq. (19) vanishes upon $\int dp$ integration and $n$ summation, and one is left with

$$\lambda_{abc} = -\frac{e^2}{\omega} \sum_n \int (dp) (m_{nd} \delta_{pa} \sum_b \epsilon_{bdc} + \text{cyclic terms}).$$  \hspace{1cm} (20)

We use the same symbol for $\lambda_{abc}$ given by Eqs. (19) or (20), even though they are equivalent only if the integration is done over the entire Brillouin zone, and summation is over all bands; this does not seem to lead to a confusion.

The validity of the entire treatment presented here is limited to frequencies that are small compared to the typical band gaps encountered in the problem. Only under this condition we can neglect interband absorption, and the dynamics is adiabatic, and hence can be reduced to a single-band kinetic equation. For instance, for a single Weyl point, the frequency of the electromagnetic wave has to be small compared to the doping level; in a two-band model of a metal with spin-split Fermi surfaces, the frequency has to be small compared to the spin splitting at the Fermi level.

We briefly comment that the absorptive counterpart of natural optical activity—the circular dichroism—comes from the imaginary part of $\lambda_{abc}$, and can be included phenomenologically by substituting [24] $\omega \to \omega + i/\tau$ into Eq. (20) [35], where $\tau$ is the relevant relaxation time. For $\omega \tau \ll 1$ we obtain a purely dissipative current, which is characterized by $j \propto B$ in an isotropic system. This current, appearing due to the existence of Berry curvature in the band structure, is the “intrinsic” analog of the same type of current found in Ref. [36], which considered electron scattering on impurities lacking an inversion center.

Finally, we would like to point out that our results are in full accord with the Onsager relations for conductivity [1,37], which in the absence of magnetic order read $\sigma_{ab}(\omega, \mathbf{q}) = \sigma_{ba}(\omega, -\mathbf{q})$. This implies that tensor $\lambda_{abc}$ satisfies

$$\lambda_{abc}(\omega) = -\lambda_{bac}(\omega).$$  \hspace{1cm} (21)

This is clearly the case for Eqs. (19) and (20). Further, the Hermitian (absorptive) part of the conductivity tensor is an even function of $\omega$, and its anti-Hermitian (dispersive) part is an odd function of $\omega$. We can thus conclude that in the absence of absorption $\lambda_{abc}(\omega)$ is a real tensor that satisfies

$$\lambda_{abc}(\omega) = -\lambda_{abc}(-\omega).$$  \hspace{1cm} (22)

Again, this holds for Eqs. (19) and (20), which were derived neglecting dissipative effects. The imaginary (absorptive) part of $\lambda_{abc}$, describing circular dichroism, is even in frequency, which also happens to be true for the aforementioned phenomenological substitution $\omega \to \omega + i/\tau$ in Eq. (20).

**B. Gyrotropic tensor: Relation to previous works**

In what follows, we find it convenient to switch to the description of gyrotropy in terms of the gyrotropic tensor. To this end we note that the third-rank tensor $\lambda_{abc}$, antisymmetric with respect to the first pair of indices, is dual to a second-rank pseudotensor—the gyrotropic tensor $\sigma_{ab}$. Indeed, both tensors have nine independent components, and change sign under inversion. The relation between the two tensors is given by [1]

$$\lambda_{abc} = \epsilon_{abcd} \sigma_{cd} = \frac{1}{2} \epsilon_{abcd} \lambda_{abcd}. \hspace{1cm} (23)$$

Using Eq. (19), we obtain

$$\lambda_{abc} = \frac{e^2}{\omega} \sum_n \int (dp) \epsilon_{np}(\partial_p f_{sp} \cdot \Omega_{np}) \delta_{ab} - \frac{e}{\omega} \sum_n \int (dp) m_{np} \partial_p f_{spa} + \frac{e}{\omega} \sum_n \int (dp) m_{np} \partial_p f_{spb}.$$  \hspace{1cm} (24)

As is well known [13], for any band structure the first term in this expression is just a complicated way to write a zero, while, for instance, it does make a contribution for a single Weyl point. This term also has to be taken into account if one considers a nonequilibrium situation, e.g., a Weyl metal, in which different Weyl points have different chemical potentials.

The trace of the gyrotropic tensor is another useful quantity one may consider. It is easier to calculate than the full gyrotropic tensor, and if nonzero, immediately signals that the gyrotropic tensor itself is nonzero. In a system with point groups of relatively high symmetry (isotropic systems in particular), the trace of the gyrotropic tensor solely determines the magnitude of dynamic CME. The expression for this trace is

$$\text{Tr} \sigma = -\frac{3e^2}{\omega} \sum_n \int (dp) \epsilon_{np}(\partial_p f_{sp} \cdot \Omega_{np})$$

$$-\frac{2e}{\omega} \sum_n \int (dp) (m_{np} \cdot \partial_p f_{sp}).$$ \hspace{1cm} (25)

There is another aspect in which the trace of the gyrotropic tensor appears to be a quantity of interest. In general, the conductivity tensor (1) implies a complicated relation between the direction of current flow and that of magnetic field. Upon switching to the description in terms of the gyrotropic tensor, one can rewrite the latter as

$$\delta_{ab} = \frac{1}{2} \text{Tr} \delta_{ab} + \delta_{gab}. \hspace{1cm} \text{Tr} \delta = 0. \hspace{1cm} (26)$$

The $\delta_{ab}$ part of this expression is easily seen to give rise to a current flowing along the magnetic field, since the corresponding tensor $\lambda_{abc} \propto \epsilon_{abc}$. In a sense, this is a “robust” contribution to CME, independent of the propagation direction of an electromagnetic wave, and its polarization direction. The other, traceless, part may also lead to a current component along the magnetic field, but it is “fine-tuned”: the magnitude
of such effect would depend on the details of wave propagation though a crystal. We therefore concentrate on calculating Trg in what follows, aiming at providing insight into the circumstances under which “robust” CME (in the sense explained above) can be observed.

Equations (17), (19), (20), (24), and (25) are the central results of this work. They do not coincide with results published in works on related subjects [22–25], which were derived for general band structures, the same as ours. We do agree with the results of Refs. [8,9] for the dynamic chiral magnetic effect associated with a single Weyl point with particle-hole symmetry. In Ref. [38] the Berry curvature and orbital magnetic moment of quasiparticles are not explicit, thus the comparison of results is difficult. However, we do qualitatively agree with the latter work in simple limits (see below), but have different prefactors in final expressions. For a particular case of a two-band model, our expressions can be shown to reduce to those of Ref. [39]. The result for the gyrotropic current of Ref. [15] was obtained for a specific model with broken time-reversal and inversion symmetry, having only two Weyl points. The result pertains to the limit of strong magnetic field, and lies outside of the applicability region of the present theory. We can confirm, however, the general conclusion that in an “ideal” Weyl metal, represented by a collection of strictly particle-hole symmetric Weyl points located, in general, at different energies there exists dynamic CME, whose magnitude is determined by the energy-space dipole moment of Berry monopoles associated with the Weyl points. It is further claimed in Ref. [15] that the chiral magnetic effect is a topological property of Weyl metals, with essentially universal magnitude. Our results that are applicable to general band structures do not confirm that observation: It appears that the existence of Weyl nodes is not even needed for a metal to have dynamic CME. We defer the discussion of specific cases that illustrate our claims until the next Section.

As far as we understand, the difference in the results of the present work and Refs. [22,24,25] is due to the fact that in the latter ones the magnetic part of the Lorentz force and the orbital magnetic moment of quasiparticles, Eq. (5), were not included in the semiclassical equations of motion, Eqs. (7). As follows from our discussion, natural optical activity comes solely from these terms, and Refs. [22,24,25] should have obtained exact zero for, say, the gyrotropic tensor. The fact that finite results were obtained in these works can be traced back to their treatment of the current contribution coming from the anomalous velocity, which we will denote $j_a$, for the time being. The corresponding expression is given by the third term in the first bracket on the right-hand side of Eq. (14):

$$j_a = -e^3 \sum_n \int (dp) E \times \Omega_{ap} f_{ap}. \quad (27)$$

As we can see, this is a completely local current. Possible nonlocality can only come from lattice constant scales, where the semiclassical description breaks down. Therefore, even for space-dependent $E(r)$ one gets zero for it to linear order in the electric field in a system with time-reversal symmetry. The latter is due to the fact that time-reversal symmetry implies that the Berry curvature is an odd function of $p$, $\Omega_{ap} = -\Omega_{pa}$, while the equilibrium distribution function is even. Further, the form of $j_a$ was essential to get the continuity equation (12) to hold. Therefore, using alternative nonlocal expressions from Refs. [22,24,25] would violate charge conservation at the semiclassical level.

We would also like to point out that the gyrotropic tensor of Eq. (24) is written as a Fermi-surface property, and is proportional to $1/\omega$. This is a distinct feature of a metallic system: the leading frequency dependence of the gyrotropic tensor in an insulator is $\omega^2$ [20,21]. The results of Refs. [22,25] also contain the $1/\omega$ frequency dependence, yet cannot be written as Fermi-surface contributions in general, and may give finite answers in band insulators; $\lambda_{abc} \propto 1/\omega$ in insulators contradicts Kramers-Kronig relations [21].

In the remainder of this section we would like to discuss under what circumstances one should expect the trace of the gyrotropic tensor to vanish, and thus obtain a robust dynamic CME. We note that the expression for the intrinsic orbital magnetic moment (5) can be rewritten as

$$m_{ap} = -e \epsilon_{ap} \epsilon_{ap} + \frac{ie}{2} \sum_{m \neq n} (\epsilon_m + \epsilon_n) \langle \delta_p \mu_{ap} | \delta_p \mu_{ap} \rangle \times \langle \mu_{ap} | \delta_p \mu_{ap} \rangle. \quad (28)$$

If one simply drops the second term on the right-hand side of this expression, and plugs the first one into Eq. (25), the latter, after partial cancellations, will turn into an expression that determines the magnitude of the static CME, discussed in detail in Appendix B [see Eq. (B4)]. It is known that such an expression vanishes in any crystal [13]. However, it is in general not correct to neglect that contribution. Moreover, in many important situations that term is the only source of nontrivial physical effects. For instance, in noncentrosymmetric Weyl metals, it is the presence of the second term in the right-hand side of (28) that gives a finite dynamic CME.

To determine when it is important to use the entire expression (28) for the orbital magnetic moment, let us restrict ourselves to the case of only two bands coming close together in energy space in some region of the Brillouin zone, and assume that the sum over the intermediate states in Eq. (28) is saturated by entries from these two bands. Then we can write that contribution to the magnetic moment for band $n$ as

$$\frac{ie}{2} \sum_{m \neq n} (\epsilon_m + \epsilon_n) \langle \delta_p \mu_{ap} | \delta_p \mu_{ap} \rangle \times \langle \mu_{ap} | \delta_p \mu_{ap} \rangle \frac{\epsilon_{ap}}{2} \Omega_{ap}. \quad (29)$$

where we denoted the other band with $m = -n$. Clearly, deviations from exact particle-hole symmetry for the two bands in question will lead to the right-hand side of Eq. (29) being finite. A simple situation in which particle-hole asymmetry leads to the only finite contribution to the gyrotropic tensor of a noncentrosymmetric metal is presented in Sec. III A.

To proceed, we observe that the band energies that enter into Eq. (29) are “absolute”: The energy origin can be chosen arbitrarily, but it has to be the same for the entire band structure. Consider now a Weyl point with chirality $Q_{\omega} = \pm 1$ located at energy $E_{\omega}$ near the Fermi level of a certain band structure, Fig. 1. Even if one assumes perfect particle-hole symmetry
around $E_w$ for this Weyl point, the right-hand side of Eq. (29) still does not vanish: $(\epsilon_{\nu p} + \epsilon_{\nu p})/2 = E_w$. Since the latter expression is multiplied by the Berry curvature in Eq. (29), and Berry curvature has a monopolelike singularity near a Weyl point, the part of the magnetic moment from Eq. (29) will make a contribution to the total gyrotropic tensor that is proportional to $Q_w E_w$. It should be now clear that if one has a collection of Weyl points (of course, with zero net chirality), located at different energies, their total contribution to the current does not vanish as long as $\sum_w Q_w E_w$ does not vanish ($w$ now labels different Weyl points). The case where such a “Berry dipole moment” in energy space does not vanish is precisely when the dynamic CME in the system is expected [15]. This case is treated in more detail in Sec. (III B).

Finally, it is not a priori clear that the gyrotropic tensor and its trace require Berry monopoles to be nonzero. In fact, they do not, and in Sec. III C we provide an example of a situation where dynamic CME exists in a system without Weyl points.

III. NATURAL OPTICAL ACTIVITY AND CHIRAL MAGNETIC EFFECT IN SIMPLE MODELS

In this section we will illustrate the expressions obtained above with specific examples of two-band models. We would like to use these as a platform to discuss under what circumstances CME appears in metallic systems.

The trace of the gyrotropic tensor (24) for a two-band system (TBS) is evaluated to be

$$\text{Tr}_g^{\text{TBS}} = -\frac{2\epsilon^2}{\omega} \sum_{\nu = \pm} \int d\epsilon_\nu (\partial_\nu f_{\nu p} \cdot \Omega_{\nu p}). \tag{30}$$

We used $\sum_{\nu \pm} \int (d\epsilon_\nu) (\partial_\nu f_{\nu p} \cdot \Omega_{\nu p}) = 0$ to write this expression. The general momentum-space Hamiltonian for such a system is

$$\hat{h}^{\text{TBS}} = \sigma \hat{d}_p + \hat{E}_p, \tag{31}$$

where $\sigma$ is a vector of Pauli matrices in the appropriate space (being the spin space in the examples to follow). The band energies are given by $\epsilon_{\nu \pm} = \epsilon_{\nu p} \pm \epsilon_{\nu p}$. Since $\epsilon_{\nu p} = 2E_p - \epsilon_{\nu p}$, the trace of the gyrotropic tensor can be rewritten as

$$\text{Tr}_g^{\text{TBS}} = -\frac{2\epsilon^2}{\omega} \sum_{\nu = \pm} \int (d\epsilon_\nu) E_p (\partial_\nu f_{\nu p} \cdot \Omega_{\nu p}). \tag{32}$$

There is no general reason for this quantity to vanish. Expression (32) can be used to make a few useful observations regarding the circumstances under which Trg does not vanish.

There are two distinct situations one may encounter in evaluating Eq. (32): (i) $E_p$ takes a constant value on isoenergetic surfaces of $\epsilon_{\nu p}$, $\epsilon_{\nu p} = \text{const}$, and (ii) it does not.

In case (i), the integral in Eq. (32) can be split into that over magnitude of $\epsilon_{\nu p}$, and a two-dimensional surface integral over isoenergetic surfaces of $\epsilon_{\nu p}$:

$$\text{Tr}_g^{\text{TBS}} = -\frac{2\epsilon^2}{\omega} \sum_{\nu = \pm} \int d\epsilon_\nu (\epsilon_{\nu p} = \epsilon) (\partial_\nu f_{\nu p}(\epsilon)) \times \int_{\epsilon_{\nu p} = \epsilon} dS \cdot \Omega_{\nu p}. \tag{33}$$

Here $E_p(\epsilon_{\nu p} = \epsilon)$ denotes the value of $E_p$ on the surface $\epsilon_{\nu p} = \epsilon$, which is the same on the entire surface by definition in case (i). The surface integral then counts the total charge of Berry monopoles inside the $\epsilon_{\nu p} = \epsilon$ surface (Fermi surface for $\epsilon = \mu$ at zero temperature). Hence, in case (i) in order to find a nonzero $\text{Tr}_g$ one must have Berry monopoles in the band structure in the first place, and then hope that the energy integral and summation over bands do not render $\text{Tr}_g$ zero. Sections III A and III B present examples where case (i) is realized, and it so happens that $\text{Tr}_g \neq 0$.

Case (ii) is interesting when $\Omega_{\nu p}$ is monopole free. Here, even though $\int_{\epsilon_{\nu p} = \epsilon} dS \cdot \Omega_{\nu p} = 0$, the fact that $E_p$ evaluates to different values on isoenergetic surfaces of $\epsilon_{\nu p}$ can disrupt the exact cancellation between Berry fluxes over a closed surface, and yield a nonzero result for Trg, and hence for dynamic CME, even without any Berry monopoles in the band structure. An example of such a situation is considered in Sec. III C.

A. Isotropic noncentrosymmetric metal

The simplest possible model showing optical activity is that of an isotropic noncentrosymmetric metal, with the single-particle Hamiltonian given by [40]

$$\hat{h}_p = \frac{p^2}{2m} - \mu + v \sigma \mathbf{p}, \tag{34}$$

where $m$ is the effective mass, and $\sigma$ is a vector of Pauli matrices operating in the spin space. Loosely speaking, this model relates to a single Weyl point the same way as the Hamiltonian of a two-dimensional electron gas with Rashba spin-orbit coupling relates to that of a surface of a three-dimensional topological insulator: If only small $\mathbf{p}$’s are considered, it describes a Weyl point with particle-hole symmetry breaking due to the mass term; if all $\mathbf{p}$’s are taken into account, there are always two Fermi surfaces with exactly opposite Berry fluxes through them. Since we are considering this example essentially for the purpose of illustration of our results, we restrict ourselves to the case of zero temperature, and $\mu > 0$, where each of the two bands has a Fermi surface.
The Hamiltonian (34) breaks all reflections (and thus the inversion), and symmetry-wise should allow natural optical activity. However, Refs. [22,25] would predict zero for the latter, while we get a nonzero result. Reference [38] reaches the same conclusion as we do, but there the overall value of the gyrotropic current at low frequencies is four times as big as ours.

Due to the isotropy of model (34), its gyrotropic tensor is given by

$$g_{ab} = \frac{1}{2} \text{Tr} \delta_{ab}. \quad (35)$$

We will evaluate separately the contributions of the two spin-split bands to Trg, Eq. (25). Having single-band results will allow us to discuss the role of particle-hole asymmetry for a true Weyl point, where there is a single Fermi surface surrounding a Berry monopole.

We label the bands of Hamiltonian of Eq. (34) with $n = \pm$, and the corresponding energies, Berry curvatures, and orbital magnetic moments are given by

$$\epsilon_{\pm} = \frac{p^2}{2m} \pm v_p, \quad \Omega_{\pm} = \mp \frac{1}{2} \hat{p}/p^2, \quad m_{\pm} = \frac{ev_p}{2} \hat{p}/p. \quad (36)$$

The Fermi momenta for the two bands, $p_{\pm}$, are found from

$$\frac{p_{\pm}^2}{2m} \pm vp_{\pm} = \mu. \quad (37)$$

Restricting ourselves to zero temperature, and evaluating trivial integrals in Eq. (25), we obtain the contributions of the two bands to the total gyrotropic tensor, $g_{\pm}$, to be (we restrict ourself to the dynamic limit only)

$$g_{\pm} = \pm \frac{e^2}{12\pi^2 \omega} \left( \mu + \frac{p_{\pm}^2}{m} \right) \delta_{ab}. \quad (38)$$

We see that the residual mass term contributes differently to $g_{\pm}$, and leads to a nonzero total $g = g_+ + g_-$,

$$g = -\frac{e^2}{12\pi^2 \omega} \left( \frac{p_+^2}{m} - \frac{p_-^2}{m} \right) \delta_{ab}. \quad (39)$$

This result can be translated into an expression for the current response to (oscillating) uniform magnetic field:

$$J_k = \frac{e^2}{12\pi^2} \left( \frac{p_+^2}{m} - \frac{p_-^2}{m} \right) B. \quad (40)$$

An analogous expression, but of magnitude four times as big, was obtained for this model in Ref. [38]. Further, formally looking like the famous chiral magnetic effect, Eq. (40) shows that there is no universality in magnitude of such an effect in the dynamic limit: It depends on the details of the band structure, like band curvature, etc. We can estimate when such corrections are important in Weyl metals. Assuming that band curvature is due to a residual mass term with a typical for narrow gap semiconductor $m \sim 0.1 m_e$, $m_e$ being the bare electron mass, and taking a typical value for the Dirac speed in Weyl metals to be [41] $v \sim 0.1 - 0.5 \times 10^5 m/s$, we see that the energy scale that controls the importance of band curvature corrections is $m^2 \sim 10 - 100$ meV. For doping levels of this order or larger, band curvature corrections need to be taken into account for a quantitative description of chiral magnetic effect in Weyl metals.

