Effects of Berry Curvature on Thermoelectric Transport

IN

Bilayer Graphene and Other Materials

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Abstract

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Berry curvature in reciprocal space

Before we discuss Berry curvature, let us consider a concrete example, a spatially fixed spin-$\frac{1}{2}$ particle in a rotating magnetic field. Suppose the magnetic field is rotating in the xy plane. This problem can be solved exactly. The time evolution of the system is governed by the Hamiltonian, $H = -\mu_B \boldsymbol{B} \cdot \boldsymbol{\sigma}$, where the rotating magnetic field $\boldsymbol{B} = (\cos \omega t, \sin \omega t, 0)$, and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is a vector containing the Pauli matrices. With the initial condition that the spin is initially pointing parallel the magnetic field, along the x axis, $\Psi(0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$. When the magnetic field rotates very slowly compared to the timescale of evolution of the system, i.e., $\omega \ll \frac{\mu_B B}{\hbar}$, it can be shown that the spin wavefunction evolves as, $\Psi(t) = \left[e^{-i\frac{\omega t}{2}} e^{i\frac{\mu_B B}{\hbar} t} \right] \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\omega t} \end{pmatrix}$.

Then, after a complete revolution of the magnetic field, at time $T = \frac{2\pi}{\omega}$, the state evolves to, $\Psi(T) = e^{-i\pi} e^{i\frac{\mu_B B}{\hbar} T} \Psi(0)$. Although the magnetic field returns to its initial value, the state acquires an additional phase factor of $e^{-i\pi} = -1$, in addition to the usual phase factor of $e^{i\frac{\mu_B B}{\hbar} T}$ (because the system remains in the instantaneous eigenstate with energy eigenvalue $-\mu_B B$).

This is an example of a geometric phase (also known as the *Pancharatnam–Berry phase*), which is the additional phase acquired by an eigenstate, when a parameter of the Hamiltonian (here the magnetic field) is varied slowly compared to the timescale ($\sim \frac{\text{energy}}{\hbar}$) of the state.

It can be shown that (see chapter 10 of [10]) if the magnetic field subtends a solid angle Ω and returns to its initial value, the accumulated geometric phase for a spin-s system would be $-s\Omega$. Here the magnetic field subtends a solid angle 2π after rotating about the xy plane, and it is a spin-$\frac{1}{2}$ system, and the geometric phase after the magnetic field completes a revolution is $-\pi$, just as we saw previously.

2.0.1 Geometric Phase and Berry Curvature

When the Hamiltonian of a system has a paramater $\boldsymbol{\lambda}$ which evolves slowly (compared to the timescale $\frac{\hbar}{\varepsilon}$ of a state $|\varepsilon\rangle$), an eigenstate of the Hamiltonian evolves as ([2], also see chapter 10 of [10] for derivation),

$$|\varepsilon(\boldsymbol{\lambda}(t))\rangle = e^{i\gamma(t)} e^{-\frac{i}{\hbar} \int_0^t \varepsilon(\boldsymbol{\lambda}(t'))dt'} |\varepsilon(\boldsymbol{\lambda}(0))\rangle \tag{2.1}$$

where the geometric phase $\gamma(t)$ is given by the expression

$$\gamma(t) = i \int_{\boldsymbol{\lambda}_i}^{\boldsymbol{\lambda}_f} \langle \varepsilon(\boldsymbol{\lambda})| \nabla_{\boldsymbol{\lambda}} |\varepsilon(\boldsymbol{\lambda})\rangle \cdot d\boldsymbol{\lambda}.$$

Its value depends on the trajectory in the parameter space $\boldsymbol{\lambda}$, not just the endpoints. The real quantity $i \langle \varepsilon(\boldsymbol{\lambda})| \nabla_{\boldsymbol{\lambda}} |\varepsilon(\boldsymbol{\lambda})\rangle = \boldsymbol{A}(\boldsymbol{\lambda})$ is known as the Berry connection [1], and its curl, $\boldsymbol{\Omega} = \nabla_{\boldsymbol{\lambda}} \times \boldsymbol{A}$ is known as the Berry curvature.

While the overall phase of the state does not affect its physical observables, if we take a linear combination of such eigenstates, each of them would evolve with a different geometric phase, and the interference of such phase factors would indeed affect the physical properties of the system. We would now see how such a geometric phase manifests in electrons moving in a lattice, when an external electromagnetic field is applied.

2.0.2   Geometric phase of electrons in a lattice

Now, let us consider an electron in a periodic potential $V(\boldsymbol{r})$ (e.g. the potential due to a lattice, without any external electromagnetic fields). Its Hamiltonian is given by $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{\boldsymbol{r}})$.

The eigenfunctions of this Hamiltonian are of the form,

$$\psi_{n,\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{n,\boldsymbol{k}}(\boldsymbol{r})$$

Here $u_{n,\boldsymbol{k}}(\boldsymbol{r})$ is a function with the same periodicity as $V(\boldsymbol{r})$ (e.g. in a lattice, it would be periodic in every unit cell). The quantity $\hbar\boldsymbol{k}$ is known as the crystal momentum and n is the band index. This result is known as Bloch's theorem (See chapter 8 of [1]). The crystal momentum is a good quantum number for an electron in a lattice, and it is conserved upto a reciprocal lattice vector (times $\hbar$). Now, we can rewrite the eigenvalue equation $\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right] \psi_{n,\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon_{n,\boldsymbol{k}} \psi_{n,\boldsymbol{k}}(\boldsymbol{r})$ as,

$$\left[\frac{\hbar^2}{2m}(\boldsymbol{k} - i\nabla)^2 + V(\boldsymbol{r})\right] u_{n,\boldsymbol{k}}(\boldsymbol{r}) = \varepsilon_{n,\boldsymbol{k}} u_{n,\boldsymbol{k}}(\boldsymbol{r}) \tag{2.2}$$

In this equation, $\boldsymbol{k}$ is just a parameter in the effective Hamiltonian. When we apply an external electromagnetic field, the crystal momentum is not anymore a good quantum number. Its evolution is governed by the Lorenz force, (See Appendix A for derivation)

$$\boxed{\hbar\dot{\boldsymbol{k}} = -e\left(\boldsymbol{E} + \langle\dot{\boldsymbol{r}}\rangle \times \boldsymbol{B}\right)} \tag{2.3}$$

As $\boldsymbol{k}$ (now a parameter of the effective Hamiltonian in Eq. (2.2)) changes, it would give rise to a geometric phase, just like Eq. (2.1). After a small time interval Δt, $\boldsymbol{k}$ would evolve to $\boldsymbol{k} + \dot{\boldsymbol{k}}\Delta t$ (we write $\dot{\boldsymbol{k}}\Delta t = \Delta\boldsymbol{k}$), and the periodic part of the Bloch wavefunction labeled with $\boldsymbol{k}$ would evolve as

$$u_{n,\boldsymbol{k}} \to e^{i\gamma(\Delta t)} e^{-i\frac{\varepsilon_{\boldsymbol{k}}\Delta t}{\hbar}} u_{n,\boldsymbol{k}+\Delta\boldsymbol{k}}, \tag{2.4}$$

where $\gamma(\Delta t) = \boldsymbol{A}(\boldsymbol{k})\cdot\Delta\boldsymbol{k}$, and $\boldsymbol{A}(\boldsymbol{k}) = i \langle u_{n,\boldsymbol{k}}| \nabla_{\boldsymbol{k}} |u_{n,\boldsymbol{k}}\rangle$ is the Berry connection [2] in the reciprocal space. Again, for a state labeled with a single $\boldsymbol{k}$, this geometric phase is an overall global phase, which would not show up in physical observables. However, if we take a linear superposition of Bloch wavefunctions with different values of $\boldsymbol{k}$, each of them would evolve with a different geometric phase $\gamma_n(\boldsymbol{k}) = \int_0^t dt' \boldsymbol{A}(\boldsymbol{k}) \cdot \frac{d\boldsymbol{k}}{dt'}$, and we would soon see that the interference of such phase factors would lead to many interesting effects.

After all, this geometric phase is an effect of the Hamiltonian not commuting with itself at different times, for different values of the parameter $\boldsymbol{k}$. It can be easily verified that the commutator of the effective Hamiltonian with itself, for two different values of $\boldsymbol{k}$, namely, $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$,

$$\left[\frac{\hbar^2}{2m}(\boldsymbol{k}_1 - i\nabla)^2 + V(\boldsymbol{r}), \frac{\hbar^2}{2m}(\boldsymbol{k}_2 - i\nabla)^2 + V(\boldsymbol{r})\right] = -\frac{i\hbar^2}{m}(\boldsymbol{k}_1 - \boldsymbol{k}_2) \cdot \nabla V(\boldsymbol{r})$$

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[1] $\langle\varepsilon(\boldsymbol{\lambda})| \nabla_{\boldsymbol{\lambda}} |\varepsilon(\boldsymbol{\lambda})\rangle$ stands for $\int d\boldsymbol{r}\varepsilon_{\boldsymbol{\lambda}}^*(\boldsymbol{r})\nabla_{\boldsymbol{\lambda}}\varepsilon_{\boldsymbol{\lambda}}(\boldsymbol{r})$, where $\varepsilon_{\boldsymbol{\lambda}}(\boldsymbol{r})$ is the suitably normalized position space wavefunction of $|\varepsilon(\boldsymbol{\lambda})\rangle$.

[2] $\langle u_{n,\boldsymbol{k}}| \nabla_{\boldsymbol{k}} |u_{n,\boldsymbol{k}}\rangle$ stands for $\int_{\text{unit cell}} d\boldsymbol{r} u_{n,\boldsymbol{k}}^*(\boldsymbol{r})\nabla_{\boldsymbol{k}} u_{n,\boldsymbol{k}}(\boldsymbol{r})$, where the normalization of $u_{n,\boldsymbol{k}}(\boldsymbol{r})$ is chosen such that $\int_{\text{unit cell}} d\boldsymbol{r}|u_{n,\boldsymbol{k}}(\boldsymbol{r})|^2 = 1$.

2.1   Effects of Berry Curvature

2.1.1   Modification of semiclassical equations of motion of a wavepacket

The probability density of the wavefunction $\psi_{n,\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_{n,\boldsymbol{k}}(\boldsymbol{r})$ is not localized anywhere, it is periodic over all unit cells (the blue curve in Fig. 2.1). We can construct a wave packet by forming a linear superposition of many such states, such that the wavepacket is localized at some point $\boldsymbol{r}_0$ in the real space (the red curve in Fig. 2.1), and its crystal momentum is also localized around a value of $\hbar\boldsymbol{k}_0$.

Although this wavepacket is localized in both real space and (crystal) momentum space, it does not violate Heisenberg's uncertainty relation, because for this wave packet, the product of the uncertainties in position and (crystal) momentum, $\Delta\boldsymbol{r}\Delta\boldsymbol{k}$ is still greater than $\frac{1}{2}$. While the wavepacket is spread over many unit cells, its spatial variation $\Delta\boldsymbol{r}$ is much smaller than the dimensions of the system, and $\Delta\boldsymbol{k}$ is much smaller than the dimensions of the Brillouin zone. As a result, in laboratory scale, the wavepacket behaves like a classical particle, with an almost localized value of position and crystal momentum.
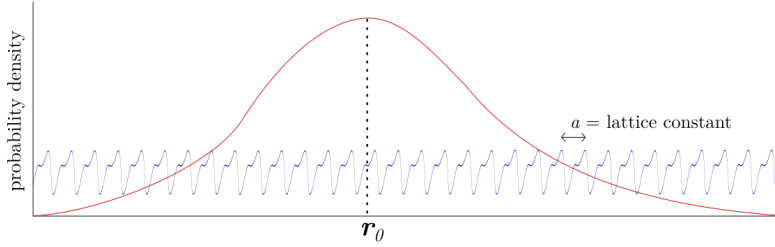
Figure 2.1: The blue curve shows the probability density of a Bloch wavefunction. It is periodic over unit cells. The red curve shows a wavepacket which is localized in real space (although it is spread over many unit cells, it is localized compared to the dimensions of the system), as well as in crystal momentum space.

It can be shown [14] that for such a wavepacket, the expectation value of the position of its center evolves as [3],

$$\boxed{\langle \dot{\boldsymbol{r}} \rangle = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} - \langle \dot{\boldsymbol{k}} \rangle \times \boldsymbol{\Omega}(\boldsymbol{k})} \tag{2.5}$$

Here, $\boldsymbol{\Omega}(\boldsymbol{k}) = \nabla_{\boldsymbol{k}} \times \boldsymbol{A}(\boldsymbol{k}) = i\langle \nabla_{\boldsymbol{k}} u_{n,\boldsymbol{k}}| \times |\nabla_{\boldsymbol{k}} u_{n,\boldsymbol{k}}\rangle$ is the Berry curvature in the reciprocal space. Also, here the energy eigenvalues are modified due to orbital magnetic moment $\boldsymbol{m}_{\boldsymbol{k}}$ of an wavepacket (more about it in Section 5.1) , $\varepsilon_{\boldsymbol{k}} = \varepsilon_0(\boldsymbol{k}) - \boldsymbol{m}_{\boldsymbol{k}} \cdot \boldsymbol{B}$, where $\varepsilon_0(\boldsymbol{k})$ is the original bandstructure energy at zero magnetic field.