### B. Weyl metal with particle-hole symmetric Weyl points

Now we would like to get expressions for the gyrotropic tensor in a simplified model of a noncentrosymmetric Weyl metal. The minimal example that would mimic the behavior of $g_{ab}$ in a real crystal is the approximation of the band structure with a collection of Weyl points. The simplest low-energy Hamiltonian in the immediate vicinity of each Weyl point, labeled by index $w$, is

$$h_w = E_w - \mu_w + \sum_{\omega} Q_{w\omega} v_{\omega w} \sigma_{\omega w}. \quad (41)$$

where $p_{\omega w}$ is the deviation in quasimomentum from the location of the Weyl point in quasimomentum space, $E_w$ is the location of the Weyl point in energy space, $\mu_w$ is the chemical potential near it (different $\mu_w$’s would correspond to a nonequilibrium situation), and the case of broken particle-hole symmetry is considered earlier in this section.

For the model of Eq. (41), the band index takes on two values $n = \pm$ around each Weyl point, with the corresponding energies given by $\epsilon_{w\pm} = E_w \pm v_{\omega w} p_{\omega w}$. The Berry curvature is given by $\Omega_{w\pm} = Q_{w\omega} p_{\omega w}/p_{\omega w}$, where $p_{\omega w}$ is the unit vector along $p_{\omega w}$; the orbital magnetic moment is $m_{w\pm} = -ev_{\omega w} p_{\omega w} \Omega_{w\pm}$. It is crucial that it is $\epsilon_{w\pm}$ that enters the first term in Eq. (24), yet it is $\epsilon_{w\pm} - E_w = \pm v_{\omega w} p$ (band splitting, rather than the individual band energy) that determines the orbital magnetic moment.

First, consider the case of equilibrium linear response, $\mu_w = \mu$ for all $w$. From Eqs. (24) and (25) it is clear that only the terms that involve the orbital magnetic moment contribute to $g_{ab}$, and one obtains

$$g_{ab} = -\frac{e^2}{6\pi^2 \omega} \sum_{w} Q_w E_w, \quad \text{Trg} = -\frac{e^2}{2\pi^2 \omega} \sum_{w} Q_w E_w. \quad (42)$$

We observe that the trace of the gyrotropic tensor is determined by the dipole moment in energy space of the Berry curvature monopoles. The gyrotropic tensor itself implies that there exists a chiral-magnetic-effect-looking current given by

$$J_k = \frac{e^2}{6\pi^2} B \sum_{w} Q_w E_w. \quad (43)$$

We now turn to a hypothetical nonequilibrium case, in which the chemical potentials in different valleys do not coincide. In practice, such a situation can be reached using a separate set of $E$ and $B$ fields, with $E \cdot B \neq 0$ to drive the Weyl points out of equilibrium using the chiral anomaly [24]. We, however, would like not to pay too much attention to the practical side of this case, and simply use it to show that Eqs. (24) and (25) give results known in the literature for this situation. For simplicity, we assume that all Weyl points are at the same energy $E_w = 0$. Under nonequilibrium conditions, one should consider both static and dynamic limits. The former is analyzed based on the expression for the current of Eq. (B3), which corresponds to $g_{ab}$ from Eq. (24) with only the first term on
TABLE I. Chiral magnetic conductivity for a Weyl metal for different cases of linear-response theory. The rows correspond to static and dynamic limits of response. The columns pertain to the equilibrium response of a Weyl metal with Weyl points located at different energies, and to nonequilibrium response of a Weyl metal with Weyl points at the same energy.

| Energy | Static | Dynamic |
|--------|--------|---------|
| $\mu$  | $E$    | $\mu$  |
| 0      | $\frac{\gamma^2}{12\pi^2} \sum_w Q_w E_w$ | $\frac{\gamma^2}{12\pi^2} \sum_w Q_w E_w$ |

the right-hand side retained. Generalizing Eq. (B5) to the case of Weyl points with different chemical potentials, one obtains

$$g_{ab} = \frac{e^2}{4\pi^2} \delta_{ab} \sum_w Q_w \mu_w,$$  

(44)

with the corresponding expression for the current,

$$j_x = \frac{e^2}{4\pi^2} B \sum_w Q_w \mu_w.$$  

(45)

This is the original expression for the static chiral magnetic effect obtained by Vilenkin [5], and many times rederived after that.

In the dynamic limit, all terms in Eq. (24) do contribute to $g_{ab}$, and we obtain

$$g_{ab} = -\frac{e^2}{12\pi^2} \delta_{ab} \sum_w Q_w \mu_w,$$  

(46)

with the corresponding expression for the current,

$$j_x = \frac{e^2}{12\pi^2} B \sum_w Q_w \mu_w.$$  

(47)

This is in full correspondence with the “chiral magnetic conductivity” results of Ref. [8], and results of Ref. [9].

We summarize the outcomes of this subsection in Table I, where we list the answers for the chiral magnetic conductivity, given by the ratio $j_x/B$, for the equilibrium case with Weyl points located at different energies, and for the nonequilibrium case with Weyl points located at different energies, for both static and dynamic situations. In Table I, the only nonzero entry of topological origin is the static chiral magnetic conductivity in the nonequilibrium case. The universal flavor of the rest of results is misleading; it is just a consequence of the simplified model of Eq. (41). The entries of third column of the table can be found in the literature. To the best of our knowledge, the bottom entry of the second column is a new result of this work.

C. Chiral magnetic effect without Berry monopoles

In Secs. III A and III B we considered examples of Hamiltonians for noncentrosymmetric metals that lead to the CME. In both cases it was the presence of linear band touchings—Weyl points—that was the culprit, even though the example of Sec. III A would not be ordinarily called a Weyl metal. Is the existence of Weyl points, or rather of Berry curvature monopoles, necessary for the existence of the chiral magnetic effect? In this section we show that the answer to that question is “no.”

To show that Berry monopoles are not required for the chiral magnetic effect, we provide an explicit example of a Hamiltonian for which the Berry curvature is monopole free, yet it exhibits the CME. We start with the simplest spin-orbit coupling Hamiltonian for a metal with noncentrosymmetric point group $C_{4v}$, given by Eq. (31) with the following $d_p$ [42]:

$$d_p^{C_4} = [\gamma p_x, -\gamma p_y, \gamma p_z, \gamma p_z \gamma (p_x^2 - p_y^2)].$$  

(48)

This Hamiltonian is symmetric under the fourfold rotation around the $z$ axis, breaks $z \to -z$ reflection, but preserves $x \to -x$ and $y \to -y$ reflections, as appropriate for the $C_{4v}$ point group. The presence of $x \to -x$ and $y \to -y$ reflections makes this group not gyrotropic (it does not show natural optical activity). To break these reflections, we choose $E_p$ in Eq. (31) as

$$E_p = \frac{p_x^2}{2m} + \gamma p_x p_y (p_z^2 - p_y^2),$$  

(49)

in which the second term does the job, keeping the fourfold rotation around $z$ intact. The total Hamiltonian thus has gyrotropic $C_4$ symmetry,

$$h^{C_4} = \frac{p_x^2}{2m} + \gamma p_x p_y (p_z^2 - p_y^2) + \sigma d_p^{C_4},$$  

(50)

and we expect that $\gamma_4$ determines the optical activity properties of this model.

The Berry curvature in the band structure that corresponds to Hamiltonian (50) is determined by the “parent” $C_{4v}$ theory:

$$\Omega_\pm = \mp \gamma v p_x p_y (p_z^2 - p_y^2) (p_z p_y - 3 p_x).$$  

(51)

This Berry curvature is obviously monopole free, it is not even singular near the origin. To calculate Trg in this case, we set the temperature to zero, and assume that the spin splitting of the band structure and breaking of $x \to -x$ and $y \to -y$ reflections are small, $\gamma p_x \gamma p_y \gamma p_z \ll \mu$, where the Fermi momentum $p_F$ is found from $p_F^2/2m = \mu$. To evaluate Eq. (32), we integrate it by parts to move the differentiation with respect to $p$ onto $E_p (\partial_\Omega_{np} = 0$ in this case), and expand the distribution function to linear order in $d_p$ and $\gamma_4$:

$$f_{\pm}(\epsilon_{\pm}) \approx f_{\alpha}(p_x^2/2m - \mu) - \partial_\alpha f_{\alpha}(p_x^2/2m - \mu) \times [\gamma_4 p_x p_y (p_z^2 - p_y^2) \pm d_p].$$  

(52)

Only the second term on the right-hand side of Eq. (52) contributes to Trg. In addition, the derivative of the Fermi function in that term restricts the integration over momenta to $p = p_F$ at zero temperature. After simple transformations, we obtain

$$Trg = \frac{e^2}{\omega} \frac{v_4 p_x^2}{\mu} \int \frac{\gamma p_x^2}{v} \left(I(p_{\perp}^2/\mu)ight),$$  

(53)

where

$$I(x) = \frac{1}{\pi^3} \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta \times \frac{x}{x^2 \cos^2 \theta + 16 \sin^6 \theta \sin^2(4\phi)}.$$  

(54)
It is easy to find asymptotic values of this integral:

\[ I(x) \approx \begin{cases} \frac{x}{\text{const}}, & \text{if } x \ll 1, \\ \frac{1}{2x^2}, & \text{if } x \gg 1. \end{cases} \]  

(55)

This nonzero result for the trace of the gyrotropic tensor illustrates the main point of this section: Berry monopoles are not needed for the dynamic chiral magnetic effect. In particular, the dynamic chiral magnetic effect is not related to the chiral anomaly in general.

IV. CONCLUSION

To summarize, we have derived completely general expressions [Eqs. (17) and (B3)] for the leading contribution to the gyrotropic current in a metallic system at low frequencies and wave vectors. To confirm our results, derived from the semiclassical kinetic equation, we performed a calculation based on the Kubo formula, which yielded identical ones.

The obtained expressions hold for frequencies and wave vectors that satisfy \( \omega, q \ll \mu, E_g \), where \( E_g \) is the relevant energy gap, and \( \nu \) is the relevant speed. The typical doping levels found in Weyl metals range 1–10 meV, which places \( \omega \) in the THz range.

The main physical conclusion is the identification of the intrinsic orbital magnetic moment of quasiparticles as the source of natural optical activity in (semi)metals. We also showed that the chiral magnetic effect in general exists in the dynamic limit (\( \omega > v q \)) in metallic systems with natural optical activity. The Weyl metal with a gyrotropic point group is such a system. However, the list of band structures showing natural optical activity (and chiral magnetic effect in particular) is not limited to the Weyl metal: The presence of Weyl points and the associated Berry monopoles is in general not required for the existence of the chiral magnetic effect and natural optical activity at low frequencies. This was also numerically confirmed in a recent paper [43].

Specializing to the case of Weyl metals, if the latter can be represented by a collection of particle-hole symmetric Weyl points near its Fermi level, the trace of the gyrotropic tensor, determining the magnitude of the dynamic CME, is determined by the energy space dipole moment of Berry monopoles, corresponding to the Weyl points. In general, this trace, as well as the magnitude of the chiral magnetic effect, is determined by peculiarities of the band structure, and is nonuniversal; we estimate the doping level above which band curvature effects are important to take into account in the description of the dynamic CME to be 10–100 meV.

Certain [44–47] Weyl metals from the monopnictide family [48] have \( C_{4v} \) point group, which is not gyrotropic [2]. One could hope to study natural optical activity in these materials upon application of an appropriate strain to reduce the point group to, say, \( C_4 \). Even in that case such a study would be complicated by their opaqueness due to high concentrations of mobile carriers. This obstacle may be possible to overcome with applying pressure, which has been reported to drive TaAs toward insulating behavior [49].

Note added: Shortly after a preprint of our work appeared [50], two other contributions came out dealing with similar topics [51,52]. The Kubo-formula-based treatment of Ref. [51] appears to be incomplete, but its conclusion that the existence of Weyl points is not required for CME is in line with ours. The treatment of Ref. [52] seems to be correct if one fixes a factor of 2 mistake in their expression for the orbital magnetic moment in a two-band model.

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APPENDIX A: DERIVATION OF (18) FROM KUBO FORMULA

In this section we rederive the expressions for the gyrotropic current, obtained above from the semiclassical kinetic equation, using Kubo formula. Given the spread of results existing in the literature, we would like to give all the details of the calculation, such that it would be straightforward (but unavoidably time consuming) to check it.

We adopt the gauge in which the electric potential is equal to zero, and seek current response to vector potential, A. The Kubo formula for the Fourier component of the current relates the latter to the vector potential, \( J_\omega^(\omega, \mathbf{q}) = \varepsilon_{\mathbf{ab}}A_\omega^{(\mathbf{q}, \omega)} \), with kernel \( \varepsilon_{\mathbf{ab}}^{(\omega, \mathbf{q})} \) given by

\[
\varepsilon_{\mathbf{ab}}^{(\omega, \mathbf{q})} = e^2 \sum_{n,n'} \int (d\mathbf{p}) \frac{\delta_n p q^2 - \delta_{n'} p q^2}{\omega - \xi_n p + q^2 + \xi_{n'} p - q^2} \\
\times \langle u_{n'} p - q^2 | \partial_a \mathbf{h} | u_n p + q^2 \rangle \langle u_n p + q^2 | \partial_b \mathbf{h} | u_{n'} p - q^2 \rangle. 
\]

(A1)

We will only consider the linear-in-\( q \) part of \( \varepsilon_{\mathbf{ab}}^{(\omega, \mathbf{q})} \), since the \( O(q^4) \) terms are completely standard. Normally, in order to compute the physical conductivity one has to subtract the diamagnetic current contribution, which amounts to redefining \( \varepsilon \) according to \( \varepsilon^{(\omega, \mathbf{q})} = \varepsilon^{(\omega, \mathbf{q})} - \lim_{\mathbf{q} \to 0} \varepsilon^{(0, \mathbf{q})} \). Since we are interested in the \( O(q) \) part of \( \varepsilon \), we do not have to worry about the diamagnetic term.

We will split the total response into the intra- and interband parts, starting with the intraband one.

1. Intraband part

For clarity and brevity, we will use \( |u_n\rangle \equiv |u_{n\mathbf{p}}\rangle, \epsilon_n \equiv \epsilon_{n\mathbf{p}}, \) \( h \equiv \hbar \mathbf{p}, \) and \( f_n \equiv f_{n\mathbf{p}}. \) For band velocity we will use \( \partial \mathbf{v}_{n\mathbf{p}} \equiv v_{n\mathbf{q}} \), and the Cartesian components of \( v_{n\mathbf{q}} \) will be denoted with letters from the beginning of Latin alphabet: \( \mathbf{v}_{n\mathbf{q}} \) denotes the \( \mathbf{c} \)th component of velocity in band \( n \).

Linear-in-\( q \) intraband contribution exists only in the static limit of Eq. (A1) (\( \omega \to 0 \) before \( q \to 0 \)). The contribution to \( \varepsilon_{\mathbf{ab}}^{(\omega, \mathbf{q})} \) that appears in the static limit we denote with \( \varepsilon_{\mathbf{ab}}^{\text{int}}^{(0, \mathbf{q})} \),

\[
\varepsilon_{\mathbf{ab}}^{\text{int}}^{(0, \mathbf{q})} \\
= -e^2 \sum_n \int (d\mathbf{p}) \frac{\delta_{n\mathbf{p}} q^2}{\xi_{n\mathbf{p}} q^2} \frac{\delta_{n\mathbf{p}} q^2}{\xi_{n\mathbf{p}} q^2} \\
\times (u_{n\mathbf{p}} q^2 | \partial_a \mathbf{h} | u_{n\mathbf{p}} q^2) (u_{n\mathbf{p}} q^2 | \partial_b \mathbf{h} | u_{n\mathbf{p}} q^2) \\
\times (u_{n\mathbf{p}} q^2 | \partial_a \mathbf{h} | u_{n\mathbf{p}} q^2) (u_{n\mathbf{p}} q^2 | \partial_b \mathbf{h} | u_{n\mathbf{p}} q^2) \\
\times (u_{n\mathbf{p}} q^2 | \partial_a \mathbf{h} | u_{n\mathbf{p}} q^2) (u_{n\mathbf{p}} q^2 | \partial_b \mathbf{h} | u_{n\mathbf{p}} q^2) \\
\times (u_{n\mathbf{p}} q^2 | \partial_a \mathbf{h} | u_{n\mathbf{p}} q^2) (u_{n\mathbf{p}} q^2 | \partial_b \mathbf{h} | u_{n\mathbf{p}} q^2).
\]
consideration the first bracket:

\[ \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle 
= \langle u_n | \partial_b \epsilon_n | u_n \rangle 
= -\frac{1}{2} q, \langle \partial_b u_n \rangle | \partial_b \epsilon_n | u_n \rangle 
= \partial_b \epsilon_n - \frac{1}{2} q, \langle \partial_b u_n \rangle | \partial_b \epsilon_n | u_n \rangle. \]

(A3)

To get the second bracket, we have to change \( a \rightarrow b \), and \( q \rightarrow -q \):

\[ \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle 
= \partial_b \epsilon_n - \frac{1}{2} q, \langle \partial_b u_n \rangle | \partial_b \epsilon_n | u_n \rangle. \]

(A4)

Then we get

\[
\mathcal{Q}_{ab}^{\text{inter}}(0, q) = -e^2 \sum_n \int (dp) \partial_a f_n \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle 
\times \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle 
\approx -e^2 \sum_n \int (dp) \partial_a f_n \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle 
\times \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle 
- v_{ba} \langle u_n | \partial_b \epsilon_n | u_n \rangle 
+ v_{ab} \langle u_n | \partial_b \epsilon_n | u_n \rangle.
\]

(A5)

Now in each term on the right-hand side we insert a resolution of identity, \( \sum_n |u_n\rangle \langle u_n| = I \), between the derivative of a bra or a ket, and a derivative of the Hamiltonian, and observe that the terms with \( n' = n \) cancel.

Further progress is possible if one uses the following identities:

\[
\langle u_n | \partial_b \epsilon_n | u_n \rangle = \delta_b \epsilon_n, \quad n = n',
\]

\[
\langle u_n | \partial_b \epsilon_{n'} | u_{n'} \rangle = (\epsilon_n - \epsilon_{n'}) \langle u_n | \partial_b u_{n'} | u_{n'} \rangle, \quad n \neq n', \quad (A6)
\]

\[
\langle u_n | \partial_b u_{n'} | u_{n'} \rangle = -\langle \partial_b u_{n'} | u_{n'} \rangle.
\]

The first two of these can be compactly written as \([53]\)

\[
\partial_b (\epsilon_n - \epsilon_{n'}) | u_{n'} \rangle = (\epsilon_n - \epsilon_{n'}) \partial_b | u_{n'} \rangle, \quad (A7)
\]

which is the form we found most useful.

Using Eq. (A7), we obtain

\[
\mathcal{Q}_{ab}^{\text{inter}}(0, q) = -e^2 \sum_{n' \neq n} \int (dp) \partial_a f_n \langle u_{np+q/2} | \partial_b (\epsilon_n - \epsilon_{n'}) | u_{np+q/2} \rangle 
\times \langle u_{np+q/2} | \partial_b (\epsilon_n - \epsilon_{n'}) | u_{np+q/2} \rangle 
+ e^2 \sum_n \int (dp) \partial_a f_n \langle u_{np+q/2} | \partial_b (\epsilon_n - \epsilon_{n'}) | u_{np+q/2} \rangle 
\times \langle u_{np+q/2} | \partial_b (\epsilon_n - \epsilon_{n'}) | u_{np+q/2} \rangle. \]

(A8)

This expression can be related to the quasiparticle orbital magnetic moment, given by

\[
m_a = \frac{ie}{2} \langle \partial_b u_a | \times (\hbar_p - \epsilon_a) | \partial_b u_a \rangle, \quad (A9)
\]

or in components:

\[
m_{ad} = \frac{ie}{2} \epsilon_{d\gamma} \langle \partial_b u_a | \times (\hbar_p - \epsilon_a) | \partial_b u_a \rangle 
\]

\[
= -\frac{ie}{2} \sum_{n' \neq n} \epsilon_{d\gamma} (\epsilon_n - \epsilon_{n'}) | \partial_b u_{n'} | u_{n'} \rangle \langle u_{n'} | \partial_b u_{n'} \rangle. \]

(A10)

From the last equation it follows that

\[
\epsilon_{d\gamma} m_{ad} = -\frac{ie}{2} \sum_{n' \neq n} \epsilon_{d\gamma} (\epsilon_n - \epsilon_{n'}) | \partial_b u_{n'} | u_{n'} \rangle \langle u_{n'} | \partial_b u_{n'} \rangle 
- (\partial_b u_{n'}) \langle u_{n'} | \partial_b u_{n'} \rangle. \]

(A11)

This allows one to rewrite Eq. (A8) as

\[
\mathcal{Q}_{ab}^{\text{inter}}(0, q) = -ie \sum_n \int (dp) \partial_a f_n q \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle 
\times \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle 
+ ie \sum_n \int (dp) \partial_a f_n q \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle 
\times \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle. \]

(A12)

The corresponding contribution to the gyrotropic current is

\[
j_{\gamma}^{\text{inter}} = -e \sum_n \int (dp) m_a \times (i \mathbf{q} \times \mathbf{A}) \partial_b f_n 
- e \sum_n \int (dp) (i \mathbf{q} \times \mathbf{m}_a) \partial_b f_n. \]

(A13)

These terms have very different semiclassical interpretation. The first one is the current that comes from energy shift in the semiclassical distribution function, Eq. (B1). There exists a related contribution that corresponds to band velocity renormalization due to energy renormalization, Eq. (6), which is a part of the intraband response, see below. The second term is equal (with the opposite sign) to the current of nonequilibrium quasiparticle magnetization. Its role in the derivation is to cancel the former contribution, coming from the intraband part of the response, in the static limit.

2. Interband part

The interband part of response is insensitive to the order of \( \epsilon \rightarrow 0 \) and \( q \rightarrow 0 \) limits. We will thus write

\[ \mathcal{Q}_{ab}^{\text{inter}}(0, q) = -e^2 \sum_{n' \neq n} \int (dp) f_{np+q/2} - f_{n'p+q/2} \]

\[ \times \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle \langle u_{np+q/2} | \partial_b \epsilon | u_{np+q/2} \rangle. \]

(A14)

There are three sources of linear-in-\( q \) terms: the distribution function difference, the difference of transition energies, and the matrix element. We consider them one by one below.
a. Distribution function contribution

The contribution to \( Q_{ab} \) that comes from \( q \) dependence of distribution functions difference for interband transitions we denote with \( Q_{\text{inter,df}}^{\text{inter,df}}(0, q) \).

\[
Q_{\text{inter,df}}^{\text{inter,df}}(0, q) = -\frac{1}{2} e^2 \sum_{n \neq n'} \int (d\mathbf{p}) \frac{q^2 f_n + q^2 f_{n'}}{\epsilon_n - \epsilon_{n'}} \langle u_n | \partial_b h | u_{n'} \rangle \langle u_{n'} | \partial_b h | u_n \rangle
\]

\[
= -\frac{1}{2} e^2 \sum_{n \neq n'} \int (d\mathbf{p}) (q \partial_p f_n + q \partial_p f_{n'}) (\epsilon_n - \epsilon_{n'}) \langle u_n | \partial_b u_{n'} | u_{n'} \rangle \langle u_{n'} | \partial_b u_n | u_n \rangle
\]

\[
= -\frac{1}{2} e^2 \sum_{n \neq n'} \int (d\mathbf{p}) (q \partial_p f_n + q \partial_p f_{n'}) (\epsilon_n - \epsilon_{n'}) \langle u_n | \partial_b u_{n'} | u_{n'} \rangle \langle u_{n'} | \partial_b u_n | u_n \rangle - \langle \partial_b u_n | \partial_b u_{n'} | u_{n'} \rangle (u_n | \partial_b u_{n'})
\]

\[
= -ie \sum_n \int (d\mathbf{p}) (q \partial_p f_n) \epsilon_n \mathbf{m}_{\text{el}}. \tag{A15}
\]

The corresponding gyrotropic current is

\[
j_g^{\text{inter,df}} = -ie \sum_{p,n} (q \partial_p f_n) \mathbf{m}_n \times \mathbf{A}. \tag{A16}\]

We note in passing that

\[
j_g^{\text{inter,df}} = -e \sum_{p,n} (\partial_p f_n \mathbf{m}_n) (\mathbf{q} \times \mathbf{A}) = -e \sum_{p,n} \partial_p f_n (v_n \mathbf{m}_n) \mathbf{B}. \tag{A17}\]

b. Transition energies

The contribution to \( Q_{ab} \) that comes from \( q \) dependence of transition energies for interband transitions we denote with \( Q_{\text{inter,te}}^{\text{inter,te}}(0, q) \).

\[
Q_{\text{inter,te}}^{\text{inter,te}}(0, q) = e^2 \sum_{n \neq n'} \int (d\mathbf{p}) \frac{f_n - f_{n'}}{(\epsilon_n - \epsilon_{n'})^2} \langle v_n c + v_{n'} c | (\partial_a u_n | \partial_a u_{n'}) \rangle (\epsilon_{n'} - \epsilon_n) \langle u_{n'} | \partial_b u_n | u_n \rangle
\]

\[
= e^2 \sum_{n \neq n'} \int (d\mathbf{p}) (f_n - f_{n'}) (v_n c + v_{n'} c) \frac{q_c}{2} (\partial_a u_n | \partial_a u_{n'}) \langle \partial_b u_{n'} | \partial_b u_n | u_n \rangle. \tag{A18}\]

Because of \( f_n - f_{n'} \), we can extend the summation to include \( n = n' \). The terms that involve products like \( f_n v_n \) and \( f_{n'} v_{n'} \) allow summation over the intermediate states, such that we obtain

\[
Q_{\text{inter,te}}^{\text{inter,te}}(0, q) = e^2 \sum_n \int (d\mathbf{p}) f_n v_n c \frac{q_c}{2} \langle \partial_b u_n | (\partial_a u_n - i \leftrightarrow j) \rangle + e^2 \sum_{n \neq n'} \int (d\mathbf{p}) f_n v_{n'} c \frac{q_c}{2} \langle (u_{n'} | \partial_a u_n) (\partial_b u_{n'} | - i \leftrightarrow j) \rangle. \tag{A19}\]

Using identity (A7), we can do more summations over intermediate states in Eq. (A19):

\[
Q_{\text{inter,te}}^{\text{inter,te}}(0, q) = e^2 \sum_{p,n} \int (d\mathbf{p}) f_n \frac{q_c}{2} \langle (\partial_b u_n | (\partial_a u_n - i \leftrightarrow j) \rangle - e^2 \sum_{p,n,n'} \int (d\mathbf{p}) f_{n'} \frac{q_c}{2} \langle (u_{n'} | \partial_a u_n) (\partial_b u_{n'} | - i \leftrightarrow j) \rangle. \tag{A20}\]

c. Matrix elements

The contribution to \( Q_{ab} \) that comes from \( q \) dependence of matrix elements for interband transitions we denote with \( Q_{\text{inter,mr}}^{\text{inter,mr}}(0, q) \).

\[
Q_{\text{inter,mr}}^{\text{inter,mr}}(0, q) = -e^2 \sum_{p,n} \int (d\mathbf{p}) \frac{f_n - f_{n'}}{(\epsilon_n - \epsilon_{n'})^2} \langle u_{n,p-q/2} | (\partial_b h | u_{n',p+q/2}) \langle u_{n',p+q/2} | (\partial_b h | u_{n,p-q/2}) \rangle. \tag{A21}\]

Using

\[
\langle u_{n,p-q/2} | \partial_b h | u_{n',p+q/2} \rangle = (\epsilon_n - \epsilon_{n'}) \langle u_{n'} | \partial_a u_n | u_n \rangle - \frac{q_e}{2} \langle \partial_a u_n | \partial_b h | u_n \rangle + \frac{q_e}{2} \langle u_n | \partial_a u_n | \partial_b h \rangle,
\]

\[
\langle u_{n',p+q/2} | \partial_b h | u_{n,p-q/2} \rangle = (\epsilon_{n'} - \epsilon_n) \langle \partial_b u_{n'} | \partial_a u_n | u_n \rangle + \frac{q_e}{2} \langle \partial_a u_n | \partial_b h | u_n \rangle - \frac{q_e}{2} \langle u_n | \partial_a u_n | \partial_b h \rangle.
\]
the linear-in-$q$ part of the matrix element contribution becomes

$$Q_{ab}^{\text{inter,me}}(0, q) = -e^2 \sum_{p,n,n'} \left( f_n - f_{n'} \right) q_n \left( \langle u_n | \partial_ah | \partial_bun \rangle \langle \partial_cun | \partial_hu_n \rangle - \langle u_n | \partial_a\epsilon_n | \partial_bu_n \rangle \langle \partial_cu_n | \partial_hu_n \rangle \right)$$

$$- \langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_a\epsilon_{n'} \rangle + \langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_a\epsilon_{n'} \rangle). \quad \text{(A22)}$$

Performing summation over intermediate states wherever possible, and exchanging $n \leftrightarrow n'$ where convenient, we obtain

$$Q_{ab}^{\text{inter,me}}(0, q) = e^2 \sum_{n} \int \langle dp \rangle f_n \frac{q_n}{2} \left( \langle \partial_bu_n | \partial_hu_n \rangle + [cab] - [cba] - [bac] \right)$$

$$+ e^2 \sum_{n,n'} \int \langle dp \rangle f_n \frac{q_n}{2} \left( \langle u_n' | \partial_bu_n \rangle \langle \partial_cu_{n'} | \partial_hu_n \rangle + \langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle \right)$$

$$+ \langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle + \langle \partial_bu_n' | \partial_cu_n \rangle \langle \partial_hu_n | \partial_u_n \rangle + \langle \partial_bu_n | \partial_cu_n \rangle \langle \partial_hu_n | \partial_u_n \rangle). \quad \text{(A23)}$$

A square bracket with a set of indices inside indicates an expression structurally identical to the preceding one, the only difference being the order in which $a$, $b$, or $c$ appears in the derivatives. The specific order is given by the contents of the bracket.

The terms in the double sums are modified according to

$$\langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle = \langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'}$$

$$\langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle = - \langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'}$$

$$\langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle = - \langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'}$$

$$\langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle = \langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'}$$

These transformations make a few more summations over $n'$ possible, and we finally arrive at

$$Q_{ab}^{\text{inter,me}}(0, q) = e^2 \sum_{n} \int \langle dp \rangle f_n \frac{q_n}{2} \left( \langle \partial_bu_n | \partial_hu_n \rangle + [cab] - [cba] - [bac] \right)$$

$$+ e^2 \sum_{n,n'} \int \langle dp \rangle f_n \frac{q_n}{2} \left( \langle u_n' | \partial_bu_n \rangle \langle \partial_cu_{n'} | \partial_hu_n \rangle + \langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle \right)$$

$$+ \langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle - \langle \partial_bu_n | \partial_cu_n \rangle \langle \partial_hu_n | \partial_u_n \rangle - \langle \partial_bu_n | \partial_cu_n \rangle \langle \partial_hu_n | \partial_u_n \rangle). \quad \text{(A24)}$$


d. Total contribution of matrix elements and transition energies

Combining Eqs. (A20) and (A24) we obtain

$$Q_{ab}^{\text{inter,me+tr}}(0, q) = e^2 \sum_{n} \int \langle dp \rangle f_n \frac{q_n}{2} \left( \langle \partial_bu_n | \partial_hu_n \rangle + \langle \partial_bu_n | \partial_hu_n \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'} \right)$$

$$+ e^2 \sum_{n,n'} \int \langle dp \rangle f_n \frac{q_n}{2} \left( \langle u_n' | \partial_bu_n \rangle \langle \partial_cu_{n'} | \partial_hu_n \rangle + \langle \partial_bu_n | \partial_cu_{n'} \rangle \langle \partial_hu_n | \partial_u_{n'} \rangle \right)$$

$$- \langle \partial_bu_n | \partial_cu_n \rangle \langle \partial_hu_n | \partial_u_n \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'}$$

$$- \langle \partial_bu_n' | \partial_cu_n \rangle \langle \partial_hu_n | \partial_u_n \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'}$$

$$- \langle \partial_bu_n' | \partial_cu_n \rangle \langle \partial_hu_n | \partial_u_n \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'} \rangle. \quad \text{(A25)}$$

It can be shown that the double-summation terms cancel out:

$$\sum_{n,n'} \int \langle dp \rangle f_n \frac{q_n}{2} \left( \langle u_n' | \partial_bu_n \rangle \langle \partial_cu_{n'} | \partial_hu_n \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'} \right)$$

$$- \langle \partial_bu_n | \partial_cu_n \rangle \langle \partial_hu_n | \partial_u_n \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'}$$

$$- \langle \partial_bu_n | \partial_cu_n \rangle \langle \partial_hu_n | \partial_u_n \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'}$$

$$- \langle \partial_bu_n | \partial_cu_n \rangle \langle \partial_hu_n | \partial_u_n \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'} \rangle \right)$$

$$= \sum_{n} \int \langle dp \rangle f_n \frac{q_n}{2} \left( \langle \partial_bu_n | \partial_hu_n \rangle + \langle \partial_bu_n | \partial_hu_n \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'} \right)$$

$$- \langle \partial_bu_n | \partial_cu_n \rangle \langle \partial_hu_n | \partial_u_n \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'} \rangle = 0. \quad \text{(A26)}$$

Thus we simply get

$$Q_{ab}^{\text{inter,me+tr}}(0, q) = e^2 \sum_{n} \int \langle dp \rangle f_n \frac{q_n}{2} \left( \langle \partial_bu_n | \partial_hu_n \rangle + \langle \partial_bu_n | \partial_hu_n \rangle \langle \epsilon_{n} - h \rangle \partial_u_{n'} \right) + [cab] + [bca] - [acb] - [cba] - [bac]. \quad \text{(A27)}$$
Since the expression in brackets is fully antisymmetric with respect to \(a, b, \) and \(c\), we can write it as
\[
\mathcal{Q}_{ab,ac+\epsilon}^{\text{linear}}(0,\mathbf{q}) = e^2 \sum_{n} \int (d\mathbf{p}) f_n \frac{q_p}{2} \epsilon_{bac} \partial_p \cdot (\partial_p u_n) \times (h + \epsilon_n) (\partial_p u_n). 
\] (A28)

3. Current in the static limit

Combining the current that corresponds to Eq. (A28) with Eq. (A17) integrated by parts, we obtain
\[
\begin{align*}
\langle \, \mathbf{j}^{\text{static}} \rangle_n &= e \sum_{n} \int (d\mathbf{p}) f_n (\partial_p m_n) (i \mathbf{q} \times \mathbf{A})_n - \frac{i}{2} e^2 \sum_{n} \int (d\mathbf{p}) f_n \partial_p \cdot (\partial_p u_n) \times (h + \epsilon_n) (\partial_p u_n) (i \mathbf{q} \times \mathbf{A})_n \\
&= \frac{i}{2} e^2 \sum_{n} \int (d\mathbf{p}) f_n \partial_p \cdot (\partial_p u_n) \times (h - \epsilon_n) (\partial_p u_n) B_n - e^2 \sum_{n} \int (d\mathbf{p}) f_n \frac{i}{2} \partial_p \cdot (\partial_p u_n) \times (h + \epsilon_n) (\partial_p u_n) B_n \\
&= -e^2 \sum_{n} \int (d\mathbf{p}) f_n i \partial_p \cdot (\partial_p u_n) \times (\partial_p u_n) B_n = -e^2 \sum_{n} \int (d\mathbf{p}) f_n i \partial_p (\epsilon_n \mathbf{\Omega}_n) B_n. 
\end{align*}
\] (A29)

After an integration by parts, this can be rewritten as
\[
\langle \, \mathbf{j}^{\text{static}} \rangle_n = e^2 \sum_{n} \int (d\mathbf{p}) \epsilon_n (\partial_p f_n \cdot \mathbf{\Omega}_n) \mathbf{B}. 
\] (A30)

This result is further discussed in Appendix B.

4. Current in the dynamic limit

In order to get the current in the dynamic limit, we just need to subtract the static contribution of the intraband response, Eq. (A13), from the total result in the static limit, since the interband part of the current is independent of the orders of limit:
\[
\begin{align*}
\langle \, \mathbf{j}^{\text{dynamic}} \rangle_n &= e^2 \sum_{p,n} \epsilon_n (\partial_p f_n \Omega_n) \mathbf{B} + \frac{e}{\omega} \sum_{p,n} (\mathbf{m}_n \cdot (i \mathbf{q} \times \mathbf{A})) \partial_p f_n + \frac{e}{\omega} \sum_{p,n} (i \mathbf{q} \times \mathbf{m}_n)(\partial_p f_n A). 
\end{align*}
\] (A31)

To obtain Eq. (17), we rewrite the current as a response to the electric field \(\mathbf{E} = i \omega \mathbf{A}\):
\[
\langle \, \mathbf{j}^{\text{dynamic}} \rangle_n = e^2 \sum_{p,n} \epsilon_n (\partial_p f_n \Omega_n) (\mathbf{q} \times \mathbf{E}) + \frac{e}{\omega} \sum_{p,n} (\mathbf{m}_n \cdot (\mathbf{q} \times \mathbf{E})) \partial_p f_n + \frac{e}{\omega} \sum_{p,n} (\mathbf{q} \times \mathbf{m}_n)(\partial_p f_n \mathbf{E}), 
\] (A32)

which is, indeed, Eq. (18).

**APPENDIX B: VANISHING CURRENT IN THE STATIC LIMIT**

The result of Eq. (A30) the equilibrium current in the case of a uniform \(\mathbf{B}\) field can be straightforwardly obtained in the context of semiclassical formalism. Below we will simply recover known results, but we nevertheless present them for completeness of our treatment. In a static magnetic field, the equilibrium distribution function at chemical potential \(\mu\) is modified according to the dispersion (6):
\[
f_{eq}(\epsilon_{np}) = f_{th}(E_{np}). 
\] (B1)

Then the equilibrium current \(\mathbf{j}_{eq}\) is given by
\[
\langle \, \mathbf{j}_{eq} \rangle = e \sum_{n} \int (d\mathbf{p}) \partial_p E_{np} f_n(E_{np}) \\
- e^2 \sum_{n} \int (d\mathbf{p}) (\partial_p \epsilon_{np} \cdot \mathbf{\Omega}_{np}) f_n(\epsilon_{np}) \mathbf{B}. 
\] (B2)

We emphasize that it is the total energy \(E_{np}\) from Eq. (6) that enters in the first term on the right-hand side of this expression, while we can use \(\epsilon_{np}\) in the second term, since it is already linear in \(\mathbf{B}\), and we are interested in linear response.

The equilibrium current \(\mathbf{j}_{eq}\) vanishes in a crystal. In the dynamic limit, the first term on the right-hand side of Eq. (14) yielded a nonzero current along the magnetic field because the electron’s velocity is shifted by \(-\partial_{\mathbf{p}}(\mathbf{m}_n \mathbf{B})\) from its unperturbed value \(\partial_{\mathbf{p}} \epsilon_{np}\). However, in the static limit, this velocity shift is exactly compensated by the shift of the energy in the distribution function, Eq. (B1). Therefore, the first term vanishes identically. The second term in Eq. (B2) has been associated with the static limit of chiral magnetic effect in the literature [5–9], and it is finite for a single Weyl point. However, when the momentum integration is extended to the entire Brillouin zone, and the summation over all bands is performed, this current vanishes due to the fact that there is zero total Berry monopole charge in the Brillouin zone [13]. The simplest way to see this explicitly is to recast the expression for the chiral-magnetic-effect-related part of the static current as a Fermi-surface property. Denoting the second term on the right-hand side of Eq. (B2) as \(\mathbf{j}_{\text{CME}}\), and integrating by parts, one obtains
\[
\langle \, \mathbf{j}_{\text{CME}} \rangle = e^2 \sum_{n} \int (d\mathbf{p}) \epsilon_{np} (\partial_p f_n \Omega_{np}) \mathbf{B}. 
\] (B3)
where we used the fact that \( \sum_{\varepsilon_n} f_{\varepsilon_n} \varepsilon_n \partial \Omega_{\varepsilon_n} = 0 \), since the momentum-space divergence of the Berry curvature is nonzero only at singularities associated with band touchings, and the signs of the monopole charges are the opposite for the two degenerate bands. By switching from integration over quasimomenta to the integration over isoenergetic surfaces and energy, one obtains at zero temperature
\[
J_{\text{CME}} = -\frac{e^2 \mu}{4\pi^2} B \sum_{\varepsilon_n} \frac{1}{\Omega_{\varepsilon_n}} \int dS_{\varepsilon_n} \cdot \Omega_{\varepsilon_n}, \quad (B4)
\]
where we switched from band summation to summation over Fermi surfaces. The orientation of \( dS_{\varepsilon_n} \) has to be chosen as the outer (inner) normal for electron (hole) Fermi surfaces, because of their opposite group velocity direction. Since the signs of the Berry curvature are also opposite for electron and hole surfaces, we conclude that the contribution of a given Weyl point is independent of the position of the chemical potential relative to its nodal energy, and the current is given by
\[
J_{\text{CME}} = \frac{e^2 \mu}{4\pi^2} B \sum_{\varepsilon_n} \Omega_{\varepsilon_n} = 0, \quad (B5)
\]
where \( \sum_{\varepsilon_n} \ldots \) denotes the sum over Weyl points, and \( \Omega_{\varepsilon_n} = \pm 1 \) is the chirality of a Weyl point.