In popular Solid State Physics textbooks, the second term in the RHS of Eq. (2.5), involving the Berry curvature is omitted (e.g. see Eq. 8.51 of [1]). This is most likely because people thought that the overall phase factor is unimportant. Also, we would soon see that the Berry curvature is identically zero unless certain symmetries are broken, and this is why its effects cannot be experimentally observed in most systems.

To see why the extra term appears, let us first investigate how we can produce such a wavepacket, which is localized in both position space and crystal momentum space. This discussion is based on Section I. of [14]. To make the wavepacket localized near $\boldsymbol{k}_0$ in the reciprocal space, consider a *real* weight function $w(\boldsymbol{k}-\boldsymbol{k}_0)$, which is sharply localized about $\boldsymbol{k} = \boldsymbol{k}_0$. Now consider a linear superposition of the Bloch wavefunctions, of the form, $\int d\boldsymbol{k}w(\boldsymbol{k}-\boldsymbol{k}_0)e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_0}\left(e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u_{n,\boldsymbol{k}}(\boldsymbol{r})\right)$. The expectation value of $\boldsymbol{k}$ of this wavefunction should be localized about $\boldsymbol{k}_0$. Then, near $\boldsymbol{r} = \boldsymbol{r}_0$, the functions $e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)}$ constructively interfere, and we would expect the wavepacket to have a

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[3]Note that this is the (group) velocity of the wavepacket. A single Bloch eigenstate does not have a definite velocity, because its density is periodic over every unit cell – it does not have an well defined position, which could move with a certain velocity.

high probability density at $\boldsymbol{r}_0$. However, the functions $u_{n,\boldsymbol{k}}(\boldsymbol{r})$ may have different phases for different values of $\boldsymbol{k}$ at the same $\boldsymbol{r} = \boldsymbol{r}_0$, and then the waves would not constructively interfere. After properly taking account of this (See Appendix B.2), the wavefunction that is localized around $\langle \boldsymbol{r} \rangle = \boldsymbol{r}_0$, and peaked at crystal momentum $\hbar \boldsymbol{k}_0$ is found to be,

$$\psi(\boldsymbol{r}, t = 0) = \int d\boldsymbol{k} w(\boldsymbol{k} - \boldsymbol{k}_0) e^{i\boldsymbol{A}(\boldsymbol{k_0}) \cdot (\boldsymbol{k} - \boldsymbol{k_0})} e^{-i\boldsymbol{k} \cdot \boldsymbol{r}_0} \left(e^{i\boldsymbol{k} \cdot \boldsymbol{r}} u_{n,\boldsymbol{k}}(\boldsymbol{r}) \right). \tag{2.6}$$

Here $\boldsymbol{A}$ is again the Berry connection. After a small time Δt, the individual Bloch wavefunctions would then evolve as in Eq. (2.4), and the wavefunction of the wavepacket would be,

$$\psi(\boldsymbol{r}, t = \Delta t) = \int d\boldsymbol{k} w(\boldsymbol{k} - \boldsymbol{k}_0) e^{i\boldsymbol{A}(\boldsymbol{k_0}) \cdot (\boldsymbol{k} - \boldsymbol{k_0})} e^{-i\boldsymbol{k} \cdot \boldsymbol{r}_0} \left(e^{i(\boldsymbol{k} + \Delta \boldsymbol{k}) \cdot \boldsymbol{r}} e^{i\boldsymbol{A} \cdot \Delta \boldsymbol{k}} e^{-i\frac{\varepsilon_{\boldsymbol{k}} \Delta t}{\hbar}} u_{n, \boldsymbol{k} + \Delta \boldsymbol{k}} \right).$$

It can be shown (See Appendix. B.4), that for this state, the expectation value of position is located at

$$\langle \boldsymbol{r} \rangle = \boldsymbol{r}_0 + \frac{\Delta t}{\hbar} \nabla_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} |_{\boldsymbol{k} = \boldsymbol{k}_0} - \Delta \boldsymbol{k}_0 \times \boldsymbol{\Omega}(\boldsymbol{k_0}).$$

The change in the expectation value of position after time Δt is then, $\frac{\Delta t}{\hbar} \nabla_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} |_{\boldsymbol{k} = \boldsymbol{k}_0} - \Delta \boldsymbol{k}_0 \times \boldsymbol{\Omega}(\boldsymbol{k_0})$. After dividing the change in position in $\langle \boldsymbol{r} \rangle$ by Δt, the expression of velocity in Eq. (2.5) follows.

2.1.2 Violation of Liouville's theorem and Modification of phase space density

We now drop the notation $\langle \cdot \rangle$ of expectation values, and denote $\langle \boldsymbol{r} \rangle \equiv \boldsymbol{r}$ and $\langle \boldsymbol{k} \rangle \equiv \boldsymbol{k}$ for a wavepacket localized at $\boldsymbol{r}$ and $\boldsymbol{k}$. Consider a point $(\boldsymbol{r}, \boldsymbol{k})$ in the phase space, with a small volume element ΔV_0 around it. The points inside the volume element ΔV_0 evolve as governed by the semiclassical equations of motion,

$$\boxed{\dot{\boldsymbol{r}} = \frac{1}{\hbar} \nabla_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} - \dot{\boldsymbol{k}} \times \boldsymbol{\Omega}(\boldsymbol{k})} \tag{2.7}$$

$$\boxed{\hbar \dot{\boldsymbol{k}} = -e \left(\boldsymbol{E} + \dot{\boldsymbol{r}} \times \boldsymbol{B} \right)} \tag{2.8}$$

and suppose, they occupy a new volume $\Delta V(t)$ around the point $(\boldsymbol{r}', \boldsymbol{k}')$ after time t. Then, the quantity

$$\Delta V(t) \left(1 + \frac{e}{\hbar} \boldsymbol{B}\left(\boldsymbol{r}(t) \right) \cdot \boldsymbol{\Omega}\left(\boldsymbol{k}(t) \right) \right)$$

remains a constant of motion [19](See Appendix C for proof).

Liouville's theorem states that the volume ΔV occupied by a fixed number of points in the phase space remains invariant as the point $(\boldsymbol{r}, \boldsymbol{k})$ flows following the equations of motion (which are obtained from a classical Hamiltonian). In other words, the phase space density remains invariant. Here, that does not hold anymore (unless either of $\boldsymbol{B}$ or $\boldsymbol{\Omega}$ is zero, or they are orthogonal so that their dot product is zero). Note that the quantity defined above is a function of the local coordinates $(\boldsymbol{r}(t), \boldsymbol{k}(t))$, and does not depend on the trajectory.

Since the number of phase space points in the volume element $\Delta \boldsymbol{k} \Delta \boldsymbol{r} \left(1 + \frac{e}{\hbar} \boldsymbol{B}\left(\boldsymbol{r}(t) \right) \boldsymbol{\Omega}\left(\boldsymbol{k}(t) \right) \right)$ remains constant in time, if the magnetic field was initially zero, and we gradually turn on a homogeneous magnetic field, the number of states in the volume $\Delta \boldsymbol{k} \Delta \boldsymbol{r} \left(1 + \frac{e}{\hbar} \boldsymbol{B}(t) \cdot \boldsymbol{\Omega}\left(\boldsymbol{k} \right) \right)$ would be equal to the number of states in the initial volume $\Delta \boldsymbol{k} \Delta \boldsymbol{r}$.

As a result, when we calculate the expectation value of any operator $\mathcal{O}$ over all states, we would have to introduce an additional factor of $\left(1 + \frac{e}{\hbar} \boldsymbol{B} \cdot \boldsymbol{\Omega}\left(\boldsymbol{k} \right) \right)$ in the integrand, to correctly take account of all the states.

$$\langle \mathcal{O} \rangle = \int \frac{d\boldsymbol{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \boldsymbol{B} \cdot \boldsymbol{\Omega}\left(\boldsymbol{k} \right) \right) \langle \mathcal{O} \rangle_{\boldsymbol{k}} \, \tilde{g}_{\boldsymbol{k}} \tag{2.9}$$

Here $\tilde{g}_{\boldsymbol{k}}$ is known as the distribution function, and counts the occupation number of electrons in a state labeled with $\boldsymbol{k}$. When no external fields are applied, in thermodynamic equilibrium, it is the Fermi distribution function, $\tilde{g}_{\boldsymbol{k}} = f_{\boldsymbol{k}} = \frac{1}{e^{\beta\left(\varepsilon_{\boldsymbol{k}}-\mu\right)}+1}$. When an electromagnetic field is applied, this equilibrium is disturbed, and we write the distribution function as $\tilde{g}_{\boldsymbol{k}} = f_{\boldsymbol{k}} + g_{\boldsymbol{k}}$, where $g_{\boldsymbol{k}}$ is the non-equilibrium part of the distribution (it is zero when there is no external electric field, or temperature gradient, or chemical potential gradient). We will see how to calculate it in Section 4.

Also, since Liouville's theorem does not hold anymore, we cannot obtain the equations of motion (2.7) and (2.8) from any (classical) effective Hamiltonian.

2.2   When do we get a non-zero Berry Curvature?

2.2.1   Spatial Inversion Symmetry

Under spatial inversion symmetry, the polar vectors change sign, $\boldsymbol{r} \to -\boldsymbol{r}$, $\boldsymbol{k} \to -\boldsymbol{k}$, $\boldsymbol{E} \to -\boldsymbol{E}$, but axial vectors like $\boldsymbol{B} \to \boldsymbol{B}$ remain unchanged. Also, since $\boldsymbol{\Omega} = \nabla_{\boldsymbol{k}} \times A$ itself is an axial vector, under spatial inversion it changes as, $\boldsymbol{\Omega}(\boldsymbol{k}) \to \boldsymbol{\Omega}(-\boldsymbol{k})$.

Then, if we apply the spatial inversion operator, the LHS of Eq. (2.5) changes sign, and then the RHS must change sign too. Then, $\dot{\boldsymbol{k}} \times \boldsymbol{\Omega}(\boldsymbol{k})$ must also change overall sign. But, under spatial inversion, $\dot{\boldsymbol{k}} \times \boldsymbol{\Omega}(\boldsymbol{k}) \to (-\dot{\boldsymbol{k}}) \times \boldsymbol{\Omega}(-\boldsymbol{k})$, and this must be equal to $-\dot{\boldsymbol{k}} \times \boldsymbol{\Omega}(\boldsymbol{k})$, and we must have,

$$\boldsymbol{\Omega}(-\boldsymbol{k}) = \boldsymbol{\Omega}(\boldsymbol{k}), \tag{2.10}$$

when spatial inversion symmetry is present.

2.2.2   Time Reversal Symmetry

Under time reversal, the quantities $\dot{\boldsymbol{r}} \to -\dot{\boldsymbol{r}}$, $\boldsymbol{k} \to -\boldsymbol{k}$ change sign, whereas $\dot{\boldsymbol{k}} \to \dot{\boldsymbol{k}}$ remains the same. The spin of the electron also flips, $\boldsymbol{\sigma} \to -\boldsymbol{\sigma}$.

If we apply the time reversal operator, the LHS of Eq. (2.5) changes sign, and then $\dot{\boldsymbol{k}} \times \boldsymbol{\Omega}(\boldsymbol{k})$ must change an overall sign too. In general, the Berry curvature depends on the band index and the spin, and it follows that when time reversal symmetry is present,

$$\boldsymbol{\Omega}_{n,\sigma}(-\boldsymbol{k}) = -\boldsymbol{\Omega}_{n,-\sigma}(\boldsymbol{k}). \tag{2.11}$$

When there is no spin orbit coupling, the spatial parts of the wavefunctions for up and down spins are the same, consequently the Berry curvatures are the same too (because the Berry Curvature $\boldsymbol{\Omega}(\boldsymbol{k}) = i \langle \nabla_{\boldsymbol{k}} u_{n,\boldsymbol{k}} | \times | \nabla_{\boldsymbol{k}} u_{n,\boldsymbol{k}} \rangle$ is a function of the spatial part of the wavefunction).

Then, when the spin orbit coupling is negligible, under time reversal symmetry,

$$\boldsymbol{\Omega}_{n,\sigma}(-\boldsymbol{k}) = -\boldsymbol{\Omega}_{n,\sigma}(\boldsymbol{k}). \tag{2.12}$$

Note: Even when the time reversal symmetry is broken due to an external magnetic field, we continue to have the same Bloch wavefunctions (when the magnetic field is low enough), and since the Berry curvature is a function of the Bloch wavefunctions, in case there was time reversal symmetry before applying the magnetic field, the result (2.12) continues to hold even after applying it (until the magnetic field is so high that the bandstructure is heavily modified, and we enter the regime of Landau levels).

2.2.3   Conditions for non-Zero Berry Curvature

As a result, when both spatial inversion and time reversal symmetry exist, and spin orbit coupling is negligible, then, combining Eq. (2.10) and Eq. (2.12) $\boldsymbol{\Omega}_{n,\sigma}(-\boldsymbol{k}) = \boldsymbol{\Omega}_{n,\sigma}(\boldsymbol{k}) = -\boldsymbol{\Omega}_{n,\sigma}(\boldsymbol{k})$, i.e. $\boldsymbol{\Omega} \equiv 0$ for any $\boldsymbol{k}$.