The result of Eq. (B4) is clearly of topological origin: each Berry monopole that corresponds to a Weyl point makes a contribution to the total current that depends only on its Berry charge and chemical potential, with a universal prefactor. The total static current \((B5)\) is also quite universal: It is a universal zero. Equations (B4) and (B5) describe static CME: In a static magnetic field, a Weyl point in a band structure makes a contribution to current that flows along the magnetic field, and whose magnitude is a universal quantity; however, the total current vanishes in equilibrium.

\[\text{References}\]

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CHAPTER 4

ONSAGER RELATIONS AND
CURRENT-INDUCED MAGNETIZATION
In this Chapter, I discuss the role of Onsager relations for the conductivity tensor in establishing its general symmetry properties, and its physical content. Based on the Onsager relations, I discuss the implications of the time-reversal (TR) symmetry for the relation between bulk gyrotropic currents and an effective surface Hall effect, which is required by the TR-symmetry. In particular, such surface Hall effect, related to the spatial change of the gyrotropic tensor invariably present near sample boundaries, is responsible for canceling the polar Kerr effect due to the bulk polarization rotation.[1, 2] In this sense, there is electromagnetic bulk-edge correspondence in gyrotropic metals. Further, studying phenomenological magnetoelectric response of a noncentrosymmetric medium, and again relying on the Onsager relations, I will show that the gyrotropic tensor also determines the so-called kinetic magnetoelectric effect, equivalent to the phenomenon of current-induced magnetization in noncentrosymmetric metals.

Let us start with a general discussion of the Onsager relations consequences for the conductivity tensor. Allowing for a moment for the possibility of time-reversal symmetry breaking in a noncentrosymmetric crystal, with the existence of magnetization $M$, the optical conductivity tensor $\sigma_{ab}(\omega, q; M)$ can be written as

$$\sigma_{ab}(\omega, q; M) \approx \sigma_{ab}(\omega) + \chi_{abc}(\omega)M_c + \lambda_{abc}(\omega)q_c, \quad (4.1)$$

for small $M$ and $q$. In this expression, $\sigma_{ab}(\omega)$ is the usual local optical conductivity, the pseudotensor $\chi_{abc}$ is the anomalous Hall effect term, and tensor $\lambda_{abc}$ describe the natural optical activity, as we have discussed in previous chapters. These tensors determine the antisymmetric part of the conductivity tensor. The Onsager relations[3] tell us:

$$\sigma_{ab}(\omega, q; M) = \sigma_{ba}(\omega, -q; -M), \quad (4.2)$$

implying that $\chi_{abc}$ and $\lambda_{abc}$ are antisymmetric with respect to the first pair of indices, which would be derived below:

$$\begin{bmatrix} \lambda_{abc} \\ \chi_{abc} \end{bmatrix} = -\begin{bmatrix} \lambda_{bac} \\ \chi_{bac} \end{bmatrix}. \quad (4.3)$$

### 4.1 Onsager relations, antisymmetry of $\lambda_{abc}$ tensor, and the bulk-surface correspondence

Let us derive Eq.(4.3) with Onsager relation[4]. Since $\chi_{abc}$ works similar to $\lambda_{abc}$, we will just derive the $\lambda_{abc}$ part of Eq.(4.3).
Any component of current density can be written as

$$j_a(r) = \int d\mathbf{r}' \sigma_{ab}(\mathbf{r}, \mathbf{r}') E_b(\mathbf{r}').$$  \hspace{0.5cm} (4.4)$$

Then, we can get a relation about the dot product of electric field and current:

$$\int d\mathbf{r}'(\mathbf{r} \cdot \mathbf{j}(\mathbf{r})) = \int d\mathbf{r}' \sigma_{ab}(\mathbf{r}, \mathbf{r}') E_b(\mathbf{r}),$$

$$= \int d\mathbf{r} \int d\mathbf{r}' \sigma_{ab}(\mathbf{r}, \mathbf{r}') E_b(\mathbf{r}),$$

$$= \int d\mathbf{r} \sigma_{ba}(\mathbf{r}, \mathbf{r}') E_a(\mathbf{r}),$$

$$= \int d\mathbf{r} \sigma_{ab}(\mathbf{r}, \mathbf{r}') E_b(\mathbf{r}),$$

$$= \int d\mathbf{r} \sigma_{ab}(\mathbf{r}, \mathbf{r}') E_b(\mathbf{r}).$$ \hspace{0.5cm} (4.5)$$

Current density in a sample with nontrivial natural optic activity can be written as

$$j_a = \sigma_{ab} E_b + \lambda_{abc} \partial_c E_b + i(\partial_c \gamma_{abc}) E_b,$$ \hspace{0.5cm} (4.6)$$

with $\gamma_{abc}$ term describing a boundary distribution to the total current density.

Express currents in Eq.(4.5) with the form shown in Eq.(4.6). For the left hand side:

$$\int d\mathbf{r}' \mathbf{E}'(\mathbf{r}) \cdot \mathbf{j}(\mathbf{r}) = \int d\mathbf{r}' \mathbf{E}'(\mathbf{r}) j_a(\mathbf{r}),$$

$$= \int d\mathbf{r}' \sigma_{ab}(\mathbf{r}, \mathbf{r}') E_b(\mathbf{r}),$$

$$= \int d\mathbf{r} \sigma_{ba}(\mathbf{r}, \mathbf{r}') E_a(\mathbf{r}),$$

$$= \int d\mathbf{r} \sigma_{ab}(\mathbf{r}, \mathbf{r}') E_b(\mathbf{r}),$$

$$= \int d\mathbf{r} \sigma_{ab}(\mathbf{r}, \mathbf{r}') E_b(\mathbf{r}).$$ \hspace{0.5cm} (4.7)$$

and for the right hand side:

$$\int d\mathbf{r} \mathbf{E}(\mathbf{r}) \cdot \mathbf{j}'(\mathbf{r}) = \int d\mathbf{r} \mathbf{E}(\mathbf{r}) \left[\sigma_{ab} E_b + \lambda_{abc} \partial_c E_b + i(\partial_c \gamma_{abc}) E_b\right],$$ \hspace{0.5cm} (4.8)$$

where we replaced index $a \leftrightarrow b$ to get the final result.
With \( \int dr E'_a(r) j_a(r) = \int dr E_a(r) j'_a(r) \), we obtain Eq.(4.3):

\[
\int dr E'_a(r) \lambda_{abc} i \partial_c E_b = -i \int dr E'_a \lambda_{bac} \partial_c E_b \\
\Rightarrow \lambda_{abc} = -\lambda_{bac},
\]

(4.9)

together with a relation between bulk contribution \( \lambda_{abc} \) and the boundary contribution \( \gamma_{abc} \):

\[
\int dr E'_a(r) i(\partial_c \gamma_{abc}) E_b = -i \int dr E'_a E_b \partial_c \lambda_{bac} + i \int dr E'_b \partial_c \gamma_{bac} \\
\Rightarrow \partial_c \gamma_{abc} = -\partial_c \lambda_{bac} + \partial_c \gamma_{bac} \\
\Rightarrow \gamma_{abc} = \frac{1}{2} \lambda_{abc}. \quad (4.10)
\]

### 4.2 Onsager relations in the magnetoelectric effect

We take the dc limit, "\( q \to 0 \) first, then \( \omega \to 0 \)" of linear response to electric field. Therefore, the response of the crystal to electromagnetic field is fully determined by the electric polarization and the magnetization:

\[
P_a(\omega, q) = \chi^{e}_{ab}(\omega) E_b(\omega, q) + i \chi^{em}_{ab}(\omega) B_b(\omega, q), \quad (4.11a)
\]
\[
M_a(\omega, q) = -i \chi^{me}_{ab}(\omega) E_b(\omega, q) + \chi^{m}_{ab}(\omega) B_b(\omega, q). \quad (4.11b)
\]

Here we only keep up to linear order of \( q \), so we can neglect the \( q \) dependence of the response tensors \( \chi^{e,m,em,me} \) as well. The magnetoelectric susceptibility \( \chi^{me}_{ab} \) describes the magnetization response to a transport electric field, known as the kinetic magnetoelectric effect[5].

A macroscopic current density can be written as

\[
j = -i \omega P(\omega, q) + iq \times M(\omega, q). \quad (4.12)
\]

If we substitute Eq.(4.11) into Eq.(4.12), and use Faraday’s law \( \mathbf{B} = q \times \mathbf{E} / \omega \), we get

\[
j_a = -i \omega \chi^{e}_{ab} E_b - i \omega \chi^{em}_{ab} \frac{\epsilon_{bcd} q_c E_d}{\omega} + i \epsilon_{abc} q_b \chi^{me}_{cd} E_d + i \epsilon_{abc} q_b \chi^{m}_{cd} \frac{\epsilon_{drs} q_r E_s}{\omega}, \quad (4.13)
\]

from which we write out the conductivity tensor

\[
\sigma_{ab} = -i \omega \chi^{e}_{ab} - i \chi^{em}_{ab} \epsilon_{bcd} q_c + i \epsilon_{abc} q_b \chi^{me}_{cd} + i \epsilon_{asc} q_s \chi^{m}_{cd} \epsilon_{drb} q_r / \omega. \quad (4.14)
\]
From Onsager relation $\sigma_{ab}(\omega, q) = \sigma_{ba}(\omega, -q)$ we get

$$
-i\omega \chi_{ab}^e - i\epsilon_{bcd}\chi_{ad}^m q_c + i\epsilon_{acd}\chi_{d}^m q_a + i\epsilon_{asc}\chi_{cd}^m q_s / \omega \\
= -i\omega \chi_{ba}^e + i\epsilon_{adc}\chi_{bd}^m q_c - i\epsilon_{bcd}\chi_{ca}^m q_d + i\epsilon_{bsc}\chi_{cd}^m q_s / \omega.
$$

(4.15)

By comparing terms in the left-hand side and those in the right-hand side, we get

$$
\chi_{ab}^e = \chi_{ba}^e, \quad \chi_{cd}^m = \chi_{dc}^m, \quad \chi_{ad}^m = \chi_{da}^m.
$$

(4.16)

### 4.3 Current-induced magnetization

The gyrotropic part of current in Eq.(4.12) can be written as

$$j_g,a = (\chi_{ad}^m e_{dcb} + \epsilon_{acd}\chi_{db}^m) q_c e_{ab} E_b,$$

(4.17)

and from the previous section we’ve already known that $\chi_{ad}^m = \chi_{da}^m$. Therefore we obtain

$$
\lambda_{abc} = (\epsilon_{acd}\chi_{db}^m - \epsilon_{bcd}\chi_{da}^m).
$$

(4.18)

$$
\Rightarrow \quad g_{ab} = \frac{1}{2}\epsilon_{cda}\lambda_{cdb} = \chi_{ab}^m - \delta_{ab} \text{Tr} \chi_{cd}^m.
$$

(4.19)

Since $\text{Tr}g = \text{Tr}g - 3\text{Tr}g = -2\text{Tr}g$, we get

$$
\chi_{ab}^m = g_{ab} - \frac{1}{2}\delta_{ab} \text{Tr}g.
$$

(4.20)

The gyrotropic tensor has been obtained in chapter 3. For a disordered system, we write it as

$$g_{ab} = \frac{e}{(\omega + \frac{i}{\tau})} \int (d\mathbf{p})(m_{pa}^\text{int} \partial_b f_0^p - \delta_{ab} m_{p}^\text{int} \cdot \partial_f f_0^p),$$

(4.21)

where $m_{p}^\text{int} = \frac{i\hbar}{\tau} (\partial_p u_p) \times (\hbar_p - \epsilon_p) |\partial_p u_p|$ is the intrinsic orbital magnetic moment. Therefore, we reach the formula for the magnetoelectric susceptibility:

$$
\chi_{ab}^m = \frac{e}{(\omega + \frac{i}{\tau})} \int (d\mathbf{p}) m_{pa}^\text{tot} \partial_b f_0^p,
$$

(4.22)

which gives the following expression for the magnetization[6]:

$$
M^\text{int} = \int (d\mathbf{p}) m_{p}^\text{int} \frac{eE \cdot \partial_f f_0^p}{(i\omega - \frac{i}{\tau})}.
$$

(4.23)

The reason we name this current as induced magnetization is that, the time-reversal parity of quantities in the left-hand side and right-hand side of the linear relationship $M \propto E$
indicates the existence of a dissipative process, in other words, a current flow in our time-reversal invariant noncentrosymmetric system[5,7].

Those “int” superscripts stand for “intrinsic”, indicating that they are just intrinsic part of contribution. To get total magnetization, we have to consider the “extrinsic” contributions: skew scattering and side-jump. The “extrinsic” contributions have a similar form as Eq.(4.23), but the orbital magnetic moments are different. As I have mentioned at the beginning of this chapter, we are doing tight binding calculation of the current induced magnetization on Tellurium. We are calculating different contributions separately, so that we are able to compare them to find which one dominates at what kind of conditions.

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CHAPTER 5

DYNAMIC CHIRAL MAGNETIC EFFECT AND
FARADAY ROTATION IN
MACROSCOPICALLY DISORDERED HELICAL
METALS

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Dynamic Chiral Magnetic Effect and Faraday Rotation in Macroscopically Disordered Helical Metals

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We develop an effective medium theory for electromagnetic wave propagation through gapless nonuniform systems with a dynamic chiral magnetic effect. The theory allows us to calculate macroscopic-disorder-induced corrections to the values of optical, as well as chiral magnetic conductivities. In particular, we show that spatial fluctuations of the optical conductivity induce corrections to the effective value of the chiral magnetic conductivity. The absolute value of the effect varies strongly depending on the system parameters, but yields the leading frequency dependence of the polarization rotation and circular dichroism signals. Experimentally, these corrections can be observed as features in the Faraday rotation angle near frequencies that correspond to the bulk plasmon resonances of a material. Such features are not expected to be present in single-crystal samples.

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Ignited by the field of topological insulators, interest in the geometric properties of band structures has spread to gapless systems now. Among the latter, Weyl semimetals seem to have attracted the largest attention, partly due to their nontrivial topological properties [1–6], and partly due to the experimental verification of their existence [7–14].

There have been a substantial number of theoretical proposals on how the geometric properties of Weyl metals manifest themselves in observable experimental quantities related, for instance, to magnetotransport [15–19], nonlocal transport [20,21], or strain [22–25] phenomena. However, in Weyl systems, or gapless topological systems in general, one necessarily deals with systems with a gapless bulk. This means that, at least in principle, they manifest all responses pertinent to a more mundane metal with the same symmetries. This implies that a careful quantitative understanding of various experiments is required in order to disentangle the geometric features of the observed responses. In particular, the omnipresent disorder effects must always be carefully studied.

In this Letter, we describe how macroscopic sample inhomogeneities affect optical tests of the dynamic chiral magnetic effect via Faraday rotation measurements. We show that in thin films of metals with low carrier concentration, macroscopic fluctuations of the local conductivity affect the frequency dependence of the measured optical polarization rotation signal, creating sharp features near the plasma edge of the metal, which are absent in single crystals.

The chiral magnetic effect (CME) is defined as the existence of a contribution to the electric current density $\mathbf{j}$, driven by a magnetic field $\mathbf{B}$, which yields the following expression for the electric current density in the simplest isotropic case:

$$\mathbf{j}(\omega) = \sigma(\omega)\mathbf{E}(\omega) + \gamma(\omega)\mathbf{B}(\omega). \quad (1)$$

The first term on the right-hand side of Eq. (1) represents the usual optical conductivity response to an electric field $\mathbf{E}$. The coefficient $\gamma(\omega)$ is in general nonzero in noncentrosymmetric crystals with gyrotropic point groups [26]. Its possible tensorial properties are discussed below. The $\omega \rightarrow 0$ limit of $\gamma(\omega)$, which can be nonzero in a metal, is known as the chiral magnetic conductivity in the literature. Here, we consider a more general case of a frequency-dependent $\gamma(\omega)$, keeping the name of the chiral magnetic conductivity for it.

There are two basic types of the CME, pertaining to the cases of a purely static, and a slowly oscillating $\mathbf{B}$ field, which are appropriately called the static and dynamic CME, respectively.

The static CME is of purely topological origin, and relies on the existence of Weyl points, and the Berry curvature monopoles associated with them, in a band structure [15,27–31]. However, the static CME does not occur in equilibrium crystals [32,33]: it requires an imbalance between the chemical potentials near Weyl points with opposite signs of the Berry monopole charges. This imbalance is in general hard to achieve, but when it is reached via the chiral anomaly, the static CME manifests itself either as the negative longitudinal magnetoresistance [15,17,34], or nonlocal voltages in thin film samples [20]. In this sense, the static CME has been observed via magnetotransport measurements in Refs. [35–38] (see Refs. [39,40] for further references and a review of recent results), and via nonlocal voltage measurements in Ref. [41].

Here, we focus on the dynamic CME, which does exist in equilibrium gyrotropic metals, and describes their linear response to slowly oscillating electromagnetic fields. Its low-frequency limit is of geometric origin: it comes from the local geometry of electronic bands, rather than their topology, and is due to the existence of the orbital magnetic...
moment of quasiparticles in systems with nonzero Berry curvature [42–44]. It also does not require the existence of Berry monopoles, but tends to be large when the monopoles are present [42,45].

Physically, the dynamic CME is a particular manifestation of the natural optical activity phenomenon [42,43]. This observation prompts an experimental measurement of the chiral conductivity \( \gamma(\omega) \) by studying the Faraday rotation of the polarization of light transmitted through a slab of gyrotropic material.

The (complex) polarization rotation angle is determined solely by the phase difference accumulated by the two circular polarizations of light as they travel through the bulk of the material [46]:

\[
\theta(\omega) = \frac{\mu_0}{2} \mathbf{r}(\omega) d,
\]

where \( d \) is the thickness of the slab in the propagation direction. The rotation angle is not affected by possible surface conduction, either [47]. Therefore, the Faraday rotation appears to be the most direct way to measure \( \gamma(\omega) \).

Here, we show that macroscopic inhomogeneities make the effective macroscopic observable \( \gamma_{\text{eff}}(\omega) \) different from its value predicted by the band structure calculations, \( \gamma_{\text{BS}}(\omega) \). In particular, \( \gamma_{\text{eff}}(\omega) \) has sharp features around the plasma edge of the metal, which is not expected for \( \gamma_{\text{BS}}(\omega) \). Instead, at frequencies large compared to the inverse momentum relaxation time on the Fermi surface, and small compared to the lowest interband splitting at the Fermi surface, \( \gamma_{\text{BS}}(\omega) \) is a real frequency-independent constant [42]. More generally, when the frequency of the incident light is not small compared to relevant band splittings, \( \gamma_{\text{BS}}(\omega) \) does depend on \( \omega \), but obviously is still not expected to have any features at the plasma edge of a metal.

In what follows, we set out to construct the effective medium theory for a macroscopically disordered sample with the CME. The effective medium theory for composite materials, and metals in particular, has been developed over the past century [48–51], but it has not been constructed for metals with natural optical activity. We fill this void below.

**General formalism.**—We assume that a nonuniform sample is characterized by macroscopic inhomogeneities, which occur on length scales large compared to the microscopic ones, like the Fermi wavelength, or elastic mean free path. The sample is then characterized by a space-dependent (optical) conductivity \( \sigma_{ab}(\mathbf{r}, \omega) \) and the CME tensor \( \gamma_{abc}(\mathbf{r}, \omega) \).

If the variation of electromagnetic fields is slow on the scale over which the response coefficients change, the electromagnetic response of a medium can be described in terms of an effective medium theory, characterized by an effective translationally invariant (nonlocal) optical conductivity tensor. The determination of this effective tensor in the presence of the CME is the central aim of this Letter.

In general, the space-dependent response coefficients can be decomposed into the sums of their volume-averaged parts, denoted with overlines, and random parts with zero averages:

\[
\sigma_{ab}(\mathbf{r}, \omega) = \overline{\sigma}_{ab}(\omega) + \delta \sigma_{ab}(\mathbf{r}, \omega),
\]

\[
\gamma_{abc}(\mathbf{r}, \omega) = \overline{\gamma}_{abc}(\omega) + \delta \gamma_{abc}(\mathbf{r}, \omega).
\]

Since the CME is a relatively weak effect, and spatial fluctuations of \( \delta \gamma_{abc} \) will lead to even weaker effects, we set \( \delta \gamma_{abc} \to 0 \) in what follows.

It should be stressed that the variation of \( \gamma_{abc} \) is inevitably present near sample boundaries; however, this variation does not play any role in the effective medium construction, and only affects the boundary conditions for electromagnetic waves scattering off a sample with the CME or natural optical activity [52,53].

In what follows, we assume ergodic behavior for fluctuations of the response coefficients, in the sense that volume averages for various quantities coincide with their ensemble averages over disorder realizations. Physically, this means that we neglect the mesoscopic fluctuations of effective medium parameters.

To construct the effective medium theory, we use the Maxwell equations to describe the sample-specific response of a disordered medium to electromagnetic fields, and then average it over the disorder realizations. The electromagnetic response of the medium is fully determined by its nonlocal optical conductivity tensor. To the lowest order in the spatial gradients of the electric field, one has the following expression for the \( \mathbf{r} \)th component of the current density in a nonuniform chiral metal:

\[
\mathbf{j}_a = \sigma_{ab}(\mathbf{r}, \omega) \mathbf{E}_b + \frac{i}{\omega} \gamma_{abc}(\omega) \nabla_c \mathbf{E}_b.
\]

This expression is the anisotropic version of Eq. (1) in view of Faraday’s law for monochromatic fields, \( \mathbf{B} = \nabla \times \mathbf{E}/i \omega \).

It is well known that, in a time-reversal system, the antisymmetric part of the optical conductivity tensor is fully determined by the spatial gradients of \( \gamma_{abc} \) [52]. Since we take \( \gamma_{abc}(\omega) \) to be equal to its spatially averaged (equally, disorder-averaged) value, \( \sigma_{ab}(\mathbf{r}, \omega) \) is a symmetric local conductivity tensor.

To proceed, we make several simplifying assumptions, which are easily relaxed within the theory developed below, but increase the clarity of the presentation. We go back to the assumption that the medium is isotropic; hence, \( \sigma_{ab} = \sigma \delta_{ab}, \gamma_{abc} = \gamma \delta_{abc} \). Under these assumptions, the expression for the current density simplifies to

\[
\mathbf{j} = [\sigma(\omega) + \delta \sigma(\omega, \mathbf{r})] \mathbf{E} + \gamma(\omega) \mathbf{B}.
\]

The fluctuations of the local conductivity tensor are assumed to be Gaussian, with a given correlator:

\[
\langle \delta \sigma(\omega, \mathbf{r}) \delta \sigma(\omega, \mathbf{r}') \rangle = K_\omega(\mathbf{r} - \mathbf{r}').
\]

The effective medium is then characterized by the effective conductivity \( \sigma_{\text{eff}} \) and the effective chiral magnetic
conductivity $\gamma_{\text{eff}}$, which relate the average current density to the average electric and magnetic fields:

$$\bar{j} = \sigma_{\text{ef}} \bar{E} + \gamma_{\text{ef}} \bar{B}. \quad (7)$$

Using the Maxwell equations, the electric field for a given realization of $\delta \sigma(\mathbf{r}, \omega)$ can be shown to satisfy

$$\nabla(\nabla \bar{E}) - \nabla^2 \bar{E} = \frac{\omega^2}{c^2} \varepsilon(\omega) \bar{E} + \frac{\gamma(\omega)}{\varepsilon_0 c^2} \nabla \times \bar{E} + \frac{i \omega}{\varepsilon_0 c^2} \delta \sigma(\mathbf{r}, \omega) \bar{E} \quad (8)$$

with

$$\varepsilon(\omega) = \varepsilon_0 + \frac{i \tilde{\varepsilon}(\omega)}{\varepsilon_0}. \quad (9)$$

The corresponding (retarded) Green’s function obeys the following equation:

$$\left( \nabla_a \nabla_b - \nabla^2 \delta_{ab} - \frac{\omega^2}{c^2} \varepsilon(\omega) \delta_{ab} + \frac{\gamma(\omega)}{\varepsilon_0 c^2} \varepsilon_{abd} \nabla_d \right) \bar{D}_{bc}(\mathbf{r}, \mathbf{r}'; \omega)$$

$$= \delta_{ac} \delta(\mathbf{r} - \mathbf{r}'). \quad (10)$$

For weak Gaussian disorder, the effective medium theory reduces [54] to the standard self-consistent Born approximation for the disorder-averaged Green’s function $\bar{D}_{bc}(\mathbf{r} - \mathbf{r}', \omega)$, which depends on the difference $\mathbf{r} - \mathbf{r}'$ due to the restored translational invariance.

Averaging over the “disorder realizations” is done according to the standard rules for systems with quenched disorder [55]. In particular, such averaging restores the translational invariance, and the medium is characterized by a self-energy in the expression for the average retarded Green’s function of the electric fields. In the Fourier space, the equation for the disorder-averaged Green’s function becomes

$$\left( q^2 \delta_{ab} - q_a q_b - \frac{\omega^2}{c^2} \varepsilon(\omega) \delta_{ab} + \frac{i \tilde{\varepsilon}(\omega)}{\varepsilon_0 c^2} \varepsilon_{abd} q_d \right) \bar{D}_{bc}(\mathbf{q}, \omega)$$

$$= \delta_{ac}. \quad (11)$$

The Feynman diagrams for the self-energy are shown in Fig. 1. In real space it is given by

$$\Sigma_{ab}(\mathbf{r} - \mathbf{r}'; \omega) = -\frac{\omega^2}{e_0^2 c^4} K_{\omega}(\mathbf{r} - \mathbf{r}') \bar{D}_{ab}(\mathbf{r} - \mathbf{r}'; \omega), \quad (12)$$

which can be rewritten in the Fourier space as

$$\Sigma_{ab}(\mathbf{q}, \omega) = -\frac{\omega^2}{e_0^2 c^4} \int (dq') K_{\omega}(\mathbf{q} - \mathbf{q}') \bar{D}_{ab}(\mathbf{q}', \omega). \quad (13)$$

where $(dq) \equiv d^3q/(2\pi^3)$, and $K_{\omega}(\mathbf{q})$ is the usual Fourier transform of $K_{\omega}(\mathbf{r})$.

To capture the CME, one has to keep the linear in $\mathbf{q}$ dependence of the self-energy. Because of the assumed isotropy of the medium, the latter can be decomposed as

$$\Sigma_{ab}(\mathbf{q}, \omega) \approx \frac{\omega^2}{c^2} \Sigma_0(\omega) \delta_{ab} + \frac{i}{\varepsilon_0 c^2} \Sigma_1(\omega) \varepsilon_{abc} q_c. \quad (14)$$

From Eq. (11) it is clear that $\Sigma_{0,1}$ play the role of corrections to the average values of $\varepsilon(\omega)$ and $\gamma(\omega)$, respectively. From Eq. (13), the expressions for $\Sigma_{0,1}$ read

$$\Sigma_0(\omega) \delta_{ab} = -\frac{1}{\varepsilon_0^2 c^4} \int (dq) K_{\omega}(\mathbf{q}) \bar{D}_{ab}(\mathbf{q}, \omega),$$

$$\Sigma_1(\omega) \varepsilon_{abc} = \frac{i \omega}{\varepsilon_0 c^2} \int (dq) \bar{D}_{ab}(\mathbf{q}, \omega) D_{bc}(\mathbf{q}', \omega). \quad (15)$$

The fact that the tensor structures on the left- and right-hand sides of these equations match is guaranteed by the isotropy of the medium.

Limiting ourselves to the linear order in $\gamma$, we finally obtain

$$\Sigma_0(\omega) = \frac{1}{3 \varepsilon_0^2 c^2} \int (dq) K_{\omega}(\mathbf{q}) \left( \frac{2}{q_d^2 - q^2} + \frac{1}{q^2} \right),$$

$$\Sigma_1(\omega) = \gamma(\omega) \frac{\omega^2}{3 \varepsilon_0^2 c^2} \int (dq) \frac{q_d K_{\omega}(\mathbf{q})}{(q_d^2 - q^2)^2}. \quad (16)$$

where $q_d^2 = (\omega^2/c^2)[\varepsilon(\omega) + \Sigma_0(\omega)]$. The effective medium parameters are given by

$$\sigma_{\text{ef}}(\omega) = \tilde{\sigma}(\omega) - i\varepsilon_0 \omega \Sigma_0(\omega),$$

$$\gamma_{\text{ef}}(\omega) = \gamma(\omega) + \Sigma_1(\omega). \quad (17)$$

Equations (16) and (17) are one of the central results of this Letter. They allow us to determine the effective medium parameters for any particular model characterized by a given correlator of optical conductivity fluctuations. It is straightforward to show that these equations reproduce the textbook effective medium theory results [56], if one neglects the self-consistency.

In the equation for $\Sigma_0$, the first term in round brackets describes the contribution from the fluctuations with two
transverse polarizations, while the second one is the contribution from the longitudinal electric field fluctuations. The latter are dispersionless, since we did not include quadratic spatial dispersion \( O(q^2) \) terms in the dielectric tensor. In general, the contribution from the transverse modes is small in the parameter \( \alpha^2 \ell^2 / c^2 \sim \ell^2 / \lambda_0^2 \), where \( \ell \) is the scale of macroscopic inhomogeneity, and \( \lambda_0 \) is the wavelength of the light with frequency \( \omega \) in vacuum.

A model with short-ranged correlations.—To apply the general expressions (16) to a nontrivial situation, we consider a metal with a low carrier density, being treated within the Drude model with a spatially dependent electron density. In practice, one may talk about a doped semiconductor, taking into account spatial fluctuations of the dopant density. We will show that the ensuing spatial fluctuations of the optical conductivity result in plasmonic features in the frequency dependence of \( \gamma_{\text{eff}}(\omega) \).

Within the Drude model, the spatially dependent optical conductivity has the following form:

\[
\sigma(\mathbf{r}, \omega) = \frac{e^2_0 \alpha^2 \rho(\mathbf{r})}{1 - i\omega\tau}.
\]

We are interested in plasmonic features in \( \gamma_{\text{eff}}(\omega) \); hence, we specialize to frequencies close to the average plasma edge, \( \omega_0 \). For \( \omega_0 \tau \gg 1 \), the conductivity can be approximated according to

\[
\sigma(\omega, \mathbf{r}) \approx \frac{i e^2_0 \alpha^2 \rho(\mathbf{r})}{\omega} + \frac{e^2_0 \alpha^2 \rho(\mathbf{r})}{\omega^2 \tau}\;\omega. \quad (19)
\]

In what follows we will neglect the real part of the conductivity, since dissipation (\( \text{Im} \Sigma_0 \neq 0 \)) will be generated by wave decay into plasmons. However, the (positive) sign of the real part of the conductivity sets the sign of \( \text{Im} \Sigma_0 \) (also positive), see below.

Writing \( \alpha^2 \rho(\mathbf{r}) = \alpha^2_0 + \delta\alpha^2 \rho(\mathbf{r}) \), with

\[
\langle \delta\alpha^2 \rho(\mathbf{r}) \delta\alpha^2 \rho(\mathbf{r}') \rangle = \Omega^2 \exp \left[ -\kappa |\mathbf{r} - \mathbf{r}'| \right]. \quad (20)
\]

we obtain

\[
K_\omega(q) = -i \frac{e^2_0 \Omega^2}{\alpha^2} \frac{8\pi \kappa}{(q^2 + \kappa^2)^2}. \quad (21)
\]

Applying Eqs. (16), we obtain a self-consistent equation for \( \Sigma_0(\omega) \):

\[
\Sigma_0(\omega) = -\frac{1}{\omega_0} \frac{\Omega^2}{3 \alpha^2} \frac{1}{1 - \frac{\omega^2}{\omega_0^2}} + \Sigma_0(\omega). \quad (22)
\]

For \( |\omega^2 - \omega_0^2| < 2 \Omega^2 / \sqrt{3} \) one has

\[
\text{Re} \Sigma_0(\omega) = \frac{\omega_0^2 - \omega^2}{2 \alpha^2}, \quad \text{Im} \Sigma_0 = \frac{1}{2} \sqrt{3} \Omega^2 \alpha^2 \left( \frac{\omega_0^2}{\omega^2} - 1 \right)^2. \quad (23)
\]

and for \( |\omega^2 - \omega_0^2| > 2 \Omega^2 / \sqrt{3} \)

\[
\text{Re} \Sigma_0(\omega) = \frac{\omega_0^2}{2 \alpha^2} - \frac{\omega_0^2}{\omega^2} \left( \frac{\omega_0^2}{\omega^2} - 1 \right)^2 - \frac{4 \Omega^2}{3 \alpha^2}, \quad \text{Im} \Sigma_0 = 0. \quad (24)
\]

Here, \( \text{sgn}(x) \) is the sign function.

Calculating \( \Sigma_1 \), we get the following expression for \( \gamma_{\text{eff}}(\omega) \):

\[
\gamma_{\text{eff}}(\omega) = \gamma(\omega) \left[ 1 + \frac{\Omega}{\alpha \kappa} \right] \frac{1}{(1 - i q \omega / \kappa)^2}. \quad (25)
\]

As before, \( q^2 = (\alpha^2 / c^2)[\epsilon(\omega) + \Sigma_0(\omega)] \).

The results of this calculation are plotted in Fig. 2. It is observed that due to the disorder-induced scattering into the dispersionless plasmons the local part of the effective dielectric tensor of the medium acquires an imaginary part sharply peaked around the plasma frequency. In turn, this translates into sharp features in the circular dichroism and polarization rotation signals, which are determined by \( \text{Im} \gamma_{\text{eff}}(\omega) \) and \( \text{Re} \gamma_{\text{eff}}(\omega) \), respectively.

The results depend strongly on the values of two dimensionless parameters: \( \Omega / \omega_0^2 \), and \( \Omega / \alpha \kappa \). The former measures the inhomogeneous broadening of the plasma edge; the appearance of the latter is tied to the structure of the expression for \( \Sigma_1 \), Eq. (16). The main contribution to the corresponding integral comes from wave vectors \( q \sim \kappa \), where \( \kappa \) is the inverse correlation length of the optical conductivity fluctuations. The parameter \( (\Omega / \alpha \kappa)^2 \) then represents the ratio of the typical disorder-induced magnetic field fluctuation in an electromagnetic wave \( q \sim \kappa \) and electric field amplitude \( E_q \), which is \( \delta B \sim \Omega^2 E_q / \alpha c \omega \), to the average magnetic field of the wave, \( B_q \sim \kappa E_q / \omega \). This parameter determines the applicability region of the theory, which is \( (\Omega / \alpha \kappa)^2 \lesssim 1 \).

It is hard to theoretically estimate the aforementioned parameters for a given material. Instead, they can be determined from the widths and maximum height of experimental peaks, analogous to those shown in Fig. 2.
For the particular model considered, the peak width scales as $\Omega^2/\omega_0^2$, while the peak values of the circular dichroism and polarization rotation signals scale roughly as $(\Omega/c \kappa)^2$ and $(\Omega/c \kappa)^4$, respectively.

In summary, we have developed the theory of disorder-induced corrections to the chiral magnetic effect and natural optical activity in samples with macroscopic inhomogeneities. The theory is applicable to situations in which the electromagnetic fields vary smoothly on the inhomogeneity scale. In particular, the theory pertains to the case of Weyl metals with low electron density, in the terahertz frequency range. In general, the disorder-induced corrections are not large in absolute magnitude, but are the primary source of the sharp frequency dependence of the chiral conductivity around the plasma edge of the metal. This observation is pertinent to any helical metals with natural optical activity, not just Weyl ones.

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CHAPTER 6

CONCLUSIONS

This work is focused on the study in the natural optical activity and chiral magnetic effect in noncentrosymmetric metals. The main part of the research is contained in Chapter 3, while the fundamental knowledge and relevant calculation methods introduced in Chapter 1 have paved the road to our work. Since this work is motivated by the recently discovery of Weyl semimetals, Chapter 2 has provided a brief review of the background of our research and the track of our reasoning: from chiral anomaly to chiral magnetic effect. Chapter 4 and Chapter 5 has pushed the study further, either by including the current induced magnetization, or by taking disorders into consideration.

We have argued that the chiral magnetic effect is essentially a specific case of the natural optical activity, and therefore, we need to study the antisymmetric part of the optical conductivity to understand both effects. In Chapter 3, a general expression (Eq.(17) in Chapter 3) for the leading contribution to the gyrotropic current in a metallic system at low frequencies and wave vectors has been derived, which is the central result of our work. This expression holds for low frequencies $\omega$ and wave vectors $q$ compared to the energy scale of the chemical potential $\mu$ and the relevant energy gap $E_g$: $\omega, vq \ll \mu, E_g$, where $v$ is the relevant speed. The main physical conclusion is that the intrinsic orbital magnetic moment of quasiparticles is the source of the natural optical activity, the dynamic chiral magnetic effect, and the current induced magnetization in (semi)metals. Unlike the static chiral magnetic effect, the dynamic chiral magnetic effect does not have a topological origin. In general, the latter one exists in metallic systems with a gyrotropic point group, and can be observed in an inversion symmetry broken Weyl semimetal that is equipped with such point groups. However, these effects, the natural optical activity, the dynamic chiral magnetic effect and the current induced magnetization, are not limited to Weyl semimetals: the presence of the Weyl points, or the associated Berry monopoles is not
required in general for the existence of these effects. Also, we have argued that the trace of the gyrotropic tensor determines the magnitude of the dynamic chiral magnetic effect in a system with a point group of relatively high symmetry, particularly in an isotropic system. The magnitude of the dynamic chiral magnetic effect can be measured by the Faraday rotation experiments. The rotatory angle $\theta$ is directly proportional to the dynamic chiral magnetic conductivity $\gamma$ and the depth of the measured material $d$: $\theta(\omega) = \frac{\mu_0}{2} \gamma(\omega)d$.

With an effective medium theory, we have shown that macroscopic inhomogeneities (the inhomogeneities occur on length scales large compared to the microscopic ones, like the Fermi wavelength, or elastic mean free path) make the effective observable chiral magnetic conductivity different from the chiral magnetic conductivity obtained by the band structure calculations. The effective one has sharp features around the plasma edge of the metal, which is not expected from the band structure calculations. The disorder-induced correction does not affect the magnitude of the effective chiral magnetic conductivity, but it is the reason for the observable sharp feature. This effective medium theory is pertinent at the circumstance of smoothly varying electromagnetic fields on the inhomogeneity scale.