Then, to get a non-zero Berry curvature [14], either time reversal or spatial inversion symmetry must be broken, or there must be significant spin orbit coupling. Note that these conditions are necessary to get a non-zero Berry curvature, but they may not be sufficient.

2.2.4 Why the effects of Berry Curvature in transport took so long to be experimentally found?

In any metal, time reversal symmetry is already present, and the spatial inversion symmetry is present in BCC, FCC and simple cubic lattices. As a result, the Berry curvature is identically zero in most metals.

Now we understand why the effects (e.g see section 3.2) of the additional term in Eq. (2.7) were not seen in early transport experiments.

A non-zero Berry curvature can present in biased Bilayer graphene, and also in topological materials like Chern Insulator and Weyl semimetal. These materials were experimentally realized in 21st century.

CITE: appropriate sources for Graphene and topological materials.

FIND: more materials where there is a non-zero Berry curvature. — MoS_2 and its valley hall effect.

2.3 Decoupling of the equations of motion and their simplification

The coupled differential equations of motion for $\dot{\boldsymbol{r}}$ and $\dot{\boldsymbol{k}}$ (Eq. (2.7) and Eq. (2.8)) can be easily decoupled with some vector algebra (See Appendix D), and the resulting decoupled equations are,

$$\dot{\boldsymbol{r}} = \frac{\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} + \frac{e}{\hbar}(\boldsymbol{E} \times \boldsymbol{\Omega}) + \frac{e}{\hbar^2}(\boldsymbol{\Omega} \cdot \frac{\partial \varepsilon}{\partial \boldsymbol{k}})\boldsymbol{B}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}} \tag{2.13}$$

$$\dot{\boldsymbol{k}} = -\frac{\frac{e}{\hbar}\boldsymbol{E} + \frac{e}{\hbar^2}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \times \boldsymbol{B} + \frac{e^2}{\hbar^2}(\boldsymbol{E} \cdot \boldsymbol{B})\boldsymbol{\Omega}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}} \tag{2.14}$$

In a *2D sample*, $\boldsymbol{\Omega}$ is along the z axis, while $\frac{\partial \varepsilon}{\partial \boldsymbol{k}}$ is in the xy plane, then $\boldsymbol{\Omega} \cdot \frac{\partial \varepsilon}{\partial \boldsymbol{k}} = 0$. Also, in *2D*, $\boldsymbol{\Omega}$ is along the z axis, whereas $\boldsymbol{k}$ is restricted to the xy plane. Then we can neglect the term $(\boldsymbol{E} \cdot \boldsymbol{B})\boldsymbol{\Omega}$ in the expression of $\dot{\boldsymbol{k}}$. Then the equations (2.13) and (2.14) simplify to,

$$\boxed{\dot{\boldsymbol{r}} = \frac{\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} + \frac{e}{\hbar}(\boldsymbol{E} \times \boldsymbol{\Omega})}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}} \tag{2.15}$$

$$\boxed{\dot{\boldsymbol{k}} = -\frac{\frac{e}{\hbar}\boldsymbol{E} + \frac{e}{\hbar^2}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \times \boldsymbol{B}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}} \tag{2.16}$$

Chapter 3

Strategy of Calculation of Thermal and Heat Currents

To calculate the total electric current density, we need to sum the expectation value of the electric current operator, $\hat{\boldsymbol{j}}_e = -e\hat{\dot{\boldsymbol{r}}}$ over all states[1], and we substitute $\left\langle \hat{\dot{\boldsymbol{r}}} \right\rangle_{\boldsymbol{k}}$ with its value in Eq. (2.15). Without the Berry curvature, the current density would be, $\left\langle \hat{\boldsymbol{j}}_e \right\rangle = \int \frac{d\boldsymbol{k}}{(2\pi)^d}(-e\dot{\boldsymbol{r}})_{\boldsymbol{k}}(f_{\boldsymbol{k}} + g_{\boldsymbol{k}})$, but in presence of the Berry curvature, we need to take account of the phase space volume correction (see Eq. (2.9)), and the expression for the current density is,

$$\left\langle \hat{\boldsymbol{j}}_e \right\rangle = \int \frac{d\boldsymbol{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}\left(\boldsymbol{k}\right) \right) (-e\dot{\boldsymbol{r}})_{\boldsymbol{k}}(f_{\boldsymbol{k}} + g_{\boldsymbol{k}}) \tag{3.1}$$

To calculate the heat current operator, consider a closed surface in a system, through which it can exchange energy in the form of heat, and also particles. From the first law of thermodynamics we know that the heat gained by the system inside this volume satisfies, $dQ = dE - \mu dN$, where μ is the chemical potential, E is the energy of the system enclosed by the surface, and N is the number of particles inside the surface. From this relation, it follows that $\boldsymbol{j}_Q = \boldsymbol{j}_E - \mu\boldsymbol{j}_N$, where $\boldsymbol{j}_Q$, $\boldsymbol{j}_E$, and $\boldsymbol{j}_N$ are the heat current density, energy current density, and number current density [2], respectively. Now we promote the current densities to their respective operators, and obtain the relation,

$$\left\langle \hat{\boldsymbol{j}}_Q \right\rangle_{\boldsymbol{k}} = \left\langle \hat{\boldsymbol{j}}_E \right\rangle_{\boldsymbol{k}} - \mu \left\langle \hat{\boldsymbol{j}}_N \right\rangle_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} \left\langle \dot{\boldsymbol{r}} \right\rangle_{\boldsymbol{k}} - \mu \left\langle \dot{\boldsymbol{r}} \right\rangle_{\boldsymbol{k}} \tag{3.2}$$

The total heat current is then given by,

$$\left\langle \hat{\boldsymbol{j}}_Q \right\rangle = \int \frac{d\boldsymbol{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}\left(\boldsymbol{k}\right) \right) (\varepsilon_{\boldsymbol{k}} - \mu)\dot{\boldsymbol{r}}_{\boldsymbol{k}}(f_{\boldsymbol{k}} + g_{\boldsymbol{k}}) \tag{3.3}$$

We can now put $d = 2$ and use the expression of $\dot{\boldsymbol{r}}$ in Eq. (2.15) to further simplify Eq. (3.1) and Eq. (3.3), and obtain [3],

$$\left\langle \hat{\boldsymbol{j}}_e \right\rangle = -e \int \frac{d\boldsymbol{k}}{(2\pi)^2}(f_{\boldsymbol{k}} + g_{\boldsymbol{k}}) \left[\frac{1}{\hbar}\frac{\partial \varepsilon_{\boldsymbol{k}}}{\partial \boldsymbol{k}} + \frac{e}{\hbar}(\boldsymbol{E} \times \boldsymbol{\Omega}(\boldsymbol{k})) \right] \tag{3.4}$$

$$\left\langle \hat{\boldsymbol{j}}_Q \right\rangle = \int \frac{d\boldsymbol{k}}{(2\pi)^2}(\varepsilon_{\boldsymbol{k}} - \mu)(f_{\boldsymbol{k}} + g_{\boldsymbol{k}}) \left[\frac{1}{\hbar}\frac{\partial \varepsilon_{\boldsymbol{k}}}{\partial \boldsymbol{k}} + \frac{e}{\hbar}(\boldsymbol{E} \times \boldsymbol{\Omega}(\boldsymbol{k})) \right] \tag{3.5}$$

---

[1]Charge of electron is $-e$ everywhere in the thesis.

[2]the electric current density is just the electron charge times the number current density, $\boldsymbol{j}_e = -e\boldsymbol{j}_N$

[3]**This is not the complete story**. There are more terms because the electron is not completely localized in the center of the wavepacket, and there can be circulating magnetization current, which play an important role. More about that in section 5.

3.1 An analysis of contribution of different terms in the above integrals

3.1.1 The contribution from the equilibrium part of the distribution, and the band structure part of the velocity is zero

$\varepsilon_0(\boldsymbol{k})$ is usually an even function of $\boldsymbol{k}$, when the system has time reversal symmetry. Then the Fermi distribution $f_{\boldsymbol{k}} = \frac{1}{1+e^{\beta(\varepsilon_0(\boldsymbol{k})-\mu)}}$ is also an even function, and the band structure part of the velocity, $\frac{\partial \varepsilon_0(\boldsymbol{k})}{\partial \boldsymbol{k}}$ is an odd function of $\boldsymbol{k}$. Then, the integrals $\int d\boldsymbol{k} f_{\boldsymbol{k}} \frac{\partial \varepsilon_0(\boldsymbol{k})}{\partial \boldsymbol{k}}$ and $\int d\boldsymbol{k} f_{\boldsymbol{k}} (\varepsilon_0(\boldsymbol{k}) - \mu) \frac{\partial \varepsilon_0(\boldsymbol{k})}{\partial \boldsymbol{k}}$ in the expressions of the electric and heat currents are zero, because the overall integrand is an odd function.

When there is a magnetic field, we get a modified energy $\varepsilon_{\boldsymbol{k}} = \varepsilon_0(\boldsymbol{k}) - \boldsymbol{m}_{\boldsymbol{k}} \cdot \boldsymbol{B}$, and this simple argument does not hold anymore. We would still expect the net transport current to be zero, when there is no external electric field or chemical potential gradient or temperature gradient, but there is a non-zero magnetic field. Then, the modified Fermi distribution function would be, $f_{\boldsymbol{k}} = f(\varepsilon_0(\boldsymbol{k})) - \boldsymbol{m} \cdot \boldsymbol{B}) = f(\varepsilon_0(\boldsymbol{k}) + \sum_{n=1}^{\infty} (-1)^n \frac{\partial^n f}{\partial \varepsilon_0^n} \frac{(\boldsymbol{m} \cdot \boldsymbol{B})^n}{n!}$.

Then, the relevant term in the electric current density would be,

$$\int \frac{d\boldsymbol{k}}{(2\pi)^d} \left[f(\varepsilon_0(\boldsymbol{k})) + \sum_{n=1}^{\infty} (-1)^n \frac{\partial^n f}{\partial \varepsilon_0^n} \frac{(\boldsymbol{m} \cdot \boldsymbol{B})^n}{n!} \right] \left[\frac{\partial \varepsilon_0(\boldsymbol{k})}{\partial \boldsymbol{k}} - \frac{\partial}{\partial \boldsymbol{k}} (\boldsymbol{m} \cdot \boldsymbol{B}) \right]$$

The zeroeth order term in magnetic field is 0, as $\int \frac{d\boldsymbol{k}}{(2\pi)^d} f(\varepsilon_0(\boldsymbol{k})) \frac{\partial \varepsilon_0}{\partial \boldsymbol{k}} = 0$, as the overall integrand is an odd function of $\boldsymbol{k}$, as explained in the previous paragraph.

Consider the term n-th order in the magnetic field,

$$\int_{\text{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} (-1)^n \frac{\partial^n f}{\partial \varepsilon_0^n} \frac{(\boldsymbol{m} \cdot \boldsymbol{B})^n}{n!} \frac{\partial \varepsilon_0(\boldsymbol{k})}{\partial \boldsymbol{k}} - (-1)^{(n-1)} \frac{\partial^{n-1} f}{\partial \varepsilon_0^{n-1}} \frac{(\boldsymbol{m} \cdot \boldsymbol{B})^{n-1}}{(n-1)!} \frac{\partial}{\partial \boldsymbol{k}} (\boldsymbol{m} \cdot \boldsymbol{B})$$

$$= (-1)^n \int_{\text{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} \left(\frac{\partial}{\partial \boldsymbol{k}} \frac{\partial^{n-1} f}{\partial \varepsilon_0^n} \right) \frac{(\boldsymbol{m} \cdot \boldsymbol{B})^n}{n!} + \frac{\partial^{n-1} f}{\partial \varepsilon_0^{n-1}} \frac{(\boldsymbol{m} \cdot \boldsymbol{B})^{n-1}}{(n-1)!} \frac{\partial}{\partial \boldsymbol{k}} (\boldsymbol{m} \cdot \boldsymbol{B})$$

$$= (-1)^n \int_{\text{BZ}} \frac{d\boldsymbol{k}}{(2\pi)^d} \frac{\partial}{\partial \boldsymbol{k}} \left[\frac{\partial^{n-1} f}{\partial \varepsilon_0^n} \frac{(\boldsymbol{m} \cdot \boldsymbol{B})^n}{n!} \right] = 0,$$

because the integral of the gradient of a periodic scalar, over the Brillouin Zone is zero (see Appendix I of [1] for proof). Similarly, it can be shown that the similar term for energy current is zero upto all orders in magnetic field.

These results are expected because there should not be any transport currents in equilibrium (in absence of electric field, chemical potential gradient or temperature gradient).

3.1.2 Terms contributing to quadratic order in external fields (we neglect them)

In Eq. (4.4) and Eq. (4.5) it has been shown that upto leading order, the non-equilibrium part of the distribution function, $g_{\boldsymbol{k}}$ is a linear function of the electromagnetic field and the gradients of chemical potential and temperature. Then, the term $g_{\boldsymbol{k}}(\boldsymbol{E} \times \boldsymbol{\Omega}(\boldsymbol{k}))$ is a quadratic function of the externally applied fields, and we neglect its contribution in the expressions of electric and heat current densities.