In particular, our work with effective medium theory is applicable to the case of Weyl semimetals with low electron density, near the terahertz frequency range. In Chapter 4, we have obtained a relation between the magnetoelectric susceptibility and the gyrotropic tensor. This relation allow us to calculate the current induced magnetization easily with the obtained gyrotropic tensor. Apparently, with all these results from theoretic derivations, the next thing to expect is the numerical calculations on models for specific materials, and then hopefully the experimental confirmations.
APPENDIX A

GENERAL EXPRESSION FOR OPTICAL CONDUCTIVITY

A general Hamiltonian

\[ H = \int d\mathbf{r} \psi^\dagger \left( \frac{\mathbf{p} - \frac{e}{c} \mathbf{A}}{2m} \right)^2 + \lambda \mathbf{\sigma} \cdot \mathbf{E} \times (\mathbf{p} - \frac{e}{c} \mathbf{A}) + U(r) - g \mu_B \mathbf{\sigma} \cdot \mathbf{B} \mathbf{\sigma} \psi \psi^\dagger. \quad (A.1) \]

give a current containing three part

\[ j = j_{\text{grad}} + j_{\text{dia}} + j_s. \quad (A.2) \]

Magnetic current from spin density is

\[ j_{\text{spin}} = \mu_B g c \nabla \times (\psi^\dagger \mathbf{\sigma} \psi). \quad (A.3) \]

Diamagnetic current

\[ j_{\text{dia}} = -\frac{e^2}{mc} \langle \psi^\dagger (\mathbf{r}) \mathbf{\sigma} \psi (\mathbf{r}) \rangle \mathbf{A} (\mathbf{r}, \tau). \quad (A.4) \]

Averaging over a unit cell, the diamagnetic current become

\[ \bar{j}_{\text{dia}} = -\frac{e^2}{mc} \frac{N_v}{V} \mathbf{A}. \quad (A.5) \]

Gradient part of the current with the form

\[ j_{\text{grad}} = \frac{eh}{2mi} (\psi^\dagger \mathbf{\nabla} \psi - \mathbf{\nabla} \psi^\dagger \cdot \psi) \quad (A.6) \]

result in

\[ j^j_{\text{grad}} (\Omega, \mathbf{q}) = Q^{ij} (\Omega, \mathbf{q}) A_j (\mathbf{q}, \Omega), \quad (A.7) \]

with

\[ Q^{ij} (\Omega, \mathbf{q}) = -\frac{e^2 N_v^2}{4mc^3 V^3} \sum_{k,n,n'} \frac{f_{n'(k-q)} - f_{nk}}{i\Omega + \frac{2\hbar}{c} (k-q)} \langle u_n' (k-q) | \left( 2\frac{\hbar}{c} \partial_{r_i} + 2\hbar k_i - h \partial_{q_i} \right) | u_{nk} \rangle \langle u_{nk}| u_{n'(k-q)} \rangle (A.8) \]

\[ [\langle u_{nk}| \left( 2\frac{\hbar}{c} \partial_{p_j} + 2\hbar k_j - h \partial_{q_j} \right) | u_{n'(k-q)} \rangle]. \quad (A.9) \]
For tight binding model:

\[ H = \sum_{ij} t_{ij}^{\alpha \beta} e^{i \pi \epsilon_k} \int_{\mathcal{K}_r} d\mathbf{r} A(r) \hat{a}_{i\alpha}^{\dagger} \hat{a}_{j\beta} \]  
(A.10)

our gradient part of current can be written as

\[ j_{\text{grad}} = \frac{e}{\hbar} \sum_{k} \hat{a}_{k-q/2, \alpha} \partial_k t_{k}^{\alpha \beta} \hat{a}_{k+q/2, \beta} \]  
(A.11)

while diamagnetic current have this form:

\[ j_{\text{dia}} = -\frac{e^2}{\hbar^2 c} \sum_{k} \hat{a}_{k-q/2, \alpha} \partial_k (A \cdot \partial_k t_{k}^{\alpha \beta}) \hat{a}_{k+q/2, \beta} \]  
(A.12)

With the help of green’s function, after a little bit calculation, we end up with an equation similar to Eq.(C.24) for tight binding model

\[ Q_{ij}(\Omega, q)_{\text{grad}} = -\frac{e^2}{\hbar^2 c} \sum_{k, n, n'} \frac{f_{n', k-q/2} - f_{n, k+q/2}}{i\Omega + \xi_{n', k-q/2} - \xi_{n, k+q/2}} \langle u_{n', k-q/2} \frac{\partial t_k}{\partial k_i} | u_{n, k+q/2} \rangle \langle u_{n, k+q/2} \frac{\partial t_k}{\partial k_j} | u_{n', k-q/2} \rangle. \]  
(A.13)

This is a useful expression known as Kubo formula. Which is the foundation of our research as we are interested in the magnetization and optical activities, so the main part is calculating optical conductivity tensor.

Detailed derivations are given in appendix B and appendix C.
APPENDIX B

DETAILED DERIVATION FOR OPTICAL CONDUCTIVITY FOR SYSTEM OF A GENERAL HAMILTONIAN

We can write a general Hamiltonian

\[
H = \int dr \psi_\sigma^\dagger \left[ \frac{\mathbf{p} - \frac{e}{c} \mathbf{A}}{2m} \right]^2 + \lambda \mathbf{\sigma} \cdot \mathbf{E} \times (\mathbf{p} - \frac{e}{c} \mathbf{A}) + U(r) - g \mu_B \mathbf{\sigma} \cdot \mathbf{B} \psi_{\sigma'}^\dagger \psi_{\sigma'}. \tag{B.1}
\]

Here we know that \( \mathbf{B} = \vec{\nabla} \times \mathbf{A} \).

Current density \( \mathbf{j} \) can be derived from the Hamiltonian by

\[
\mathbf{j} = -e \frac{\delta H}{\delta \mathbf{A}}. \tag{B.2}
\]

Therefore, we can get a general formula of current density \( \mathbf{j} \) (we neglect spin orbit interaction \( \lambda \mathbf{\sigma} \cdot \mathbf{E} \times (\mathbf{p} - \frac{e}{c} \mathbf{A}) \) in our calculation):

\[
\mathbf{j} = \frac{e\hbar}{2mi} (\psi_\sigma^\dagger \nabla \psi_{\sigma'} - \nabla \psi_\sigma^\dagger \psi_{\sigma'}) - \frac{e^2}{mc} \psi_\sigma^\dagger \psi_{\sigma'} \mathbf{A} + \text{magnetization current from spin density.} \tag{B.3}
\]

Naturally \( \mathbf{j} \) has three parts, as shown in Eq.(B.3):

\[
\mathbf{j} = \mathbf{j}_{\text{grad}} + \mathbf{j}_{\text{dia}} + \mathbf{j}_s. \tag{B.4}
\]

\( \mathbf{j}_s \) come from the spin-magnetic interaction part of the hamiltonian. \( \mathbf{j}_{\text{dia}} \) is the diamagnetic current. \( \mathbf{j}_{\text{grad}} \) is just the first part of Eq.(B.3), involving gradient of \( \psi_{\sigma'} \). We are going to study them separately.
### B.1 Magnetic current from spin density

\[ j_s^i = c \frac{\delta}{\delta A_i} \int d\mathbf{r} \psi^\dagger B \mathbf{\nabla} \times \mathbf{A} \cdot \sigma \psi \]  
(B.5)

\[ = \mu_B g_c \frac{\delta}{\delta A_i} \int d\mathbf{r} (\psi^\dagger \sigma_{\nu \nu'} \psi_{\nu'}) \cdot \mathbf{\nabla} \times \mathbf{A} \]  
(B.6)

\[ = \mu_B g_c \frac{\delta}{\delta A_i} \int d\mathbf{r} s_i \epsilon_{ijk} \partial_j A_k \]  
(B.7)

\[ = - \mu_B g_c \frac{\delta}{\delta A_i} \int d\mathbf{r} (\partial_j s_i) \epsilon_{ijk} \delta_{lk} \]  
(B.8)

\[ = - \mu_B g_c (\epsilon_{jil} \partial_j s_i) \]  
(B.9)

\[ = - \mu_B g_c (\epsilon_{jil} \partial_j s_i). \]  
(B.10)

Here, we denote \( \mathbf{s} = \psi^\dagger \sigma \psi \).

Now we can write down our final result:

\[ j_{\text{spin}} = \mu_B g_c \mathbf{\nabla} \times (\psi^\dagger \sigma \psi). \]  
(B.12)

### B.2 Diamagnetic current

\[ j_{\text{dia}} = - \frac{e^2}{mc} \langle \psi^\dagger_{\nu} (\mathbf{r}) \psi_{\nu} (\mathbf{r}) \rangle \mathbf{A}(\mathbf{r}, \tau). \]  
(B.13)

Expand \( \psi_{\nu} \):

\[ \psi_{\nu}(\mathbf{r}) = \sum_{nk} \phi_{nk\nu}(\mathbf{r}) a_{nk}. \]  
(B.14)

Therefore, we have

\[ j_{\text{dia}} = - \frac{e^2}{mc} \sum_{nk} \phi^*_{nk\nu} \phi_{nk'\nu'} \langle a_{nk\nu'}^\dagger a_{nk'} \rangle \mathbf{A}(\mathbf{r}, \tau) \]  
(B.15)

\[ = - \frac{e^2}{mc} \sum_{nk\nu} |\phi_{nk\nu}|^2 f_{nk} \mathbf{A}(\mathbf{r}, \tau) \]  
(B.16)

\[ = - \frac{e^2}{mc} \sum_{nk\nu} \frac{1}{V} |u_{nk\nu}(\mathbf{r})|^2 f_{nk} \mathbf{A}(\mathbf{r}, \tau). \]  
(B.17)

\( f_{nk} \) is Pauli-Dirac distribution function. Average diamagnetic current over a unit cell:

\[ \bar{j}_{\text{dia}} = - \frac{e^2}{mc} \sum_{nk\nu} \frac{1}{V v_0} \int_{v_0} d\mathbf{p} |u_{nk\nu}(\mathbf{r})|^2 f_{nk} \mathbf{A}(\mathbf{r}, \tau). \]  
(B.18)
Since particle number

\[ N = \int d\mathbf{r} \langle \psi^\dagger \sigma \psi \rangle \]  
\[ = \int d\mathbf{r} \sum_{nk} \frac{|u_{nk}|^2}{V} f_{nk} \]  
\[ = \sum_{nk} \frac{1}{V} \int d\rho |u_{nk}|^2 f_{nk} \]  
\[ = \sum_{nk} \frac{1}{V_0} \int d\rho |u_{nk}|^2 f_{nk}, \]  

We can simplify our final result as

\[ \bar{j}_{dia} = -\frac{e^2}{mc} \frac{N}{V} \cdot \mathbf{A}. \]  

\[ \textbf{B.3 Gradient part of the current} \]

The gradient part of the current has been given by Eq.(B.3):

\[ j_{\text{grad}} = \frac{e\hbar}{2mi}(\psi^\dagger \nabla \psi^\sigma - \nabla \psi^\dagger \sigma \cdot \psi^\sigma). \]  

Obviously, the eigenvalue of \( j_{\text{grad}} \) can be achieved by

\[ \langle j_{\text{grad}}(\mathbf{r}, \tau) \rangle = \frac{e\hbar}{2mi} \lim_{\mathbf{r} \to \mathbf{r}'} \sum_{c} G_{cc'}(\mathbf{r}, \mathbf{r}'; \tau, \tau + \delta), \]

with Green’s function

\[ G_{cc'}(\mathbf{r}, \mathbf{r}'; \tau, \tau') = -\langle T_{\tau} \psi_c(\mathbf{r}, \tau) \psi^\dagger_{c'}(\mathbf{r}', \tau') \rangle. \]  

We need to calculate \( G_{cc'}(\mathbf{r}, \mathbf{r}'; \tau, \tau') \) first.

Hamiltonian as shown is Eq.(B.1) can be written as

\[ H = \int d\mathbf{r} \psi^\dagger_{\sigma} \hat{h}_{\sigma\sigma^\prime} \psi_{\sigma^\prime}, \]

\[ \hat{h} := \hat{h}_0 + \hat{U} = \hat{h}_0 - \frac{e}{2mc} (\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}). \]  

With Matsubara \( \tau = it \), we have

\[ (-\frac{\partial}{\partial \tau} - \hat{h}) G(\mathbf{r}, \mathbf{r}'; \tau, \tau') = \delta(\mathbf{r} - \mathbf{r}') \delta(\tau - \tau'). \]

Also, for free electron,

\[ (-\frac{\partial}{\partial \tau} - \hat{h}_0) G_0 = 1. \]
Therefore we have
\[ (G_0^{-1} - U) G(r, r', \tau, \tau') = \delta(r - r') \delta(\tau - \tau'). \] (B.31)

Expand \( G \) to the first order:
\[ G = G_0 + G_0 U G_0. \] (B.32)

with
\[ G_0 = \sum_{nk} \frac{|nk\rangle \langle nk|}{i\varepsilon - \zeta_{nk}}, \quad \zeta_{nk} := \varepsilon_{nk} - \mu. \] (B.33)

Now we can write
\[ j_{\text{grad}}(r, \tau) = \frac{e}{2mi} \lim_{r' \rightarrow r} \left( \partial_r - \partial_{r'} \right) \int dr_1 d\tau_1 G_{\sigma\sigma'}(r, r_1; \tau, \tau_1) U(r_1, \tau_1) G_{\sigma'\sigma}(r_1, r'; \tau_1, \tau + \delta), \] (B.34)

with
\[ G_{\sigma\sigma'}(r, r' \tau, \tau') = \sum_{nk} \frac{\psi_{nk\sigma'}(r, \tau) \psi_{nk\sigma'}^*(r', \tau')}{i\varepsilon - \zeta_{nk}}, \] (B.35)

and
\[ U = -\frac{e}{2mc}(p \cdot A_\tau + A_\tau \cdot p). \] (B.36)

Fourier Transformation for \( A \):
\[ A_\tau(r) = \frac{1}{V} \sum_{q, \Omega} A_{q, \Omega} e^{iqr - i\Omega\tau}. \] (B.37)

Green’s function only depends on the difference:
\[ G_{\sigma\sigma'}(r, r' \tau, \tau') = \sum_{nk} \frac{\psi_{nk\sigma'}(r) \psi_{nk\sigma'}^*(r')}{i\varepsilon - \zeta_{nk}} e^{-i\varepsilon(\tau - \tau')} \] (B.38)

Taking all these into Eq.(B.34), we can get
\[
\mathbf{j}_{\text{grad}}(\mathbf{r}, \tau) = \frac{e \hbar}{2m_i} \lim_{\tau' \to \tau} (\partial_\tau - \partial_{\tau'}) \sum_{\Omega, \epsilon, n, k} \int d\mathbf{r}_1 d\mathbf{r}_1 T \sum_{\epsilon'} \psi_{\epsilon nk}^* (\mathbf{r}_1) \psi_{\epsilon'n'k'}^* (\mathbf{r}_1) \frac{1}{i \epsilon - \tilde{\epsilon}_{nk}} e^{-i \epsilon (\tau - \tau_1)} \tag{B.39}
\]

\[
\cdot \left[ - \frac{e}{2mc} (\mathbf{p} \cdot \mathbf{A}_\Omega (\mathbf{r}_1) + \mathbf{A}_\Omega (\mathbf{r}_1) \cdot \mathbf{p}) e^{-i \Omega_1 \tau} \right] T \sum_{\epsilon'} \psi_{\epsilon'n'k'}^* (\mathbf{r}_1) \psi_{\epsilon'n'k'}^* (\mathbf{r}) \frac{1}{i \epsilon' - \tilde{\epsilon}_{n'k'}} e^{-i \epsilon' (\tau_1 - \tau - \delta)} \tag{B.40}
\]

\[
\frac{e \hbar}{2m_i} \lim_{\tau' \to \tau} (\partial_\tau - \partial_{\tau'}) \sum_{\Omega, \epsilon, n, k} \int d\mathbf{r}_1 T \sum_{\epsilon} \psi_{\epsilon nk}^* (\mathbf{r}_1) \psi_{\epsilon nk}^* (\mathbf{r}_1) \frac{1}{i \epsilon - \tilde{\epsilon}_{nk}} e^{-i \epsilon \tau} \tag{B.41}
\]

\[
\cdot \left[ - \frac{e}{2mc} (\mathbf{p} \cdot \mathbf{A}_\Omega (\mathbf{r}_1) + \mathbf{A}_\Omega (\mathbf{r}_1) \cdot \mathbf{p}) \right] T \sum_{\epsilon'} \psi_{\epsilon'n'k'}^* (\mathbf{r}_1) \psi_{\epsilon'n'k'}^* (\mathbf{r}) \frac{1}{i \epsilon' - \tilde{\epsilon}_{n'k'}} e^{i \epsilon' (\tau + \delta) \frac{1}{T} \delta_{\epsilon - \Omega - \epsilon', 0}} \tag{B.42}
\]

\[
\frac{e \hbar}{2m_i} \lim_{\tau' \to \tau} (\partial_\tau - \partial_{\tau'}) \sum_{\Omega, \epsilon, n, k} \int d\mathbf{r}_1 T \sum_{\epsilon} \psi_{\epsilon nk}^* (\mathbf{r}_1) \psi_{\epsilon nk}^* (\mathbf{r}_1) \frac{1}{i \epsilon - \tilde{\epsilon}_{nk}} e^{-i \epsilon \tau} \tag{B.43}
\]

\[
\cdot \left[ - \frac{e}{2mc} (\mathbf{p} \cdot \mathbf{A}_\Omega (\mathbf{r}_1) + \mathbf{A}_\Omega (\mathbf{r}_1) \cdot \mathbf{p}) \right] \frac{i \psi_{\epsilon'n'k'}^* (\mathbf{r}_1) \psi_{\epsilon'n'k'}^* (\mathbf{r})}{i (\epsilon - \Omega) - \tilde{\epsilon}_{n'k'}} e^{i (\epsilon - \Omega) (\tau + \delta)} \tag{B.44}
\]

\[
\frac{e \hbar}{2m_i} \lim_{\tau' \to \tau} (\partial_\tau - \partial_{\tau'}) \sum_{\Omega, \epsilon, n, k} \int d\mathbf{r}_1 T \sum_{\epsilon} \psi_{\epsilon nk}^* (\mathbf{r}_1) \psi_{\epsilon nk}^* (\mathbf{r}_1) \frac{1}{i \epsilon - \tilde{\epsilon}_{nk}} e^{-i \epsilon \tau} \tag{B.45}
\]

\[
\cdot \left[ - \frac{e}{2mc} (\mathbf{p} \cdot \mathbf{A}_\Omega (\mathbf{r}_1) + \mathbf{A}_\Omega (\mathbf{r}_1) \cdot \mathbf{p}) \right] \frac{i \psi_{\epsilon'n'k'}^* (\mathbf{r}_1) \psi_{\epsilon'n'k'}^* (\mathbf{r})}{i (\epsilon - \Omega) - \tilde{\epsilon}_{n'k'}} e^{-i \Omega \tau} \tag{B.46}
\]

\[
= \sum_{\Omega} \mathbf{j}_\Omega (\mathbf{r}) e^{-i \Omega \tau}. \tag{B.47}
\]

Since

\[
T \cdot \sum_{\epsilon} \frac{1}{i \epsilon - \tilde{\epsilon}_{nk}} \cdot \frac{1}{i (\epsilon - \Omega) - \tilde{\epsilon}_{nk}} = \frac{f_{n'k'} - f_{nk}}{i \Omega + \tilde{\epsilon}_{n'k'} - \tilde{\epsilon}_{nk}}, \tag{B.48}
\]
\[ j(t) = \sum_{\sigma, n, k, \sigma', n', k'} \frac{f_{n'k'} - f_{nk}}{i\Omega + \tilde{\xi}_{n'k'} - \tilde{\xi}_{nk}} \frac{e\hbar}{2m^*} \lim_{\delta r \to 0} (\partial_{\delta r} - \partial_{\delta r'}) \int dr_1 \psi_{nk}\psi_{nk'}^\ast (r_1) \]  
(B.49)

\[
\begin{align*}
\partial_t \psi_{nk}\psi_{nk'}^\ast (r_1) & \left( \frac{\hbar}{i} \partial_{\delta r} - \frac{\hbar}{i} \partial_{\delta r'} \right) \psi_{nk'}(r_1) + A_{Q}(r_1) \cdot \frac{\hbar}{i} \partial_{\delta r} \psi_{nk'}(r_1) \\
& - \psi_{nk}\psi_{nk'}^\ast (r_1) \left( \frac{\hbar}{i} \partial_{\delta r} + \frac{\hbar}{i} \partial_{\delta r'} \right) \psi_{nk'}(r_1) \\
& = - \frac{e^2}{4m^2 eV} \sum_{\sigma, n, k, \sigma', n', k'} \frac{f_{n'k'} - f_{nk}}{i\Omega + \tilde{\xi}_{n'k'} - \tilde{\xi}_{nk}} \int dr_1 \\
& \left( \psi_{nk}\psi_{nk'}^\ast (r_1) \left[ A_{Q}(r_1) e^{i\mathbf{q} \cdot \mathbf{r}_1} \left( \frac{2\hbar}{i} \partial_{\delta r} + \hbar \mathbf{q} \right) \psi_{nk'}(r_1) - \frac{\hbar}{i} \partial_{\delta r} \psi_{nk'}(r_1) \right] \\
& - \psi_{nk}(r_1) e^{i\mathbf{q} \cdot \mathbf{r}_1} \left( \frac{2\hbar}{i} \partial_{\delta r} + \hbar \mathbf{q} \right) \psi_{nk'}(r_1) \right) \\
& = - \frac{e^2}{4m^2 eV^2} \sum_{\sigma, n, k, \sigma', n', k'} \frac{f_{n'k'} - f_{nk}}{i\Omega + \tilde{\xi}_{n'k'} - \tilde{\xi}_{nk}} \int dr_1 e^{i(\mathbf{k} - \mathbf{k'}) \cdot \mathbf{r}_1} \\
& \left( \psi_{nk}\psi_{nk'}^\ast (r_1) \left[ u_{nk}\psi_{nk'}(r_1) \left( \frac{2\hbar}{i} \partial_{\delta r} + 2\hbar \mathbf{k} + \hbar \mathbf{q} \right) u_{nk'}(r_1) \right] \\
& - \psi_{nk}(r_1) \left( \frac{2\hbar}{i} \partial_{\delta r} + 2\hbar \mathbf{k} + \hbar \mathbf{q} \right) u_{nk'}(r_1) \right)
\end{align*}
\]  
(B.50)