3.1.3 Terms contributing to linear order in external fields

The rest of the terms ($f_{\boldsymbol{k}}(\boldsymbol{E} \times \boldsymbol{\Omega})$ and $g_{\boldsymbol{k}} \frac{\partial \varepsilon_{\boldsymbol{k}}}{\partial \boldsymbol{k}}$) are linear in the external electric field, and chemical potential gradient, and temperature gradient, and henceforth, we would only consider these terms.

3.2   An illustration of the above procedure: the Anomalous Hall effect and quantized off-diagonal electric conductivity

When there is a non-zero Berry curvature, a sample can show a Hall response even in absence of a magnetic field, and more astonishingly, the Hall conductance is quantized. This is known as the anomalous Hall effect.

Suppose we apply an electric field along x direction on a 2D sample, and the magnetic field $\boldsymbol{B} = 0$. There are no temperature gradient or chemical potential gradient.

It can be shown that $g_{\boldsymbol{k}} = \frac{\partial f}{\partial \varepsilon} \frac{\tau}{\hbar} \frac{\partial \varepsilon}{\partial \boldsymbol{k}} \cdot e\boldsymbol{E}$, upto linear order in $\boldsymbol{E}$ (this is a special case of Eq. (4.4), with $\boldsymbol{B} = 0$). Ignoring the terms with quadratic and zero contribution, (See section 3.1.2 and 3.1.1), the electric current $\left\langle \hat{\boldsymbol{j}}_e \right\rangle = -e \int \frac{d\boldsymbol{k}}{(2\pi)^2} \left[f_{\boldsymbol{k}} \frac{e}{\hbar} (\boldsymbol{E} \times \boldsymbol{\Omega}(\boldsymbol{k})) + g_{\boldsymbol{k}} \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \boldsymbol{k}} \right]$. The second term contributes to σ_{xx}, and it is nothing but a regular Ohmic response (analyzed in section 4.0.1). The first term [4] leads to a current perpendicular to the applied electric field,

$$\left\langle \hat{\boldsymbol{j}}_e \right\rangle_y = \frac{e^2}{2\pi\hbar} \boldsymbol{E}_x \int \frac{d\boldsymbol{k}}{2\pi} f_{\boldsymbol{k}} \boldsymbol{\Omega}(\boldsymbol{k}) = \frac{e^2}{2\pi\hbar} \boldsymbol{E}_x \int_{\text{filled}} \frac{d\boldsymbol{k}}{2\pi} \boldsymbol{\Omega}(\boldsymbol{k}).$$

For a fully filled band, the integral of $\frac{1}{2\pi}\boldsymbol{\Omega}(\boldsymbol{k})$ over the first Brillouin zone is an integer, and it is called the first Chern Number (see 7.4.1), which we denote as $\mathcal{C}$. Then, the off-diagonal part of the conductivity tensor is *quantized*[5],

$$\sigma_{xy} = \frac{\boldsymbol{j}_y}{\boldsymbol{E}_x} = \frac{e^2}{2\pi\hbar} \mathcal{C}.$$

Here we have a current along y axis, while the external electric field is along the x axis. This is like the Hall effect, but *without* a magnetic field, hence it is called the *Anomalous* Hall effect.

Note that this is *not* the Quantum Hall Effect, where the diagonal conductivity σ_{xx} also becomes quantized under very high magnetic fields, and the bandstructures are replaced by Landau levels. In this paper we are working in the low magnetic field regime, and in this particular context of anomalous Hall effect, the magnetic field is zero.

3.2.1   When do we get non-zero Anomalous Hall response?

When time reversal symmetry is present, the Berry curvature is an odd function, $\boldsymbol{\Omega}(\boldsymbol{k}) = -\boldsymbol{\Omega}(-\boldsymbol{k})$, and its integral over the Brillouin zone is zero (consequently, the Chern number is zero). Therefore, we need a *broken time reversal symmetry* to get Anomalous Hall Effect.

3.3   Einstein and Onsager relations

In linear regime of thermoelectric transport, we can express the electric and thermal currents as,

$$\begin{aligned}
\left\langle \hat{\boldsymbol{j}}_e \right\rangle &= \overset{\leftrightarrow}{L}_{11} \cdot \left(\boldsymbol{E} + \nabla \frac{\mu}{e} \right) + \overset{\leftrightarrow}{L}_{12} \cdot (-\nabla T) \\
\left\langle \hat{\boldsymbol{j}}_Q \right\rangle &= \overset{\leftrightarrow}{L}_{21} \cdot \left(\boldsymbol{E} + \nabla \frac{\mu}{e} \right) + \overset{\leftrightarrow}{L}_{22} \cdot (-\nabla T)
\end{aligned} \tag{3.6}$$

---

[4]It is to be noted that this is due to the intrinsic Fermi distribution function, and is independent of scattering (which is responsible for the non-equilibrium part of the distribution function, $g_{\boldsymbol{k}}$).

[5]The factor of $(1 + \frac{e}{\hbar} \boldsymbol{B} \cdot \boldsymbol{\Omega})$ gets canceled in the numerator (from the phase space connection) and the denominator (from the expression of $\dot{\boldsymbol{r}}_{\boldsymbol{k}}$), as seen in Eq. (3.4) and Eq. (3.5), and the fact that the "Anomalous Hall response is quantized" holds true even when there is a non-zero magnetic field.

Here $\overset{\leftrightarrow}{L}_{ij}$ $(i,j \in 1,2)$ are tensors, they act on a vector to give a vector. $\overset{\leftrightarrow}{L}_{11}$ is the electric conductivity, $\overset{\leftrightarrow}{L}_{22}$ is the thermal conductivity[6], and $\overset{\leftrightarrow}{L}_{12}$, $\overset{\leftrightarrow}{L}_{21}$ are related to the Seebeck and Peltier coefficients.

The symmetry between $\boldsymbol{E} \longleftrightarrow \frac{1}{e}\nabla\mu$ is known as the *Einstein relation*. Physically speaking, the thermoelectric response for an electric field and an equivalent chemical potential gradient would be identical.

Experimentally, it is found that

$$\overset{\leftrightarrow}{L}_{21} = T \overset{\leftrightarrow}{L}_{12} . \tag{3.7}$$

Relations like this are known as *Onsager relation*s. In this particular case, the Onsager relation is equivalent to the relation between the Seebeck and Peltier coefficients (See chapter 6).

These quantities are often expressed [17] in the alternative notation $\overset{\leftrightarrow}{L}_{11} = \overset{\leftrightarrow}{\sigma}$, $\overset{\leftrightarrow}{L}_{12} = \overset{\leftrightarrow}{\alpha}$, $\overset{\leftrightarrow}{L}_{21} = \overset{\leftrightarrow}{\tilde{\alpha}}$, $\overset{\leftrightarrow}{L}_{22} = \overset{\leftrightarrow}{\kappa}$.

3.3.1 (Apparent) Violation of Einstein and Onsager Relations in presence of Berry Curvature

While the theoretical validations of the Einstein and the Onsager relations have been established (see chapter 7 of [23] and chapter 8 of [1]), they are tricky to establish when a Berry curvature is present.

For an example, consider the Anomalous Hall effect. It happens due to the equilibrium part of the electronic distribution (the Fermi distribution function), and the Berry curvature part ($\boldsymbol{E} \times \boldsymbol{\Omega}$) of the velocity of the electron wavepacket. However, there are no terms like $\nabla\mu \times \boldsymbol{\Omega}$ or $\nabla T \times \boldsymbol{\Omega}$. As a result, apparently, there are no off-diagonal thermoelectric response when $\boldsymbol{E} = 0$ (but $\nabla\mu \neq 0$ or $\nabla T \neq 0$), and both Einstein and Onsager relations are violated.

Resolution: In presence of the Berry curvature, the Bloch wavepacket can have a orbital magnetic moment (see Chapter 5), i.e., the electron density is circulating about its center of mass (more specifically, the local value of the momentum, $\psi^*(\boldsymbol{r})(-i\hbar\nabla_{\boldsymbol{r}})\psi(\boldsymbol{r})$ circulates about the center $\boldsymbol{r}_0$). This circulating current is known as the magnetization current, $\boldsymbol{j}_M = \nabla \times \boldsymbol{M}$, which cannot be measured in transport experiments. The current measured in transport experiments is the transport current, which is obtained by subtracting the magnetization current from the total current, $\boldsymbol{j}_{\mathrm{tr}} = \boldsymbol{j} - \boldsymbol{j}_M$. It can be theoretically shown that the Onsager and the Einstein relations are valid for the transport electric current and the transport heat current.

In the next chapter, we show that the Einstein and the Onsager relations remain valid for current densities arising from the non-equilibrium part of the distribution, after which we would get back to resolving the issue of violation of the Einstein and Onsager relations for Anomalous Hall terms.

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[6]Here we denoted thermal conductivity as the heat current per unit temperature gradient, at zero electric field or chemical potential. Sometimes, thermal conductivity is denoted as heat current per unit temperature gradient, when the net electric current is zero (an internal electrochemical potential gradient is generated to maintain zero electric current, but that internal electrochemical potential gradient in turn contributes to the heat current). In that case, it can be shown that (see Eq. 13.56 of [1]) the heat current (i.e. the heat conductivity, because we set $\nabla T = 1$) is $\overset{\leftrightarrow}{L}_{22} - \overset{\leftrightarrow}{L}_{21} (\overset{\leftrightarrow}{L}_{11})^{-1} \overset{\leftrightarrow}{L}_{12}$. But this additional term is a small correction, it is of the order $\left(\frac{k_B T}{\varepsilon_F}\right)^2$.

Chapter 4

Boltzmann Transport Equation and its solution

A Bloch wavefunction is an eigenstate of the periodic potential of a perfect lattice, as if, an electron in a Bloch wavefunction can move throughout the system without getting scattered by the ions. However, in a real system, there are lattice defects, lattice vibrations (phonons) and impurities, all of which scatter the electron to a different state. In equilibrium, the electron distribution function reduces to the Fermi distribution, $f_{\bm{k}} = \frac{1}{e^{\beta(\varepsilon_{\bm{k}} - \mu)} + 1}$. When an external electromagnetic field, or a chemical potential gradient, or a thermal gradient is applied, the local distribution is modified due to scattering between different states. When the system is perturbed slightly out of equilibrium (i.e. when the external electromagnetic fields are much smaller than the atomic fields), the distribution is slightly modified from the Fermi distribution, $\tilde{g}_{\bm{k}} = f_{\bm{k}} + g_{\bm{k}}$, where $|g_{\bm{k}}| \ll f_{\bm{k}}$. To calculate $g_{\bm{k}}$, we employ the following idea. Consider an electron wavepacket in the phase space point $(\bm{r}, \bm{k})$, and it evolves according to the equations of motion. Then, the rate of change of the distribution function is given by the convective derivative in the phase space, $\left[\frac{\partial}{\partial t} + \dot{\bm{k}} \cdot \frac{\partial}{\partial \bm{k}} + \dot{\bm{r}} \cdot \frac{\partial}{\partial \bm{r}} \right] \tilde{g}_{\bm{k}}$. The scattering processes would try to bring it back to the local equilibrium, and we expect it to be faster when the deviation from the equilibrium is more. Then, phenomenologically, we can write that the convective derivative is proportional to the deviation from equilibrium, with the proportional constant being the scattering timescale $\tau_{\bm{k}}$, the timescale over which the distribution exponentially reaches a local equilibrium. This assumption is known as the relaxation time approximation, and under this approximation, the non-equilibrium part of the distribution function follows the Boltzmann Transport Equation (BTE), $\left[\frac{\partial}{\partial t} + \dot{\bm{k}} \cdot \frac{\partial}{\partial \bm{k}} + \dot{\bm{r}} \cdot \frac{\partial}{\partial \bm{r}} \right] \tilde{g}_{\bm{k}} = -\frac{g_{\bm{k}}}{\tau}$. The scattering timescale can in general depend on $\bm{k}$. We would soon see that only the values of $\bm{k}$ on the Fermi surface would contribute a non-zero amount to the transport, and we assume that there is a constant scattering time τ on the Fermi surface.

This formalism is based on Chapter 7 of [23], where the author has calculated the electric and thermal conductance tensors in the absence of Berry curvature. Here, we extend the formalism for a non-zero Berry curvature. When the external fields are time independent, we can drop the explicit partial derivative with respect to time, and the Boltzmann Transport Equation can be cast into the form,

$$\frac{g}{\tau} + \dot{\bm{k}} \cdot \frac{\partial}{\partial \bm{k}} g + \dot{\bm{r}} \cdot \frac{\partial}{\partial \bm{r}} g = -\dot{\bm{k}} \cdot \frac{\partial}{\partial \bm{k}} f - \dot{\bm{r}} \cdot \frac{\partial}{\partial \bm{r}} f. \tag{4.1}$$

Using the decoupled equations of motion, right hand side of Eq. (4.1) simplifies to (see Appendix E.1),

$$\frac{\partial f}{\partial \varepsilon} \frac{1}{1 + \frac{e}{\hbar} \bm{B} \cdot \bm{\Omega}} \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \bm{k}} \cdot \left[e\bm{E} + \nabla \mu + \nabla T \frac{\varepsilon - \mu}{T} \right].$$

Here we see that we can exchange $\bm{E} \leftrightarrow \nabla \mu$, i.e., the Einstein relation holds. We would show that the Onsager relation holds as well. We assume that the fields are constant in space, and drop the

term containing $\frac{\partial g}{\partial \boldsymbol{r}}$.

Validity of neglecting this term: When we solve the equation after discarding this term, we would find that (See Eq. (4.4)) this term ($\dot{\boldsymbol{r}} \cdot \frac{\partial g}{\partial \boldsymbol{r}}$) is second order in the applied fields. Then upto linear order, we can discard this term. Then, the BTE becomes,

$$\frac{g}{\tau} - \frac{\frac{e}{\hbar}\boldsymbol{E} + \frac{e}{\hbar^2}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \times \boldsymbol{B}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}} \cdot \frac{\partial}{\partial \boldsymbol{k}} g = \frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \cdot \left[e\boldsymbol{E} + \nabla \mu + \nabla T \frac{\varepsilon - \mu}{T}\right] \quad (4.2)$$

We can further simplify this equation. If we neglect the term $\boldsymbol{E} \cdot \frac{\partial g}{\partial \boldsymbol{k}}$ in the LHS, we would find (in the next section) that g is a linear function of the electric field, the chemical potential gradient, and the temperature gradient. Then, $\boldsymbol{E} \cdot \frac{\partial g}{\partial \boldsymbol{k}}$ would be quadratic in the applied fields, and the solution would remain self-consistent if we neglect it. In other words, if we first neglect it, find the solution, and treat this terms as a perturbation, it would turn out to be quadratic, and we would neglect it anyway. Finally, the equation we would have to solve is,

$$\boxed{\frac{g}{\tau} - \underbrace{\frac{\frac{e}{\hbar^2}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \times \boldsymbol{B}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}} \cdot \frac{\partial}{\partial \boldsymbol{k}} g}_{\text{treated as a perturbation}} = \frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \cdot \left[e\boldsymbol{E} + \nabla \mu + \nabla T \frac{\varepsilon - \mu}{T}\right]} \quad (4.3)$$

We treat the second term in the LHS as a perturbation. An order of the magnitude estimate in Appendix F shows that the magnetic field needs to be of the order of hundreds of Tesla for this term to be of the same magnitude as the other term, $\frac{g}{\tau}$. Since the magnetic field in the laboratories are much less than that, we can treat it as a perturbation. We would see that this term gives rise to the (ordinary) Hall effect, that is why we would not completely neglect it.

4.0.1 Solution for $\boldsymbol{B} \neq 0$, $\boldsymbol{\Omega} \neq 0$, $\boldsymbol{E} \neq 0$, $\nabla \mu = \nabla T = 0$

The solution of the equation (4.3) is (see Appendix E.2),

$$g = \frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{\tau}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}}\cdot e\boldsymbol{E} + \frac{\frac{e\tau}{\hbar^2}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{\partial \varepsilon}{\partial \boldsymbol{k}}\cdot \boldsymbol{B} \times \left[\frac{\partial}{\partial \boldsymbol{k}}\left[\frac{\frac{\partial f}{\partial \varepsilon}\tau}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\right]\frac{e\boldsymbol{E}}{\hbar}\cdot\frac{\partial \varepsilon}{\partial \boldsymbol{k}} + \frac{\frac{\partial f}{\partial \varepsilon}\tau}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\left[(\frac{e}{\hbar}\boldsymbol{E} \cdot \frac{\partial}{\partial \boldsymbol{k}})\frac{\partial \varepsilon}{\partial \boldsymbol{k}}\right]\right] \quad (4.4)$$

Verification: When $\boldsymbol{\Omega} = 0$, and $\varepsilon = \frac{\hbar^2 k^2}{2m^*}$, this term produces an electric conductivity tensor, $\overset{\leftrightarrow}{\sigma} = \frac{ne^2\tau}{m^*}\begin{pmatrix} 1 & \omega_c\tau \\ -\omega_c\tau & 1 \end{pmatrix}$.

Regular Ohmic conduction:

When $\boldsymbol{B} = 0$, we get $g = \frac{\partial f}{\partial \varepsilon}\frac{\tau}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \cdot \boldsymbol{E}$.

4.0.2 Solution for $\boldsymbol{B} \neq 0$, $\boldsymbol{\Omega} \neq 0$, $\boldsymbol{E} = 0$, $\nabla \mu \neq 0$, $\nabla T \neq 0$

Here the solution of (4.3) upto linear order in external fields is (see Appendix E.3),

$$g = \frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{\tau}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}}\cdot \boldsymbol{S} + \frac{\frac{e\tau}{\hbar^2}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{\partial \varepsilon}{\partial \boldsymbol{k}}\cdot \boldsymbol{B} \times \left[\frac{\partial}{\partial \boldsymbol{k}}\left[\frac{\frac{\partial f}{\partial \varepsilon}\tau}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\right]\frac{\boldsymbol{S}}{\hbar}\cdot\frac{\partial \varepsilon}{\partial \boldsymbol{k}} + \frac{\frac{\partial f}{\partial \varepsilon}\tau}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\left[\left(\frac{1}{\hbar}\boldsymbol{S} \cdot \frac{\partial}{\partial \boldsymbol{k}}\right)\frac{\partial \varepsilon}{\partial \boldsymbol{k}}\right]\right] \quad (4.5)$$

with $\boldsymbol{S} = \nabla \mu + \frac{\varepsilon - \mu}{T}\nabla T$.

Since the Boltzmann Transport Equation (4.3) is linear, when there is a non-zero electric field as well as a chemical potential gradient and temperature gradient, we can add the solutions in Eq. (4.4) and Eq. (4.5). In other words, the form of Eq. (4.5) remains, and we only need to substitute $\boldsymbol{S} = e\boldsymbol{E} + \nabla \mu + \frac{\varepsilon - \mu}{T}\nabla T$.

4.0.3 Validity of the Einstein and Onsager relations due to the non-equilibrium part of the distribution

Einstein Relation: We can interchange $e\boldsymbol{E}$ and $\nabla\mu$, and the form of the equations (4.4) and (4.5) remain the same. Then, the Einstein relation holds for the currents arising from the non-equilibrium part of the distribution.

Onsager Relation: In Eq. (4.5), ∇T always comes with a factor of $\frac{\varepsilon-\mu}{T}$, and to find the heat current, we need to multiply with an additional factor of $(\varepsilon - \mu)$ (see Eq. (3.3)). It follows that the contribution to $\overset{\leftrightarrow}{L}_{12}$ and $\overset{\leftrightarrow}{L}_{21}$ are the same upto a factor of $\frac{1}{T}$, and the Onsager relation (see Eq. (3.7)) holds for these contributions.

Chapter 5

Resolution of the Apparent Violation of Einstein and Onsager Relations with Orbital Magnetization

5.1 Orbital Magnetic Moment

While an wavepacket like that in Eq. (2.6) is localized around a point (say, $\boldsymbol{r}_0$), it the electron is not completely localized at that point, and can have an angular momentum due to the rotation about that point (in classical sense). As an analogy, if we could replace the electron probability density with the density of a classical charged fluid, that fluid could rotate about its center of mass, and would have an angular momentum due to that rotation, and consequently, a magnetic moment. We call this the orbital magnetic moment of an electron wavepacket,

$$\boldsymbol{m_k} = -\frac{e}{2m} \langle \psi_{\boldsymbol{k},\boldsymbol{r}_0} | (\hat{\boldsymbol{r}} - \boldsymbol{r}_0) \times \hat{\boldsymbol{p}} | \psi_{\boldsymbol{k},\boldsymbol{r}_0} \rangle \tag{5.1}$$

This is just a generalization of the formula $\boldsymbol{m} = (-e)g\frac{\boldsymbol{L}}{2m}$, with the Lande-$g$ factor set to 1, as this magnetic moment is due to the spatial motion of the electron, and not due to its spin angular
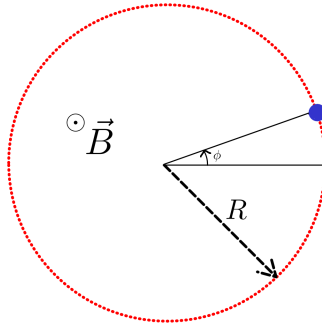

Figure 5.1: A free particle on a ring. A magnetic field $\boldsymbol{B}$ is applied perpendicular to the plane of the ring.

momentum. Note that m is the bare electron mass (not the effective mass of a Bloch state).[1]

5.1.1   An example

For a free electron moving in a ring of radius R (Fig. 5.1), the eigenfunctions of the Hamiltonian are $\psi_n(\phi) = \frac{1}{2\pi R}e^{in\phi}$, with energy eigenvalue, $\varepsilon_0(n) = \frac{\hbar^2 n^2}{2mR^2}$ It has an orbital angular momentum $n\hbar$ about the center of the ring, and a magnetic moment $m_z = -\frac{e}{2m}n\hbar$. When a magnetic field perpendicular to the center of mass is applied, the eigenfunctions remain the same, but the energy eigenvalues are modified to, $\varepsilon(n) = \frac{1}{2mR^2}(n\hbar + \frac{eBR^2}{2})^2$. Then, upto linear order in the magnetic field, the energy eigenvalue is, $\varepsilon(n) = \frac{1}{2mR^2}(n^2\hbar^2 + n\hbar eBR^2) = \varepsilon_0(n) - m_z B$.

While the density of this wavefunction is spread over all the ring, we can consider a localized wavepacket with the most significant contribution from this wavefunction, and that wavepacket would have almost the same magnetic moment, and the same energy eigenvalue.

5.2   Is the orbital magnetic moment caused by the Berry Curvature?

No. Consider a free particle moving in a ring. The eigenfunctions would have zero Berry curvature, but there is a net magnetic moment.

5.3   Modified Expression for Electric Current Density

Let us look back and try to see why we got an apparent violation of the Einstein and Onsager relations for the Anomalous Hall Effect, in Section 3.3.1. In the anomalous Hall effect, we got a term like $\boldsymbol{E} \times \int d\boldsymbol{k}\boldsymbol{\Omega}(\boldsymbol{k})$, but there were no terms like $\nabla\mu \times \boldsymbol{\Omega}(\boldsymbol{k})$, or $\nabla T \times \boldsymbol{\Omega}(\boldsymbol{k})$. The electric field enters through the solution of the semiclassical equation o f velocity, whereas the gradient of the chemical potential and the gradient of the temperature entered through the out of equilibrium part of the distribution function.

To get this term, we need to use the fact that the wavepacket has a finite width, an electron in a Bloch wavepacket centered at $\boldsymbol{r}_0$ can be found at $\boldsymbol{r}_1 \neq \boldsymbol{r}_0$, and it can contribute to the current at $\boldsymbol{r}_1$ ($\neq \boldsymbol{r}_0$). As an analogy, the total electron density near an atom in a insulator is not just the electron density of that atom, but the sum of electron densities belonging to all the atoms, evaluated at that point. Of course, atoms far away from the point would contribute very less, but nearby atoms can contribute significantly. Previously, when we calculated $\langle j \rangle(\boldsymbol{r}_1)$, we only considered the contribution of the Bloch wavepacket localized at $\boldsymbol{r}$.

Let us try to find the expectation value of a general operator $\mathcal{O}$ at a point $\boldsymbol{r}_1$. We would consider the sum of the contributions of all wavepackets centered at a point $\boldsymbol{r}_0$, and sum over all $\boldsymbol{r}_0$. That is, [18]

$$\left\langle \hat{\mathcal{O}} \right\rangle(\boldsymbol{r}_1) = \int d\boldsymbol{r}_0 \int \frac{d\boldsymbol{k}}{(2\pi)^d}(f+g)(1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega})\langle\psi_{\boldsymbol{k},\boldsymbol{r}_0}|\frac{1}{2}\{\hat{\mathcal{O}},\delta(\hat{\boldsymbol{r}}-\boldsymbol{r}_1)\}|\psi_{\boldsymbol{k},\boldsymbol{r}_0}\rangle$$

Here $\hat{\boldsymbol{r}}$ is the position operator that acts on the states. $\boldsymbol{r}_1$ is just a parameter, and here $\boldsymbol{r}_1$ acting on a state has to be understood as the operator $\boldsymbol{r}_1\mathcal{I}$, with $\mathcal{I}$ being the identity operator acting on the Hilbert space. And, $\frac{1}{2}\{\hat{\mathcal{O}},\delta(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)\}$ denotes the Hermitized operator $\frac{\hat{\mathcal{O}}\delta(\hat{\boldsymbol{r}}-\boldsymbol{r}_1)+\delta(\hat{\boldsymbol{r}}-\boldsymbol{r}_1)\hat{\mathcal{O}}}{2}$, in case $\hat{\boldsymbol{r}}$ and $\hat{\mathcal{O}}$ does not commute. $|\psi_{\boldsymbol{k},\boldsymbol{r}_0}\rangle$ is the Bloch wavepacket with the expectation values of position and crystal momentum being $\boldsymbol{r}_0$, and $\boldsymbol{k}$, respectively.