Here we used Bloch wave function

\[ \psi_{nk}(r) = \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{r}} u_{nk}(r). \]  
(B.64)

Since \( u_{nk}(r) \) is a periodic function:

\[ u_{nk}(r) = u_{nk}(r + \mathbf{R}). \]  
(B.65)
\[ \int_{-\infty}^{\infty} dr_1 e^{i(q-k+k') \cdot r_1} u^*_n(k,k') (r_1) (2\frac{\hbar}{i}\partial_{r_1} + 2\hbar k' + \hbar q) u_{n'}(k',r_1) \] (B.66)

\[ = \int_{-\infty}^{\infty} dr_1 e^{i(q-k+k') \cdot (r_1+R)} u^*_n(k,k') (r_1+R) (2\frac{\hbar}{i}\partial_{r_1} + 2\hbar k' + \hbar q) u_{n'}(k',r_1+R) \] (B.67)

\[ = \int_{-\infty}^{\infty} dr_1 e^{i(q-k+k') \cdot (r_1+R)} u^*_n(k,k') (r_1) (2\frac{\hbar}{i}\partial_{r_1} + 2\hbar k' + \hbar q) u_{n'}(k',r_1) \] (B.68)

We have

\[ (q - k + k') \cdot R = 2\pi n, \quad n = 0, \pm 1, \pm 2, \ldots \] (B.69)

As all these vectors \( q, k, k' \) are within Brillouin Zone, our \((q - k + k') \cdot R\) can only take the value \( 0, \pm 2\pi n \). But we are concerned with the \( q \to 0 \) result at last. When \( q \to 0 \), \((q - k + k') \cdot R\) can only take the value 0. Therefore, we neglect \( \pm 2\pi n \) terms in our calculation. However, as a reminder, if we want to get \( \sigma(q, \omega) \) for a larger \( q \), we should include \( \pm 2\pi n \) terms.

\[ \int_{-\infty}^{\infty} dr_1 e^{i(q-k+k') \cdot r_1} u^*_n(k,k') (r_1) (2\frac{\hbar}{i}\partial_{r_1} + 2\hbar k' + \hbar q) u_{n'}(k',r_1) \] (B.70)

\[ = \sum_R \int_{r_0} dr \ u^*_n(k,k') (r) (2\frac{\hbar}{i}\partial_{r} + 2\hbar k' + \hbar q) u_{n'}(k',r) \delta_{q-k+k',0} \] (B.71)

\[ = N \langle u_{n'k'} | (2\frac{\hbar}{i}\partial_{r} + 2\hbar k' + \hbar q) | u_{n'k'} \rangle \delta_{q-k+k',0} \] (B.72)

Therefore, we can get our \( j_\Omega(r) \) simplified as

\[ j_\Omega(r) = - \frac{e^2 N}{4m^2 c V^2} \sum_{q',e,k} \int_{n,n'} \frac{f_{n'k} - f_{nk}}{i\Omega + \xi_{n'(k-q')} - \xi_{nk}} \{ \psi^*_n(k,q) \psi_{n'(k,q')} (r) \} \frac{\hbar}{i} \partial_{r} \psi_{nk'} (r) \] (B.73)

\[ - \psi_{nk'} (r) \frac{\hbar}{i} \partial_{r} \psi^*_n(k,q)(r) \} [\langle u_{nk} | (2\frac{\hbar}{i}\partial_{r} + 2\hbar k - \hbar q) | u_{n'(k-q)} \rangle \cdot A_{q',\Omega} \] (B.74)

\[ = - \frac{e^2 N}{4m^2 c V^2} \sum_{q',e,k} \int_{n,n'} \frac{f_{n'k} - f_{nk}}{i\Omega + \xi_{n'(k-q')} - \xi_{nk}} \{ e^{iq'r} u^*_n(k,q) (\hbar k + \frac{\hbar}{i} \partial_{r}) u_{nk'} (r) \} \] (B.75)

\[ = - \frac{e^2 N}{4m^2 c V^2} \sum_{q',e,k} \int_{n,n'} \frac{f_{n'k} - f_{nk}}{i\Omega + \xi_{n'(k-q')} - \xi_{nk}} \{ e^{iq'r} u^*_n(k,q) (\hbar k + \frac{\hbar}{i} \partial_{r}) u_{nk'} (r) \} \] (B.76)

\[ = - \frac{e^2 N}{4m^2 c V^2} \sum_{q',e,k} \int_{n,n'} \frac{f_{n'k} - f_{nk}}{i\Omega + \xi_{n'(k-q')} - \xi_{nk}} \{ e^{iq'r} u^*_n(k,q) (\hbar k + \frac{\hbar}{i} \partial_{r}) u_{nk'} (r) \} \] (B.77)

\[ - u_{nk'} (r) (\hbar (q - k) + \frac{\hbar}{i} \partial_{r}) u^*_n(k,q) (r) \} [\langle u_{nk} | (2\frac{\hbar}{i}\partial_{r} + 2\hbar k - \hbar q) | u_{n'(k-q)} \rangle \cdot A_{q',\Omega} \] (B.78)

Do Fourier Transformation

\[ j_\Omega(q) = \int d\mathbf{r} j_\Omega(r) e^{-iqr}. \] (B.79)
First, let us do partial integral to simplify it a little bit:

\[
\int d\boldsymbol{r}e^{i\mathbf{q} \cdot \mathbf{r}} \{ u_{n'}^{*}(\mathbf{k-q}')_{c}(\mathbf{r})(\hbar \mathbf{k} + \frac{\hbar}{i} \partial_{\mathbf{r}})u_{nk\mathbf{r}}(\mathbf{r}) - u_{nk\mathbf{r}}(\mathbf{r})(\hbar (\mathbf{q-k}) + \frac{\hbar}{i} \partial_{\mathbf{r}})u_{n'}^{*}(\mathbf{k-q}')_{c}(\mathbf{r}) \} = \int d\boldsymbol{r}e^{i\mathbf{q} \cdot \mathbf{r}} \{ u_{n'}^{*}(\mathbf{k-q}')_{c}(\mathbf{r})(\hbar \mathbf{k} + \frac{\hbar}{i} \partial_{\mathbf{r}})u_{nk\mathbf{r}}(\mathbf{r}) - u_{nk\mathbf{r}}(\mathbf{r})(\hbar (\mathbf{q-k}) + \frac{\hbar}{i} \partial_{\mathbf{r}})u_{n'}^{*}(\mathbf{k-q}')_{c}(\mathbf{r}) \}
\]

(B.80)

(B.81)

(B.82)

Same analysis process as what we did from Eq.(B.69) to Eq.(B.72) give us similar result

\[
\int d\boldsymbol{r}e^{i\mathbf{q} \cdot \mathbf{r}} u_{n'}^{*}(\mathbf{k-q}')_{c}(\mathbf{r})(2\hbar \mathbf{k} - \hbar \mathbf{q} + 2\frac{\hbar}{i} \partial_{\mathbf{r}})u_{nk\mathbf{r}}(\mathbf{r})
\]

(B.83)

(B.84)

Substitute it into Eq.(B.78) and Eq.(B.79), we get

\[
\hat{j}_{\Omega}(\mathbf{q}) = -\frac{e^{2}N^{2}}{4m^{2}c^{3}} \sum_{k,n,n'} i\Omega + \tilde{\xi}_{n}(\mathbf{k-q}) - \tilde{\xi}_{nk} \langle u_{n'}^{*}(\mathbf{k-q}) | (2\frac{\hbar}{i} \partial_{\mathbf{r}} + 2\hbar \mathbf{k} - \hbar \mathbf{q}) | u_{nk} \rangle \]

(B.85)

(B.86)

\begin{align*}
\langle u_{nk} | (2\frac{\hbar}{i} \partial_{\mathbf{r}} + 2\hbar \mathbf{k} - \hbar \mathbf{q}) | u_{n'}^{*}(\mathbf{k-q}) \rangle \cdot \mathbf{A}_{\mathbf{q},\Omega}
\end{align*}

B.4 Prove that \( \hat{j}_{\text{grad}}(\Omega \rightarrow 0, \mathbf{q} \rightarrow 0) + \hat{j}_{\text{dia}} = 0. \)

Denote Eq.(B.1) as

\[
\hat{H} = \int d\mathbf{r} \psi_{\mathbf{r}}^\dagger \hat{h}_{\mathbf{r}} \psi_{\mathbf{r}}
\]

(B.87)

\[
\hat{h} = \frac{(\mathbf{p} - \frac{e}{c}\mathbf{A})^{2}}{2m} + \lambda \mathbf{r} \cdot \mathbf{E} + (\mathbf{p} - \frac{e}{c}\mathbf{A}) + U(\mathbf{r}) - g_{\mu} \mathbf{B} \cdot \mathbf{r}.
\]

(B.88)

\(\hat{h}\) have eigenstate \( \psi_{nk\mathbf{r}}(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{V}}} e^{ik\mathbf{r} \cdot \mathbf{r}} u_{nk\mathbf{r}}(\mathbf{r}) \), with corresponding eigenvalue as \( \epsilon_{nk} \):

\[
\hat{h}_{\mathbf{r}} | u_{nk} \rangle = \epsilon_{nk} | u_{nk} \rangle.
\]

(B.89)

Now we neglect the spin-orbit interaction as what we did before. We want to prove that when \( \Omega \rightarrow 0, \mathbf{q} \rightarrow 0 \), the gradient part of the current density

\[
\hat{j}_{\text{grad}}^{i}(\Omega, \mathbf{q}) = -\frac{e^{2}N^{2}}{4m^{2}c^{3}} \sum_{k,n,n'} i\Omega + \tilde{\xi}_{n}(\mathbf{k-q}) - \tilde{\xi}_{nk} \langle u_{n'}^{*}(\mathbf{k-q}) | (2\hbar \hat{p}^{j} + 2\hbar \mathbf{k}^{j} - \hbar \mathbf{q}^{j}) | u_{nk} \rangle \]

(B.91)

\[
\langle u_{nk} | (2\hbar \hat{p}^{j} + 2\hbar \mathbf{k}^{j} - \hbar \mathbf{q}^{j}) | u_{n'}^{*}(\mathbf{k-q}) \rangle \mathbf{A}_{\mathbf{q},\Omega}
\]

cancels diamagnetic current density

\[
\hat{j}_{\text{dia}}^{i}(\Omega, \mathbf{q}) = -\frac{e^{2}}{mc} N A_{\mathbf{q},\Omega}^{i}.
\]

(B.92)
Write

\[ j^i_{q\Omega} = Q^{ij}_{q\Omega} A^j_{q\Omega} \]  \hspace{1cm} (B.93)

Now we try to prove that these two \( Q \)s are same with opposite sign.

**B.4.1 Diagonal contribution \( n = n' \) (intraband)**

From Eq. (B.91), we have our intraband

\[
\lim_{\Omega \to 0} Q^{ij}_{q\Omega} = - \frac{e^2 N^2}{4m^2 c V^3} \sum_{k,n} \left( \frac{\partial f_{nk}}{\partial \xi_{nk}} \right) \cdot q \langle u_{nk} | \left( 2 \hbar \hat{p}^i + 2 \hbar k^i \right) | u_{nk} \rangle \langle u_{nk} | \left( 2 \hbar \hat{p}^j + 2 \hbar k^j \right) | u_{nk} \rangle. \]  \hspace{1cm} (B.94)

Here

\[ f_{nk} = f_{th}(\xi_{nk}), \]  \hspace{1cm} (B.95)

\( f_{th} \) is the thermal distribution function.

\[
\frac{\partial f_{nk}}{\partial k} = \frac{\partial f_{th}(\xi_{nk})}{\partial \xi_{nk}} \cdot \frac{\partial \xi_{nk}}{\partial k}. \]  \hspace{1cm} (B.96)

Therefore, we have

\[
\lim_{\Omega \to 0} Q^{ij}_{q\Omega} = - \frac{e^2 N^2}{4m^2 c V^3} \sum_{k,n} \left( \frac{\partial f_{th}(\xi_{nk})}{\partial \xi_{nk}} \right) \cdot \frac{\partial \xi_{nk}}{\partial k} \cdot q \langle u_{nk} | \left( 2 \hbar \hat{p}^i + 2 \hbar k^i \right) | u_{nk} \rangle \langle u_{nk} | \left( 2 \hbar \hat{p}^j + 2 \hbar k^j \right) | u_{nk} \rangle. \]  \hspace{1cm} (B.97)

Take the derivative of \( k \) to each side of Eq. (B.89):

\[
\partial_k h_k | u_{nk} \rangle + \hat{h}_k \partial_k | u_{nk} \rangle = \partial_k \varepsilon_{nk} | u_{nk} \rangle + \varepsilon_{nk} \partial_k | u_{nk} \rangle. \]  \hspace{1cm} (B.98)

Applying \( \langle u_{nk} | \) to the left side, we get

\[
\langle u_{nk} | \partial_k h_k | u_{nk} \rangle = \partial_k \varepsilon_{nk} \langle u_{nk} | u_{nk} \rangle = \frac{V}{N} \partial_k \varepsilon_{nk} = \frac{V}{N} \partial_k \xi_{nk}. \]  \hspace{1cm} (B.99)

From Eq. (B.88), we see that, up to the lowest order

\[
\partial_k h_k \approx \frac{\hbar \hat{p} + \hbar k}{m}. \]  \hspace{1cm} (B.100)

Substitute it back to Eq. (B.97), we have

\[
\lim_{\Omega \to 0} Q^{ij}_{q\Omega} = - \frac{e^2}{c V} \sum_{k,n} \frac{\partial f_{th}(\xi_{nk})}{\partial \xi_{nk}} \frac{\partial \xi_{nk}}{\partial k_i} \frac{\partial \xi_{nk}}{\partial k_j} \]  \hspace{1cm} (B.101)

\[
= \frac{e^2}{c V} \sum_{k,n} \frac{\partial^2 \xi_{nk}}{\partial k_i \partial k_j} f_{th}(\xi_{nk}). \]  \hspace{1cm} (B.102)
By taking a second derivative to Eq.(B.89) \( \partial_k \partial_j \langle \hat{h}_k | u_{nk} \rangle = \epsilon_{nk} | u_{nk} \rangle \), we get

\[
\partial_k \left( \frac{\hat{p}_j + k_j}{m} | u_{nk} \rangle + \hat{h}_k \partial_j | u_{nk} \rangle \right) = \partial_k \left( \partial_k \epsilon_{nk} | u_{nk} \rangle + \epsilon_{nk} \partial_j | u_{nk} \rangle \right). 
\]

(B.103)

\[
\Rightarrow \quad \frac{\hat{p}_j + k_j}{m} \partial_k | u_{nk} \rangle + \frac{1}{m} \delta_{ij} | u_{nk} \rangle + \frac{\hat{p}_i + k_i}{m} \partial_j \langle \hat{h}_k | u_{nk} \rangle + \hat{h}_k \partial_i, \partial_j | u_{nk} \rangle 
\]

(B.104)

\[
= \partial_k \partial_j \epsilon_{nk} | u_{nk} \rangle + \partial_k \epsilon_{nk} \partial_j | u_{nk} \rangle + \partial_k \epsilon_{nk} \partial_k | u_{nk} \rangle + \epsilon_{nk} \partial_k \partial_j | u_{nk} \rangle.
\]

(B.105)

applying \( \langle u_{nk} \rangle \) to the left, we have

\[
\frac{\partial^2 \epsilon_{nk}}{\partial k \partial j} = \frac{1}{m} \delta_{ij} + \frac{1}{v_0} \langle u_{nk} \rangle |(\frac{\hat{p}_j + k_j}{m} - \partial_k \epsilon_{nk})\partial_j | u_{nk} \rangle + \frac{1}{v_0} \langle u_{nk} \rangle |(\frac{\hat{p}_i + k_i}{m} - \partial_k \epsilon_{nk})\partial_k | u_{nk} \rangle.
\]

(B.106)

Finally, we get the intraband contribution:

\[
\lim_{\Omega \to 0} Q_{ij}^{\text{intr}} = \frac{e^2}{c V} \sum_{k,n} f_{\text{th}}(\xi_{nk}) \frac{\delta_{ij}}{m} + \frac{1}{v_0} \langle u_{nk} \rangle |(\frac{\hat{p}_j + k_j}{m} - \partial_k \epsilon_{nk})\partial_j | u_{nk} \rangle 
\]

(B.107)

\[
+ \frac{1}{v_0} \langle u_{nk} \rangle |(\frac{\hat{p}_i + k_i}{m} - \partial_k \epsilon_{nk})\partial_j | u_{nk} \rangle \}
\]

(B.108)

\[
= \frac{e^2 N}{m c V} \delta_{ij} + \frac{e^2}{c V v_0} \sum_{k,n} f_{\text{th}}(\xi_{nk}) \langle u_{nk} \rangle |(\frac{\hat{p}_j + k_j}{m} - \partial_k \epsilon_{nk})\partial_j | u_{nk} \rangle
\]

(B.109)

\[
+ \frac{e^2}{c V v_0} \sum_{k,n} f_{\text{th}}(\xi_{nk}) \langle u_{nk} \rangle |(\frac{\hat{p}_i + k_i}{m} - \partial_k \epsilon_{nk})\partial_j | u_{nk} \rangle.
\]

(B.110)

### B.4.2 Off-diagonal contribution \( n \neq n' \) (interband)

From Eq.(B.91), we have the interband

\[
\lim_{\Omega \to 0} Q_{ij}^{\text{inter}} = -\frac{e^2 N^2}{4 m^2 c V^3} \sum_{k,n \neq n'} f_{n''k} - f_{n'k} \langle u_{n'k} | (2 \hbar \hat{p}^j + 2 \hbar k^j) | u_{nk} \rangle \langle u_{nk} | (2 \hbar \hat{p}^j + 2 \hbar k^j) | u_{n'k} \rangle.
\]

(B.111)

In order to get \( \langle u_{n'k} | (2 \hbar \hat{p}^j + 2 \hbar k^j) | u_{nk} \rangle \), we left multiply \( \langle u_{n'k} \rangle \) to Eq.(B.98):

\[
\langle u_{n'k} | \partial_k \hat{h}_k | u_{nk} \rangle + \epsilon_{n',k} \langle u_{n'k} | \partial_k | u_{nk} \rangle = \partial_k \epsilon_{nk} \langle u_{n'k} | u_{nk} \rangle + \epsilon_{nk} \langle u_{n'k} | \partial_k | u_{nk} \rangle.
\]

(B.112)

\[
\Rightarrow \quad \langle u_{n'k} | \partial_k \hat{h}_k | u_{nk} \rangle = \langle u_{n'k} | \frac{\hbar \hat{p}^j + \hbar k^j}{m} | u_{nk} \rangle = (\xi_{nk} - \xi_{n',k}) \langle u_{n'k} | \partial_k | u_{nk} \rangle.
\]

(B.113)

Substituting it to Eq.(B.111), we get

\[
\lim_{\Omega \to 0} Q_{ij}^{\text{inter}} = \frac{e^2 N^2}{c V^3} \sum_{k,n \neq n'} \frac{f_{n''k} - f_{n'k}}{\xi_{n''k} - \xi_{n'k}} (\xi_{n''k} - \xi_{n'k})^2 \langle u_{n'k} | \partial_k | u_{nk} \rangle \langle u_{nk} | \partial_k | u_{n'k} \rangle
\]

(B.114)

\[
= \frac{e^2 N^2}{c V^3} \sum_{k,n,n'} (f_{n''k} - f_{n'k})(\xi_{n''k} - \xi_{n'k}) \langle u_{n'k} | \partial_k | u_{nk} \rangle \langle u_{nk} | \partial_k | u_{n'k} \rangle
\]