Now, since the state is spread around $\boldsymbol{r}_0$, we can take that into account by expanding the delta function (upto leading order),

$$\delta(\boldsymbol{r}_1 - \hat{\boldsymbol{r}}) = \delta((\boldsymbol{r}_1 - \boldsymbol{r}_0) - (\hat{\boldsymbol{r}} - \boldsymbol{r}_0)) \approx \delta(\boldsymbol{r}_1 - \boldsymbol{r}_0) - (\hat{\boldsymbol{r}} - \boldsymbol{r}_0)\cdot\nabla_{\boldsymbol{r}_1}\delta(\boldsymbol{r}_1 - \boldsymbol{r}_0)$$

---

[1]See Appendix G for some discussion on the mass entering in different relations.

Using this, we get,

$$
\begin{aligned}
\left\langle \hat{\mathcal{O}} \right\rangle (\boldsymbol{r}_1) = &\int \frac{d\boldsymbol{k}}{(2\pi)^d} (f + g)(1 + \frac{e}{\hbar} \boldsymbol{B} \cdot \boldsymbol{\Omega}) \left\langle \psi_{\boldsymbol{k},\boldsymbol{r}_1} \right| \hat{\mathcal{O}} \left| \psi_{\boldsymbol{k},\boldsymbol{r}_1} \right\rangle \\
&- \nabla_{\boldsymbol{r}_1} \cdot \int \frac{d\boldsymbol{k}}{(2\pi)^d} (f + g)(1 + \frac{e}{\hbar} \boldsymbol{B} \cdot \boldsymbol{\Omega}) \left\langle \psi_{\boldsymbol{k},\boldsymbol{r}_1} \right| \frac{1}{2} \{ \hat{\mathcal{O}}, (\hat{\boldsymbol{r}} - \boldsymbol{r}_1) \} \left| \psi_{\boldsymbol{k},\boldsymbol{r}_1} \right\rangle
\end{aligned}
\tag{5.2}
$$

We would work with this leading order expansion of the Delta function. For the current density operator, we need to separately take the three components of $\hat{\boldsymbol{j}} = -e\frac{\hat{\boldsymbol{p}}}{m}$ to be $\hat{\mathcal{O}}$.

Let us define the tensor,

$$
\mathcal{M}_{i,j} = \left\langle \psi_{\boldsymbol{k},\boldsymbol{r}_1} \right| \frac{1}{2} \{ -e\frac{\hat{p}_j}{m}, (\hat{\boldsymbol{r}} - \boldsymbol{r}_1)_i \} \left| \psi_{\boldsymbol{k},\boldsymbol{r}_1} \right\rangle
$$

where i, j runs from $1, 2, \ldots d$. It can be shown that (see Appendix H) $\mathcal{M}_{i,j}$ is completely anti-symmetric [8]. Then, in 3D universe (the sample can still be 2 dimensional), we can construct a vector, whose components are, $m_i = \frac{1}{2}\epsilon_{ijk}\mathcal{M}_{jk}$ ([8]). It can be shown (see Appendix H) that this is nothing but the orbital magnetic moment, defined in Eq. (5.1). We can also invert the relation, $\mathcal{M}_{jk} = m_i \epsilon_{ijk}$.

Note that we can rewrite the new term as,

$$
\begin{aligned}
&- \nabla_{\boldsymbol{r}_1} \cdot \int \frac{d\boldsymbol{k}}{(2\pi)^d} (f + g)(1 + \frac{e}{\hbar} \boldsymbol{B} \cdot \boldsymbol{\Omega}) \left\langle \psi_{\boldsymbol{k},\boldsymbol{r}_1} \right| \frac{1}{2} \{ \hat{\mathcal{O}}, (\hat{\boldsymbol{r}} - \boldsymbol{r}_1) \} \left| \psi_{\boldsymbol{k},\boldsymbol{r}_1} \right\rangle \\
&= -\partial_i \int \frac{d\boldsymbol{k}}{(2\pi)^d} (f + g)(1 + \frac{e}{\hbar} \boldsymbol{B} \cdot \boldsymbol{\Omega}) \left\langle \psi_{\boldsymbol{k},\boldsymbol{r}_1} \right| \frac{1}{2} \{ \hat{\mathcal{O}}, (\hat{\boldsymbol{r}} - \boldsymbol{r}_1)_i \} \left| \psi_{\boldsymbol{k},\boldsymbol{r}_1} \right\rangle,
\end{aligned}
$$

with sum over i implied. Then to get the μ-th component of $\left\langle \hat{\boldsymbol{j}} \right\rangle$, we take $\hat{\mathcal{O}} = -e\frac{\hat{p}_\mu}{m}$. We denote $[dk] = \frac{d\boldsymbol{k}}{(2\pi)^d}(1 + \frac{e}{\hbar} \boldsymbol{B} \cdot \boldsymbol{\Omega})$. We get,

$$
\begin{aligned}
&- \partial_i \int [dk] (f + g) \mathcal{M}_{i\mu} \\
&= -\partial_i \int [dk] (f + g) m_\nu \epsilon_{\nu i \mu} \\
&= +\partial_i \int [dk] (f + g) m_\nu \epsilon_{i\nu\mu}
\end{aligned}
$$

This is the μ-th component of $\nabla \times \int \frac{d\boldsymbol{k}}{(2\pi)^d}(f + g)(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega})\boldsymbol{m_k}$. When the electric field, chemical potential gradient and the temperature gradients are constant, we can drop the term $\nabla \times \int d\boldsymbol{k} g(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega})\boldsymbol{m_k}$, because g is already a linear function of $\boldsymbol{E}$, $\nabla\mu$ and ∇T.

Finally we get,

$$
\left\langle \hat{\boldsymbol{j}}_e \right\rangle = -e \int \frac{d\boldsymbol{k}}{(2\pi)^d} g_{\boldsymbol{k}} \frac{1}{\hbar} \frac{\partial \varepsilon_{\boldsymbol{k}}}{\partial \boldsymbol{k}} + f_{\boldsymbol{k}} \frac{e}{\hbar} (\boldsymbol{E} \times \boldsymbol{\Omega}(\boldsymbol{k})) + \nabla \times \int \frac{d\boldsymbol{k}}{(2\pi)^d} f_{\boldsymbol{k}} \left(1 + \frac{e}{\hbar} \boldsymbol{B} \cdot \boldsymbol{\Omega} \right) \boldsymbol{m_k}.
\tag{5.3}
$$

This equation has a simple interpretation. The net current is the contribution of the center of mass movements of the wavepackets, as well as due to the rotation about their individual centers of mass. We want to calculate the properties of the anomalous Hall effect, where $\boldsymbol{B} = 0$. Then the expression simplifies to

$$
\left\langle \hat{\boldsymbol{j}}_e \right\rangle \Big|_{\boldsymbol{B}=0} = -e \int \frac{d\boldsymbol{k}}{(2\pi)^d} g_{\boldsymbol{k}} \frac{1}{\hbar} \frac{\partial \varepsilon_0(\boldsymbol{k})}{\partial \boldsymbol{k}} + f_{\boldsymbol{k}} \frac{e}{\hbar} (\boldsymbol{E} \times \boldsymbol{\Omega}(\boldsymbol{k})) + \nabla \times \int \frac{d\boldsymbol{k}}{(2\pi)^d} f_{\boldsymbol{k}} \boldsymbol{m_k}.
\tag{5.4}
$$

5.4 Total Magnetization of the system

Due to the orbital moment of the Bloch wavepackets, the system gets a net non-zero magnetization, which leads to circulating along its edges. However, the net magnetization density is slightly

different from the sum of the individual orbital magnetic moments. This is because, the phase space density changes when as we turn on a magnetic field (even in the limit of a zero magnetic field, see the expression of $\boldsymbol{M}^e$ below). Under zero external electric field, and zero chemical potential gradient and temperature gradient, the Gibbs free energy of the system is [20],

$$G = -\frac{1}{\beta} \sum_{\boldsymbol{k}} \log\left(1 + e^{-\beta(\varepsilon_{\boldsymbol{k}} - \boldsymbol{m}_{\boldsymbol{k}} \cdot \boldsymbol{B} - \mu)}\right)$$

$$= -\frac{1}{\beta} \int \frac{d\boldsymbol{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}\right) \log\left(1 + e^{-\beta(\varepsilon_{\boldsymbol{k}} - \boldsymbol{m}_{\boldsymbol{k}} \cdot \boldsymbol{B} - \mu)}\right)$$

Then the magnetization is,

$$\boldsymbol{M}^e = \left.\frac{\partial G}{\partial \boldsymbol{B}}\right|_{\boldsymbol{B}=0}$$
$$= \frac{1}{\beta} \int \frac{d\boldsymbol{k}}{(2\pi)^d} \frac{e}{\hbar}\boldsymbol{\Omega}(\boldsymbol{k}) \log\left(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k}) - \mu)}\right) + \int \frac{d\boldsymbol{k}}{(2\pi)^d} f\boldsymbol{m}_{\boldsymbol{k}} \tag{5.5}$$

The circulating magnetization current is,

$$\boldsymbol{j}_M^e = \nabla \times \boldsymbol{M}^e$$
$$= \nabla \times \int \frac{d\boldsymbol{k}}{(2\pi)^d} f\boldsymbol{m}_{\boldsymbol{k}} + \nabla\mu \times \int \frac{d\boldsymbol{k}}{(2\pi)^d} \frac{e}{\hbar}\boldsymbol{\Omega}(\boldsymbol{k})f + \frac{\nabla T}{T} \times \int \frac{d\boldsymbol{k}}{(2\pi)^d} \frac{e}{\hbar}\boldsymbol{\Omega}(\boldsymbol{k})f_{\boldsymbol{k}}(\varepsilon_0(\boldsymbol{k}) - \mu) \tag{5.6}$$
$$+ \frac{\nabla T}{T} \times \int \frac{d\boldsymbol{k}}{(2\pi)^d} \frac{e}{\hbar}\boldsymbol{\Omega}(\boldsymbol{k})k_B T \log\left(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k}) - \mu)}\right)$$

We cannot measure this circulating magnetization current in transport experiments, what we measure is the transport current, which is obtained by subtracting the magnetization current from the total current,

$$\boxed{\begin{aligned} \boldsymbol{j}^e{}_{\text{transport}} &= \left\langle \hat{\boldsymbol{j}}_e \right\rangle - \boldsymbol{j}^e{}_M \\ &= \int \frac{d\boldsymbol{k}}{(2\pi)^d}(-e)g_{\boldsymbol{k}}\frac{1}{\hbar}\frac{\partial\varepsilon_0(\boldsymbol{k})}{\partial\boldsymbol{k}} - f_{\boldsymbol{k}}\frac{e^2}{\hbar}\left(\left[\boldsymbol{E} + \frac{\nabla\mu}{e}\right] \times \boldsymbol{\Omega}(\boldsymbol{k})\right) \\ &\quad - \frac{\nabla T}{T} \times \int \frac{d\boldsymbol{k}}{(2\pi)^d}\frac{e}{\hbar}\boldsymbol{\Omega}(\boldsymbol{k})\left[f_{\boldsymbol{k}}(\varepsilon_0(\boldsymbol{k}) - \mu) + k_B T \log\left(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k}) - \mu)}\right)\right] \end{aligned}} \tag{5.7}$$

We now see that the *Einstein relation* is valid because we can exchange $\boldsymbol{E} \leftrightarrow \frac{\nabla\mu}{e}$ (the validity of the Einstein relation in the non-equilibrium distribution $g_{\boldsymbol{k}}$ has already been shown in section 4.0.3). To show that the Onsager relation is valid, we need to find the modified expression of the heat current, taking into account of the magnetization density.