(B.115)
B.4.3 Total contribution

By combining the interband and intraband result we get in section 4.1 and section 4.2, we get the \( Q(\Omega \to 0, q \to 0) \) of gradient part of the current

\[
\lim_{\Omega \to 0} \lim_{q \to 0} Q_{ij}^{\Omega} = \frac{e^2 N}{m c V} \delta_{ij} + \frac{e^2}{c V v_0} \sum_{k,n} f_{nk} \langle u_{nk} \vert (\hat{p}_j + k_j) - \partial_{k_j} \epsilon \rangle \partial_{k_j} \vert u_{nk} \rangle
\]

\[+ \frac{e^2}{c V v_0} \sum_{k,n} f_{nk} \langle u_{nk} \vert (\hat{p}_j + k_j) - \partial_{k_j} \epsilon \rangle \frac{\langle u_{nk} \vert u_{nk} \rangle}{v_0} \partial_{k_j} \vert u_{nk} \rangle \]

\[= \frac{e^2 N}{m c V} \delta_{ij} + \frac{e^2}{c V v_0} \sum_{k,n} f_{nk} \langle u_{nk} \vert (\hat{p}_j + k_j) \partial_{k_j} \vert u_{nk} \rangle \]

\[+ \frac{e^2}{c V v_0} \sum_{k,n} f_{nk} \langle u_{nk} \vert (\hat{p}_j + k_j) \partial_{k_j} \vert u_{nk} \rangle \]

\[= \frac{e^2 N}{m c V} \delta_{ij} + \frac{e^2}{c V v_0} \sum_{k,n} f_{nk} \langle u_{nk} \vert (\hat{p}_j + k_j) \partial_{k_j} \vert u_{nk} \rangle \]

\[+ \frac{e^2}{c V v_0} \sum_{k,n} f_{nk} \langle u_{nk} \vert (\hat{p}_j + k_j) \partial_{k_j} \vert u_{nk} \rangle \]

\[= \frac{e^2 N}{m c V} \delta_{ij} + \frac{e^2}{c V v_0} \sum_{k,n} f_{nk} \langle u_{nk} \vert (\hat{p}_j + k_j) \partial_{k_j} \vert u_{nk} \rangle \]

\[+ \frac{e^2}{c V v_0} \sum_{k,n} f_{nk} \langle u_{nk} \vert (\hat{p}_j + k_j) \partial_{k_j} \vert u_{nk} \rangle \]

\[= \frac{e^2 N}{m c V} \delta_{ij}
\]

Finally, we reach the result

\[
j_{\text{grad}}^i(\Omega \to 0, q \to 0) = \frac{e^2 N}{m c V} \delta_{ij} A^i_{\Omega, q} = \frac{e^2 N}{m c V} A^i_{\Omega, q}.
\]

Obviously, it cancels the diamagnet current

\[
\jmath^i_{\text{dia}}(\Omega, q) = -\frac{e^2 N}{m c V} A^i_{\Omega, q}
\]

with \( \Omega \to 0, q \to 0 \). We have no net current when \( \Omega \to 0, q \to 0 \). QED.
B.5 Conclusion

A general Hamiltonian

\[
H = \int dr \, \psi^\dagger (p - eA/c)^2/2m + \lambda \sigma \cdot E \times (p - eA) + U(r) - g\mu B \cdot \sigma \psi^\dagger \psi.
\]  

(B.131)

give a current containing three part

\[
j = j_{\text{grad}} + j_{\text{dia}} + j_s.
\]  

(B.132)

Magnetic current from spin density is

\[
j_{\text{spin}} = \mu_B g c \vec{\nabla} \times (\psi^\dagger \sigma \psi).
\]  

(B.133)

Diamagnetic current

\[
j_{\text{dia}} = -\frac{e^2}{mc} \langle \psi^\dagger(r) \psi^\dagger(r) \rangle A(r, \tau).
\]  

(B.134)

Averaging over a unit cell, the diamagnetic current become

\[
\bar{j}_{\text{dia}} = -\frac{e^2}{mc} \frac{N}{V} \cdot A.
\]  

(B.135)

Gradient part of the current with the form

\[
j_{\text{grad}} = \frac{e\hbar}{2mi} (\psi^\dagger \nabla \psi^\dagger - \nabla \psi^\dagger \cdot \psi^\dagger)
\]  

(B.136)

result in

\[
j_{\text{grad}}(\Omega, q) = -\frac{e^2 N^2}{4m^2 c^2 V^3} \sum_{k,\eta, n} \frac{f_n'(k-q) - f_{nk}}{i\Omega + \zeta_n'(k-q) - \zeta_{nk}} \langle u_n'(k-q) | (2\hbar \frac{\partial}{\partial r} + 2\hbar k - hq) | u_{nk} \rangle
\]  

\[
\langle u_{nk} | (2\hbar \frac{\partial}{\partial r} + 2\hbar k - hq) | u_{n'(k-q)} \rangle \cdot A_{q,\Omega}.
\]  

(B.137)

We have proven that, ignoring the current from spin density, the net current vanish when \( \Omega \to 0, q \to 0 \).
APPENDIX C

DETAILED DERIVATION OF OPTICAL CONDUCTIVITY IN TIGHT BINDING MODEL

For Tight Binding model, the Hamiltonian on the presence of $A$ should be written as

$$H = \sum_{ij} h_{ij}^{\alpha\beta} \epsilon_r \int_a^b dr \, A(r) \, \hat{a}_i^{\alpha} \hat{a}_j^{\beta}. \quad (C.1)$$

After some careful calculation we can get

$$j = j_{\text{grad}} + j_{\text{dia}}, \quad (C.2)$$

$$j_{\text{grad}} = \frac{e}{\hbar} \sum_k \hat{a}_k^{\alpha} \partial_k h_{ij}^{\alpha\beta} \hat{a}_{k+\frac{q}{2}, \beta}, \quad (C.3)$$

$$j_{\text{dia}} = -\frac{e^2}{\hbar^2 c} \sum_k \hat{a}_k^{\alpha} \partial_k (A \partial_k h_{ij}^{\alpha\beta}) \hat{a}_{k+\frac{q}{2}, \beta}. \quad (C.4)$$

Write $j(k, \omega) = Q_{ij}(k, \omega) A_j(k, \omega)$, we can calculate the response kernel. With the help of Green’s Function, we can get the result for gradient part of current density (in Matsubara representation):

$$Q_{ij}(q, \Omega) = -\frac{e^2}{\hbar^2 c} \sum_{m,k} \text{Tr} \left[ \frac{\partial h}{\partial k_i} G^M(k+q/2, \epsilon_m + \Omega) \frac{\partial h}{\partial k_j} G^M(k-q/2, \epsilon_m) \right], \quad (C.5)$$

$$= -\frac{e^2}{\hbar^2 c} \sum_{k,n,n'} \frac{f_{n', k-q/2} - f_{n, k+q/2}}{i\Omega + \delta_{n', k-q/2} - \delta_{n, k+q/2}} \langle n', k - \frac{q}{2} | \frac{\partial h}{\partial k_i} | n, k + \frac{q}{2} \rangle \langle n, k + \frac{q}{2} | \frac{\partial h}{\partial k_j} | n', k - \frac{q}{2} \rangle. \quad (C.6)$$

Detailed calculation has been attached below.

C.1 The expression of the current density

The Hamiltonian for tight binding model can be written as

$$H = \sum_{ij} h_{ij}^{\alpha\beta} (A) a_i^{\alpha} a_j^{\beta}, \quad (C.7)$$
where
\[ h_{ij}^{\alpha\beta}(A) = h_{ij}^{\alpha\beta} e^{ie \int_{A}^{R} drA(r)} \] (C.8)
\[ \approx h_{ij}^{\alpha\beta}(R_i - R_j) [1 + \frac{ie}{\hbar c} (R_i - R_j) A(\frac{R_i + R_j}{2})]. \] (C.9)

Do Fourier transformation
\[ h_{k}^{\alpha\beta}(A) = \sum_{R} e^{-ik \cdot R} h_{ij}^{\alpha\beta}(R_i - R_j) [1 + \frac{ie}{\hbar c} (R_i - R_j) A(\frac{R_i + R_j}{2})] \] (C.10)
\[ = h_{ij}^{\alpha\beta}(k) + \frac{ie}{\hbar c} \sum_{R} e^{-ik \cdot R} (R \cdot A) h_{ij}^{\alpha\beta}(R) \] (C.11)
\[ = h_{ij}^{\alpha\beta}(k) + \frac{ie}{\hbar c} \sum_{R} -\frac{1}{i} A \cdot (\partial_k e^{-ik \cdot R}) h_{ij}^{\alpha\beta}(R) \] (C.12)
\[ = h_{ij}^{\alpha\beta}(k) - \frac{e}{\hbar c} A \cdot \partial_k h_{ij}^{\alpha\beta}. \] (C.13)

Now we need to calculate the current density. We are going to use the continuity equation
\[ \dot{\rho} + i q \cdot j = 0 \]
(remember \( \rho_i = e a_i a_{i+} \)) to reach \( j \).

Fourier transformation can give us
\[ H = \sum_{ij} h_{ij}^{\alpha\beta} a_{i+}^{\dagger} a_{j-} = \sum_{k} h_{ij}^{\alpha\beta}(k) a_{k+}^{\dagger} a_{k-}, \quad \rho_q = e \sum_{k} a_{k+}^{\dagger} a_{k+q,\alpha}. \] (C.14)

Therefore,
\[ -i q \cdot j = \dot{\rho} + i q \cdot j = \frac{ie}{\hbar} \sum_{k,p} [a_{k+}^{\dagger} h_k a_k, a_{p+q}^{\dagger} a_{p+q}] \] (C.15)
\[ = \frac{ie}{\hbar} \sum_{k,p} [a_{k+}^{\dagger} h_k a_k, a_{p+q}^{\dagger} a_{p+q}] + [a_{k+}^{\dagger} h_k, a_{p+q}^{\dagger} a_{p+q}] a_k \] (C.16)
\[ = \frac{ie}{\hbar} \sum_{k,p} a_{k+}^{\dagger} h_k a_{k+q} - a_{k+}^{\dagger} h_k a_{k+q} \] (C.17)
\[ = \frac{ie}{\hbar} \sum_{k,p} a_{k+}^{\dagger} (h_k - h_{k+q}) a_{k+q} \] (C.18)

For small \( q \)’s we get
\[ j_{grad} = \frac{e}{\hbar} \sum_{k} a_{k+q/2,\alpha}^{\dagger} \partial_k h_{ij}^{\alpha\beta}(A) a_{k+q/2,\beta}, \] (C.19)

and \( h_{k}^{\alpha\beta}(A) \) is given by Eq.(C.13). Therefore, we reach our final result.
\[ j = j_{\text{grad}} + j_{\text{dia}}, \]  
\[ j_{\text{grad}} = \frac{e}{\hbar} \sum_k a_k^{\dagger} d_{k-q/2,a}^{\beta} a_{k+q/2,\beta}, \]  
\[ j_{\text{dia}} = -\frac{e^2}{\hbar^2 c} \sum_k a_k^{\dagger} d_{k-q/2,a} (A_k d_k^{\alpha \beta}) a_{k+q/2,\beta}. \]

### C.2 Calculation of the response kernel

#### C.2.1 linear response

\[ \hat{H} = \hat{H}_0 + \delta \hat{H}, \quad \delta \hat{H} = -\frac{1}{c} \int dr \, j(r) A(r) = -\frac{1}{cV} \sum_q j_q A_q \]  
\[ i \frac{\partial}{\partial t} |\text{En}(t)\rangle = \hat{H} |\text{En}(t)\rangle. \]  

Write the eigenstate \(|\text{En}(t)\rangle\) as the evolution of the state at \(t = 0\), or \(|\text{En}(t)\rangle = e^{-i\hat{H}_0 t} \hat{U}(t)|\text{En}\rangle\).

Then Eq.(C.24) becomes

\[ i \frac{\partial}{\partial t} |\text{En}(t)\rangle = \hat{H}_0 e^{-i\hat{H}_0 t} \hat{U}(t)|\text{En}\rangle + i e^{-i\hat{H}_0 t} \frac{\partial \hat{U}(t)}{\partial t} |\text{En}\rangle; \]  
\[ = \hat{H}_0 e^{-i\hat{H}_0 t} \hat{U}(t)|\text{En}\rangle + \delta \hat{H} e^{-i\hat{H}_0 t} \hat{U}(t)|\text{En}\rangle. \]  
\[ \Rightarrow i \frac{\partial \hat{U}(t)}{\partial t} |\text{En}\rangle = e^{i\hat{H}_0 t} \delta \hat{H} e^{-i\hat{H}_0 t} \hat{U}(t)|\text{En}\rangle = \delta \hat{H}(t) \hat{U}(t)|\text{En}\rangle. \]  
\[ \Rightarrow \hat{U}(t) = 1 - i \int_{-\infty}^{t} \delta \hat{H}(t') \hat{U}(t') dt'. \]

To the first order of \(\delta \hat{H}\):

\[ \hat{U}(t) = 1 - i \int_{-\infty}^{t} \delta \hat{H}(t') dt'. \]  

Now we can calculate the expectation value of the current density

\[ j(r, t) = \langle \text{En}(t) | \hat{j}(r, t) | \text{En}(t) \rangle = \langle \text{En}(t) | j(r) | \text{En}(t) \rangle - neA(r, t) \]
\[ = \langle \text{En} | (1 + i \int_{-\infty}^{t} \delta \hat{H}(t') dt') e^{i\hat{H}_0 t} j(r) e^{-i\hat{H}_0 t} (1 - i \int_{-\infty}^{t} \delta \hat{H}(t') dt') | \text{En} \rangle - neA(r, t) \]
\[ = \langle \text{En} | j(r) | \text{En} \rangle + i \int_{-\infty}^{t} dt' \langle \text{En} | [\delta \hat{H}(t'), j(r, t)] | \text{En} \rangle - neA(r, t) \]
\[ = i \int_{-\infty}^{t} dt' \langle \text{En} | [\delta \hat{H}(t'), j(r, t)] | \text{En} \rangle - neA(r, t). \]
\[ j_i(r, t) = \int_{-\infty}^{+\infty} dx' \sum_j Q_{ij}(r - x', t - t') A_j(x', t'), \]
\[ Q_{ij}(r - x', t - t') = -i\theta(t - t') \frac{1}{c} \langle \text{En} | [j_i(r, t), j_j(x', t')] | \text{En} \rangle - ne\delta_{ij} \delta(r - x') \delta(t - t'). \]
C.2.2  Do Fourier transformation and Wick’s contraction

\[ j(k, \omega) = \int \! d\tau d^3r \, j(r, \tau) e^{-i k \cdot r + i\omega \tau} \]  (C.36)

\[ = \int \! d\tau dt \int \! d\tau' d^3r \sum_j Q_{ij}(r - r', t - t') A_j(r', t') e^{-i k \cdot r + i\omega \tau} \]  (C.37)

\[ = \int \! d\tau dt \int \! d\tau' d^3r \int \! (dq)d\Omega Q_{ij}(q, \Omega) e^{i q(r - r') - i\Omega(t - t')} \int \! (dq')d\Omega' A_j(q', \Omega') e^{i q' r' - i\Omega' t'} e^{-i k \cdot r + i\omega \tau} \]  (C.38)

\[ = \int \! (dq)d\Omega (dq')d\Omega' \delta_{q,k}\delta_{\omega,\Omega}\delta_{q,q'}\delta_{\Omega',\Omega} Q_{ij}(q, \Omega) A_j(q', \Omega') \]  (C.39)

\[ = Q_{ij}(k, \omega) A_j(k, \omega). \]  (C.40)

Ignore diamagnetic current.

\[ Q_{ij}(k, t - t') = \int \! d\tau d^3r' Q_{ij}(r - r', t - t') e^{-i k \cdot (r' - r)} \]  (C.41)

\[ = \int \! d\tau d\tau' [-i\theta(t - t') \frac{1}{c} \langle En | [j_i(r, t), j_j(r', t')] | En \rangle] e^{-i k \cdot (r' - r)} \]  (C.42)

\[ = \int \! d\tau d\tau' (dq)(dq') [-i\theta(t - t') \frac{1}{c} \langle En | [j_i(q, t), j_j(q', t')] | En \rangle e^{i q \cdot (r' - r')} \]  (C.43)

\[ = \int \! (dq)(dq') [-i\theta(t - t') \frac{1}{c} \langle En | [j_i(q, t), j_j(q', t')] | En \rangle \delta_{q,k}\delta_{q',-k} \]  (C.44)

\[ = -i\theta(t - t') \frac{1}{c} \langle En | [j_i(k, t), j_j(-k, t')] | En \rangle. \]  (C.45)

\[ \Rightarrow \quad Q_{ij}(k, \tau - \tau') = \frac{1}{c} \langle T_r | [j_i(k, \tau), j_j(-k, \tau')] \rangle. \]  (C.46)

Take Eq.(C.3) in to the equation above, and set \( \tau' = 0 \), we can get

\[ Q_{ij}(q, \tau) = \frac{e^2}{\hbar^2 c} \sum_{k, p} \frac{\partial h^{a\beta}}{\partial k_i} \frac{\partial h^{\gamma\delta}}{\partial p_j} \langle T_r | a_{k - q/2, \alpha}^\dagger (\tau) a_{k+q/2, \beta} \rangle. \]  (C.47)

Wick’s contraction gives

\[ Q_{ij}(q, \tau) = -\frac{e^2}{\hbar^2 c} \sum_{k, p} \frac{\partial h^{a\beta}}{\partial k_i} \frac{\partial h^{\gamma\delta}}{\partial p_j} \langle T_r a_{k - q/2, \delta} a_{k+q/2, \gamma} \rangle \langle T_r a_{k+q/2, \beta} \rangle. \]  (C.48)

\[ = -\frac{e^2}{\hbar^2 c} \sum_k \frac{\partial h^{a\beta}}{\partial k_i} \frac{\partial h^{\gamma\delta}}{\partial k_j} G^M_{\alpha\beta}(k - q/2, -\tau) G^M_{\gamma\delta}(k + q/2, \tau). \]  (C.49)

Do Fourier transformation for the response kernel, with \( G^M(p, \tau) = \frac{1}{\beta} \sum_n e^{-i\epsilon_n \tau} G^M(p, \epsilon_n) \), we obtain
\[ Q_{ij}(q, \Omega) = \int d\tau e^{i\Omega\tau} Q_{ij}(q, \tau) \]  
\[ = -\frac{e^2}{\hbar^2 c} \sum_{\mathbf{k}} \frac{\partial h^{\alpha\beta}}{\partial k_i} \frac{\partial h^{\gamma\delta}}{\partial k_j} \int d\tau \frac{1}{\beta^2} \sum_{m,n} e^{i\epsilon_m \tau} G^M_{\delta\alpha}(\mathbf{k} - q/2, \epsilon_m) e^{-i\epsilon_n \tau} G^M_{\beta\gamma}(\mathbf{k} + q/2, \epsilon_n) e^{i\Omega\tau} \]  
\[ = -\frac{e^2}{\hbar^2 c} \sum_{m,k} \frac{\partial h^{\alpha\beta}}{\partial k_i} \frac{\partial h^{\gamma\delta}}{\partial k_j} G^M_{\delta\alpha}(\mathbf{k} - q/2, \epsilon_m) G^M_{\beta\gamma}(\mathbf{k} + q/2, \epsilon_m + \Omega) \]  
\[ = -\frac{e^2}{\hbar^2 c} \sum_{m,k} \text{Tr}\left[ \frac{\partial h}{\partial k_i} G^M(\mathbf{k} + q/2, \epsilon_m + \Omega) \frac{\partial h}{\partial k_j} G^M(\mathbf{k} - q/2, \epsilon_m) \right] \]  
\[ \text{Input the general express of the Masubara Green’s Function, we finally obtain} \]

\[ Q_{ij}(q, \Omega) = -\frac{e^2}{\hbar^2 c} \sum_{m,k,n,n'} \text{Tr}\left[ \frac{\partial h}{\partial k_i} |n, \mathbf{k} + \frac{q}{2}\rangle \langle n, \mathbf{k} + \frac{q}{2}| \frac{\partial h}{\partial k_j} |n', \mathbf{k} - \frac{q}{2}\rangle \langle n', \mathbf{k} - \frac{q}{2}| \right] \]  
\[ = -\frac{e^2}{\hbar^2 c} \sum_{m,k,n,n'} \text{Tr}\left[ \frac{\partial h}{\partial k_i} |n, \mathbf{k} + \frac{q}{2}\rangle \langle n, \mathbf{k} + \frac{q}{2}| \frac{\partial h}{\partial k_j} |n', \mathbf{k} - \frac{q}{2}\rangle \langle n', \mathbf{k} - \frac{q}{2}| \right] \]  
\[ = -\frac{e^2}{\hbar^2 c} \sum_{m,k,n,n'} \text{Tr}\left[ \frac{\partial h}{\partial k_i} |n, \mathbf{k} + \frac{q}{2}\rangle \langle n, \mathbf{k} + \frac{q}{2}| \frac{\partial h}{\partial k_j} |n', \mathbf{k} - \frac{q}{2}\rangle \langle n', \mathbf{k} - \frac{q}{2}| \right] \]  
\[ \text{Input the general express of the Masubara Green’s Function, we finally obtain} \]