5.5   Modified Expression for Heat Current Density

We can use a similar approach for the heat current density, and it can be shown that [20] the total heat current is,

$$\left\langle \hat{\boldsymbol{j}}_Q \right\rangle = \int \frac{d\boldsymbol{k}}{(2\pi)^d}(\varepsilon_0(\boldsymbol{k}) - \mu)\left[g_{\boldsymbol{k}}\frac{1}{\hbar}\frac{\partial\varepsilon_0(\boldsymbol{k})}{\partial\boldsymbol{k}} + \frac{e}{\hbar}f_{\boldsymbol{k}}(\boldsymbol{E} \times \boldsymbol{\Omega}(\boldsymbol{k}))\right] - \boldsymbol{E} \times \int \frac{d\boldsymbol{k}}{(2\pi)^d}f_{\boldsymbol{k}}\boldsymbol{m}_{\boldsymbol{k}} \tag{5.8}$$

Here the magnetic field has been set to zero, and terms upto linear order in Electric field has been taken. This is the total energy current density, and is the sum of transport and magnetization energy currents. Just like the case of electric current, the magnetization current is the curl of energy magnetization, which is [7], $\boldsymbol{M}^E = \boldsymbol{M}_0^E + \phi(\boldsymbol{r})\boldsymbol{M}^N$. Here $\boldsymbol{M}_0^E$ is the energy magnetization at zero electric field (we call it the bare energy magnetization), and $\boldsymbol{M}^N$ is the number density magnetization (whose curl is the number current density, i.e. the electric current density divided by

the electric charge), and $\phi(\boldsymbol{r}) = e\boldsymbol{E} \cdot \boldsymbol{r}$ is the potential energy due to the electric field. In presence of an electric field, we need to add this additional term because the charges would carry the potential energy. Both the bare energy magnetization $\boldsymbol{M}_0^E$ and the number density magnetization $\boldsymbol{M}^N = \frac{\boldsymbol{M}^e}{-e}$ are functions of the chemical potential μ and temperature T. Then we can rewrite the energy magnetization as, $\boldsymbol{M}^E = \boldsymbol{M}_0^E - (\boldsymbol{E} \cdot \boldsymbol{r})\boldsymbol{M}^e$. Here $\boldsymbol{M}_0^E$

Then, the magnetization energy current density is,

$$\boldsymbol{j}_M^E = \nabla \times \boldsymbol{M}_0^E - \boldsymbol{E} \times \boldsymbol{M}^e - \underbrace{(\boldsymbol{E} \cdot \boldsymbol{r})\nabla \times \boldsymbol{M}^e}_{\text{2nd order quantity}}$$

Here $\nabla \times \boldsymbol{M}^e$ is already a function of $\nabla\mu$ and ∇T, and the term $(\boldsymbol{E} \cdot \boldsymbol{r})\nabla \times \boldsymbol{M}^e$ is of the second order, and we drop it. It follows that,

$$\boldsymbol{j}_M^E = \nabla\mu \times \frac{\partial \boldsymbol{M}_0^E}{\partial\mu} + \nabla T \times \frac{\partial \boldsymbol{M}_0^E}{\partial T} - \boldsymbol{E} \times \boldsymbol{M}^e$$

$$= \nabla\mu \times \frac{\partial \boldsymbol{M}_0^E}{\partial\mu} + \nabla T \times \frac{\partial \boldsymbol{M}_0^E}{\partial T} - \boldsymbol{E} \times \int \frac{d\boldsymbol{k}}{(2\pi)^d}\boldsymbol{m}(\boldsymbol{k})f_k + k_B T \frac{e\boldsymbol{\Omega}}{\hbar}\log\Big(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k})-\mu)}\Big)$$

Then, the transport energy current density is,

$$\boldsymbol{j}_{\text{transport}}^E = \boldsymbol{j}_{\text{total}}^E - \nabla \times \boldsymbol{M}^E$$

$$= \int \frac{d\boldsymbol{k}}{(2\pi)^d}\varepsilon_0(\boldsymbol{k})\left[g_{\boldsymbol{k}}\frac{1}{\hbar}\frac{\partial\varepsilon_0(\boldsymbol{k})}{\partial\boldsymbol{k}} + \frac{e}{\hbar}f_{\boldsymbol{k}}(\boldsymbol{E} \times \boldsymbol{\Omega}(\boldsymbol{k}))\right]$$

$$+ \boldsymbol{E} \times \int \frac{d\boldsymbol{k}}{(2\pi)^d}k_B T\frac{e\boldsymbol{\Omega}}{\hbar}\log\Big(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k})-\mu)}\Big) - \nabla\mu \times \frac{\partial \boldsymbol{M}_0^E}{\partial\mu} - \nabla T \times \frac{\partial \boldsymbol{M}_0^E}{\partial T}$$

And the transport heat current density is,

$$
\begin{aligned}
\boldsymbol{j}_{\text{transport}}^Q &= \boldsymbol{j}_{\text{transport}}^E - \mu\boldsymbol{j}_{\text{transport}}^N = \boldsymbol{j}_{\text{transport}}^E - \frac{\mu}{-e}\boldsymbol{j}_{\text{transport}}^e \\
&= \int \frac{d\boldsymbol{k}}{(2\pi)^d}(\varepsilon_0(\boldsymbol{k}) - \mu)\frac{1}{\hbar}\frac{\partial\varepsilon_0(\boldsymbol{k})}{\partial\boldsymbol{k}}g_k \\
&\quad + \boldsymbol{E} \times \int \frac{d\boldsymbol{k}}{(2\pi)^d}\left[(\varepsilon_0(\boldsymbol{k}) - \mu)\frac{e}{\hbar}\boldsymbol{\Omega}f_k + k_B T\frac{e\boldsymbol{\Omega}}{\hbar}\log\Big(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k})-\mu)}\Big)\right] \\
&\quad + \int \frac{d\boldsymbol{k}}{(2\pi)^d}(-\mu)\frac{1}{\hbar}\nabla\mu \times \boldsymbol{\Omega}f_k \\
&\quad - \frac{\mu}{\hbar}\int \frac{d\boldsymbol{k}}{(2\pi)^d}\frac{\nabla T}{T} \times \boldsymbol{\Omega}\left[f_k\left(\varepsilon_0(\boldsymbol{k})_k - \mu\right) + k_B T\log\Big(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k})-\mu)}\Big)\right] \\
&\quad - \nabla\mu \times \frac{\partial \boldsymbol{M}_0^E}{\partial\mu} - \nabla T \times \frac{\partial \boldsymbol{M}_0^E}{\partial T}
\end{aligned}
\tag{5.9}
$$

5.5.1 Validity of the Onsager relation, and the Einstein relation in the heat current density

Einstein Relation

In the second and third terms, there is some asymmetry between $e\boldsymbol{E}$ and $\nabla\mu$. For the *Einstein relation* (symmetry between $e\boldsymbol{E}$ and $\nabla\mu$) to hold, we must have a term like

$$(e\boldsymbol{E} + \nabla\mu) \times \int \frac{d\boldsymbol{k}}{(2\pi)^d}\frac{\boldsymbol{\Omega}}{\hbar}\left[(\varepsilon_0(\boldsymbol{k}) - \mu)f_k + k_B T\log\Big(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k})-\mu)}\Big)\right].$$

The missing terms must come from $-\nabla\mu \times \frac{\partial \boldsymbol{M}_0^E}{\partial\mu}$.

We must have, for Einstein relation to hold,

$-\nabla\mu \times \frac{\partial \boldsymbol{M}_0^E}{\partial \mu} = \nabla\mu \times \int \frac{d\boldsymbol{k}}{(2\pi)^d} \frac{\boldsymbol{\Omega}}{\hbar} \left[\varepsilon_0(\boldsymbol{k}) f_k + k_B T \log\left(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k})-\mu)}\right) \right]$, i.e.,

$$-\frac{\partial \boldsymbol{M}_0^E}{\partial \mu} = \int \frac{d\boldsymbol{k}}{(2\pi)^d} \frac{\boldsymbol{\Omega}}{\hbar} \left[\varepsilon_0(\boldsymbol{k}) f_k + k_B T \log\left(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k})-\mu)}\right) \right] \qquad (5.10)$$

Onsager Relation

We have already seen in section (4.0.3) that the Onsager relation is valid for the non-equilibrium distribution. For the equilibrium distribution, in the expression of $\boldsymbol{j}_{\text{transport}}^Q$ (Eq. (5.9)), we have the term, $\boldsymbol{E} \times \int \frac{d\boldsymbol{k}}{(2\pi)^d} \left[(\varepsilon_0(\boldsymbol{k}) - \mu)\frac{e}{\hbar}\boldsymbol{\Omega} f_k + k_B T \frac{e\boldsymbol{\Omega}}{\hbar} \log\left(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k})-\mu)}\right) \right]$, and in the expression of $\boldsymbol{j}_{\text{transport}}^e$ (Eq. (5.7)), we had, $-\frac{\nabla T}{T} \times \int \frac{d\boldsymbol{k}}{(2\pi)^d} \frac{e}{\hbar}\boldsymbol{\Omega}(\boldsymbol{k}) \left[f_{\boldsymbol{k}}(\varepsilon_0(\boldsymbol{k}) - \mu) + k_B T \log\left(1 + e^{-\beta(\varepsilon_0(\boldsymbol{k})-\mu)}\right) \right]$, and the Onsager relation is valid for the terms contributing to $\overset{\leftrightarrow}{L}_{12}$ and $\overset{\leftrightarrow}{L}_{21}$.

Chapter 6

Thermopower, Seebeck, Peltier and Nernst effects

Chapter 7

Chern Number in different Models

We saw that the Anomalous Hall conductivity is proportional to the Chern Numner. In this section we would look at different systems, and discuss their Berry curvature and Chern numbers.

7.1 Monolayer and Bilayer Graphene

Graphene is a two dimensional sheet of Carbon atoms, arranged in a honeycomb lattice. It is actually a single layer of graphite, and indeed, graphene is created in lab by exfoliating a later of graphite with a scotch tape. Although previously used as a theoretical toy model, graphene was isolated and characterized by Geim and Novoselov et al. [11] in 2004. It shows many wonderful electronic properties. Its band structure has a linear energy-momentum dispersion [12] relation at certain points, like that of a massless relativistic particle. It can show integer, half-integer [22] and fractional [3] Quantum Hall effects. Graphene is a semimetal. It has a gapless dispersion, but the density of states is zero at the band touching point.

We can stack two graphene sheets on top of each other, to form bilayer graphene and twist the two layers to some small angle. Twisted bilayer graphene can show superconductivity [4] at some specific twist angles (e.g. 1.1°), known as magic angles.

(a)   (b)

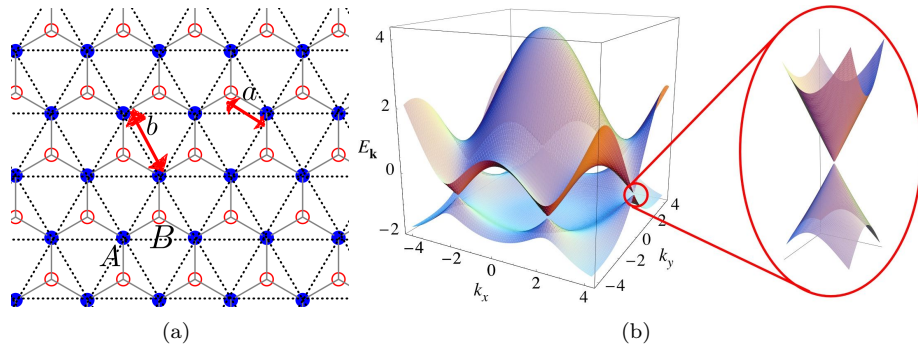Figure 7.1: (a) Lattice structure of graphene. The blue sites are marked as A, and the red, hollow sites are marked as B. The distance between two carbon atoms is a, and the lattice constant of the triangular lattice is $b = 2a\cos 30^{\circ}$. (b) Band structure of monolayer Graphene. The Dirac cones near the $\boldsymbol{K}$ points has been shown in the inset. Figure reprinted with permissions from [5]

7.2   Brillouin Zone and Band Structure

The 2D hexagonal structure does not form a lattice because the sites labelled A and B do not feel the same environment around them. However, we can describe the periodic structure of the system in terms of a triangular lattice with a basis of A and B atoms [16]. The Brillouin Zone is also hexagonal. Usually the origin of the reciprocal space is denoted as Γ. Among the six corners, any two next nearest corners can be connected by a reciprocal lattice vectors, and they are equivalent. As a result, only two of the six corners are independent. They are usually denoted by $\boldsymbol{K}(\frac{2\pi}{3b}, \frac{2\pi}{\sqrt{3}b})$ and $\boldsymbol{K}'(\frac{4\pi}{3b}, 0)$. Experimentally, graphene shows linear dispersion about these points.

To calculate the band structure of monolayer graphene, we can use a tight binding model with nearest neighbor hopping and equal on-site energy on all the sites (which we can set to zero). Then the Hamiltonian is, $H_0 = -t \sum_{\boldsymbol{R}} \sum_{\boldsymbol{r} \in \text{nearest neighbors}} |B(\boldsymbol{r} + \boldsymbol{R})\rangle \langle A(\boldsymbol{R})| + h.c.$.

We can write this in the reciprocal space,

$$H_0 = -t \sum_{\boldsymbol{k}} |\boldsymbol{k}\rangle \langle \boldsymbol{k}| \left[\sigma_x \left(1 + \cos\left(\frac{k_x b}{2} + \frac{k_y b \sqrt{3}}{2}\right) + \cos(k_x b) \right) + \sigma_y \left(\sin\left(\frac{k_x b}{2} + \frac{k_y b \sqrt{3}}{2}\right) + \sin(k_x b) \right) \right],$$

where $|A\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|B\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \equiv |A\rangle \langle B| + |B\rangle \langle A|$, and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \equiv -i |A\rangle \langle B| + i |B\rangle \langle A|$.

The energy eigenvalues of a Hamiltonian of the form $H = \boldsymbol{d} \cdot \boldsymbol{\sigma}$ are $\pm \sqrt{d_x^2 + d_y^2 + d_z^2}$. Using this formula, we can calculate the energy eigenvalues, $\varepsilon_{\boldsymbol{k}} = \pm t \sqrt{3 + 2 \cos \frac{k_x b}{2} \cos(k_y b \frac{\sqrt{3}}{2}) + 2 \cos k_x b}$.

The bandstructure is plotted in Fig. 7.1. The energy eigenvalues become 0 at $\boldsymbol{K}(\frac{2\pi}{3b}, \frac{2\pi}{\sqrt{3}b})$ and $\boldsymbol{K}'(\frac{4\pi}{3b}, 0)$ points. If we Taylor expand the energy eigenvalues about these points, the leading order terms are linear,

$$\varepsilon_q = \left[\frac{\sqrt{3}}{2} tb \right] q,$$

where $q = |\boldsymbol{k} - \boldsymbol{K}|$, or $|\boldsymbol{k} - \boldsymbol{K}|'$.

This dispersion is similar to that of a massless relativistic particle, and in two dimension, the energy-momentum relation forms a cone, termed as the Dirac cone (see Fig. 7.1(b)).

We can break the symmetry between the A, B sublattice points by introducing different on-site energies. This can be achieved by growing graphene on a Boron Nitride substrate, or by instead using a single layer Boron Nitride crystal instead (it also forms a hexagonal structure similar to graphene, with B and N atoms on the A and B sites, or vice versa.)

Then, the tight binding Hamiltonian would be, $H = H_0 + \sum_{\boldsymbol{R}} \varepsilon_A |A(\boldsymbol{R})\rangle \langle A(\boldsymbol{R})| + \varepsilon_B |B(\boldsymbol{R})\rangle \langle B(\boldsymbol{R})|$. Leaving out the constant $\frac{\varepsilon_A + \varepsilon_B}{2}$, we get,

$$\begin{aligned} H = \sum_{\boldsymbol{k}} |\boldsymbol{k}\rangle \langle \boldsymbol{k}| \bigg[&-t\sigma_x \left(1 + \cos\left(\frac{k_x b}{2} + \frac{k_y b \sqrt{3}}{2}\right) + \cos(k_x b) \right) \\ &- t\sigma_y \left(\sin\left(\frac{k_x b}{2} + \frac{k_y b \sqrt{3}}{2}\right) + \sin(k_x b) \right) + m\sigma_z \bigg], \end{aligned} \qquad (7.1)$$

with m being $\frac{\varepsilon_A - \varepsilon_B}{2}$.

The dispersion about $\boldsymbol{K}$ or $\boldsymbol{K}'$ points would be, $\varepsilon_q = \sqrt{m^2 + \frac{3t^2 b^2}{4} q^2}$, which is similar to $E = \sqrt{p^2 c^2 + m^2 c^4}$, the dispersion relation of a massive relativistic particle.

7.2.1   Berry Curvature and Chern Number

The Hamiltonian of any two-level system can be written as $\boldsymbol{d} \cdot \boldsymbol{\sigma}$, with $\boldsymbol{d} = (d_x, d_y, d_z)$ and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. If $d_{x,y,z}$ are functions of $\boldsymbol{k}$, then the z component of Berry curvature of the

ground state can be written as (see [15] for proof),

$$\Omega_z = \frac{1}{2}\hat{d} \cdot \left(\frac{\partial \hat{d}}{\partial k_x} \times \frac{\partial \hat{d}}{\partial k_y}\right) \tag{7.2}$$

(and cyclically exchange x, y, z for other components). Since the model has time reversal symmetry, $\mathbf{\Omega}(-\mathbf{k}) = -\mathbf{\Omega}(\mathbf{k})$, and the Chern number of monolayer graphene would be 0, and there would be no anomalous Hall response.

7.2.2   Selective Valley Population and Valley Chern Number

While the Chern number of the whole Band is zero (it is also zero if the bands are partially populated, because in equilibrium, the two valleys would be equally populated, and they have opposite Berry curvatures), the valleys can be selectively populated [9] with circularly polarized light. Let us first see what is the Chern number of a single Dirac cone (stretched upto infinite momentum) is.

Chern Number of a Single, Infinite Dirac Cone

Consider the Hamiltonian $H(\mathbf{k}) = k_x\sigma_x + k_y\sigma_y + m\sigma_z$. It has a dispersion relation $\varepsilon_{\mathbf{k}} = \pm\sqrt{k^2 + m^2}$. Here $\mathbf{d} = (k_x, k_y, m)$. Using the formula in Eq. (2.1), we get, $\mathbf{\Omega} = \frac{m}{2(k_x{}^2 + k_y{}^2 + m^2)^{3/2}}\hat{z}$. The corresponding Chern number is,

$$\mathcal{C} = \frac{1}{2\pi}\int_0^\infty \frac{m}{2\left(k^2 + m^2\right)^{3/2}}2\pi k\, dk = \frac{1}{2}.$$

This fractional Chern number is not of much concern, because we are not integrating over a closed, periodic surface.

Note that $\mathcal{C} = 0$ for $m = 0$, but it is $\frac{1}{2}$ for any finite but non-zero m.

7.2.3   Chern Number of a Single Valley in the Brillouin Zone

For simplicity, we can choose $t = -1$ in Eq. (7.1) (in other words, we scale the parameter m accordingly), and find the Chern Number for a single Valley in the Brillouin Zone. This can inded be experimentally achieved with cirlularly polarized electromagnetic waves [9]. This calculation is done in Mathematica (code available at [13]). We define a valley as the collection of points in the BZ, which are closer to one Dirac point than the other.
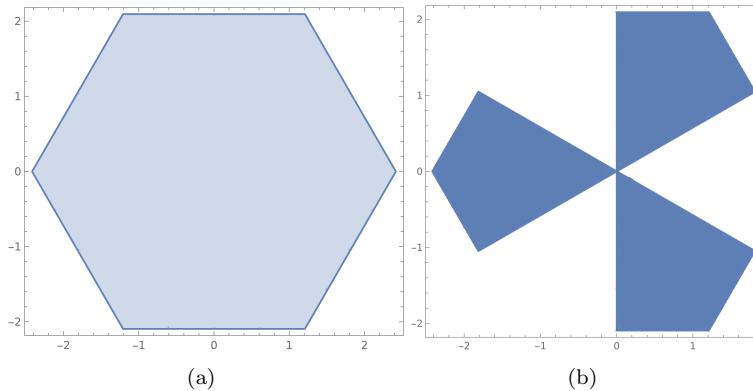

Figure 7.2: (a) The Brillouin Zone of a triangular lattice. (b) A single valley in the Brillouin Zone.

In the numerical calculation, it was found that the valley Chern number is zero when the mass term $m = 0$, while $\mathcal{C} \to \mp\frac{1}{2}$ as $m \to 0^+$ and 0^-. And, for the other valley, $\mathcal{C} \to \pm\frac{1}{2}$ as $m \to 0^+$ and 0^-. For large values of m, the valley Chern number gradually decreases, and approaches 0.
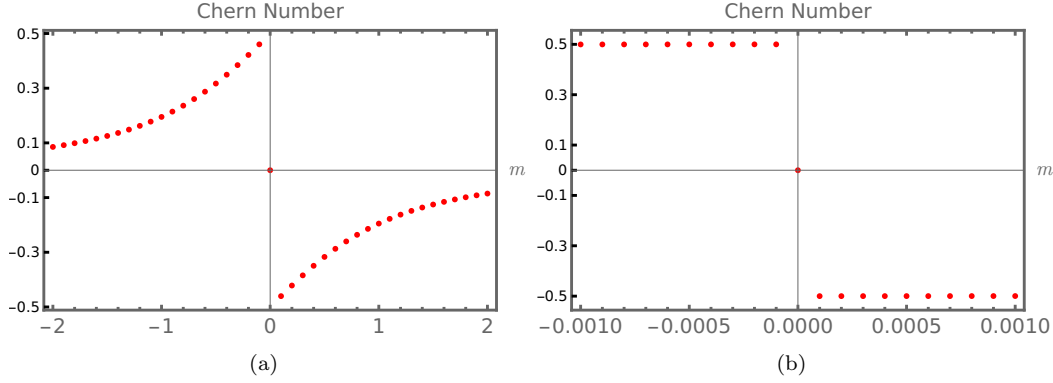
Figure 7.3: (a) Valley Chern Number as a function of m. (b) $\mathcal{C} \to \pm 0.5$ for very small values of m.

This fractional value of valley Chern number is, again, not of any concern because we did not integrate over the whole Brillouin Zone.

Note the valley Chern number is 0 exactly at $m = 0$, but it is $\pm\frac{1}{2}$ in the limit of $m \to 0$.

7.3   Bilayer Graphene and Effective Two Band Hamiltonian

In bilayer graphene, the electron can hop between the two layers, as well as within individual layers. Due to the interlayer hopping, the Dirac cones of the two layers would be hybridized.

We denote the localized Wannier functions as, $|A, 1\rangle = (1, 0, 0, 0)^T$, $|A, 2\rangle = (0, 1, 0, 0)^T$, $|B, 1\rangle = (0, 0, 1, 0)^T$ and $|B, 2\rangle = (0, 0, 0, 1)^T$, where A, B stand for the the sublattice, and $1, 2$ denote the layer index. Here we use the model proposed by Zhang, MacDonald and Mele [21], where the effective Hamiltonian near a Dirac Cone can be written as a sum of three terms,

$$H = H_1 + H_{int} + H_2.$$

Here H_1 is the intra-layer hopping Hamiltonian of monolayer graphene, $H_1 = \nu q_x \sigma_x \tau_0 + q_y \sigma_y \tau_0$, where $\nu = \pm 1$ depending on whether the Hamiltonian is describing the $\boldsymbol{K}$ or $\boldsymbol{K}'$ valley. The matrices $\sigma_{x,y,z}$ act on the A, B degree of freedom, while the matrices $\tau_{x,y,z}$ act on the degree of freedom of the two layers. H_{int} is the inter-layer hopping Hamiltonian [1]. When A site on the top layer hybridize with the A sites in the bottom layer, we can write, $H_{int} = \frac{\gamma(\sigma_x \tau_x + \sigma_y \tau_y)}{2}$, with γ being the hopping amplitude. We can also put an electric field perpendicular to the plane of the graphene sheets, and the two layers would have different potentials. This is modeled with the term, $H_2 = \Delta \sigma_0 \tau_z$.

7.3.1   Strategy for finding effective low energy Hamiltonian

If we find the eigenvectors for a general value of q_x, q_y, and write the Hamiltonian in terms of them, the effective Hamiltonian would be diagonal in them, $H_{eff} = d_z \sigma_z$. But, the Berry curvature (Eq. (7.2)) is always zero for such a Hamiltonian. We have to fix a value of (q_x, q_y), find a low energy basis, and then find the effective Hamiltonian in this basis. To find the effective

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[1]int stands for inter-layer, **not** interaction. The electrons are assumed to be non-interacting in this model.
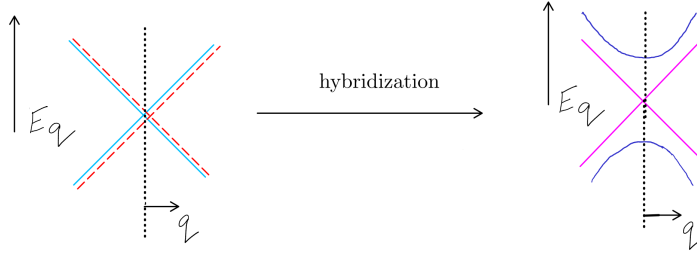
Figure 7.4: The Dirac cones of the two graphene layers (sky blue and red) are hybridized to form four bands. We want to calculate the effective Hamiltonian in the low energy subspace, comprising of the bands colored pink.

low energy subspace, we consider H_0 as a perturbation (notice that $H_0 = 0$ at $q_x = q_y = 0$.) Let us put $\gamma = 1$ for simplicity (i.e., we scale all other quantities with γ.)

$$\text{Then, } H_{int} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \text{ and } H_{int} + H_2 = \begin{pmatrix} \Delta & 0 & 0 & 0 \\ 0 & -\Delta & 1 & 0 \\ 0 & 1 & \Delta & 0 \\ 0 & 0 & 0 & -\Delta \end{pmatrix}.$$

The eigenvectors of H_{int} are, $|\phi_1\rangle \underbrace{=}_{E=0} (1,0,0,0)^T, |\phi_2\rangle \underbrace{=}_{E=0} (0,0,0,1)^T, |\phi_3\rangle \underbrace{=}_{E=1} \frac{1}{\sqrt{2}}(0,1,1,0)^T,$

$|\phi_4\rangle \underbrace{=}_{E=-1} \frac{1}{\sqrt{2}}(0,1,-1,0)^T.$

Let $P = |\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|$, the projector in the low energy subspace, and $Q = 1 - P = |\phi_3\rangle\langle\phi_3| + |\phi_4\rangle\langle\phi_4|$, the projector in the high energy subspace. Then, the effective form of H_1 in the low energy subspace would be, using the standard formula of degenerate perturbation theory,

$$H_{1,2} = PH_{int}P + PH_1Q\frac{1}{PH_{int}P - QH_{int}Q}QH_1P.$$

Since $PH_{int}P$ is already 0, we have, $H_{1,2} = -PH_1Q\frac{1}{H_{int}}QH_1P$. With all the quantities already defined, this calculation is straightforward to do, and we get (see Appendix I for details), $H_{1,2} = \begin{pmatrix} 0 & -(\nu q_x - iq_y)^2 \\ -(\nu q_x + iq_y)^2 & 0 \end{pmatrix} = -(q_x^2 - q_y^2)\tilde{\sigma}_x - 2\nu q_x q_y \tilde{\sigma}_y.$

$|\phi_1\rangle$ and $|\phi_2\rangle$, defined above, are also eigenvectors of H_2, with eigenvalues Δ and $-\Delta$, respectively.

$$(H_2)_{|\phi_1\rangle,|\phi_2\rangle} = \begin{pmatrix} \Delta & 0 \\ 0 & -\Delta \end{pmatrix} = \Delta\tilde{\sigma}_z$$

Since this term is already diagonal, we don't need to do calculate second order perturbation of this term.

Then the effective Hamiltonian in the low energy subspace is,

$$(H_{eff})_{|\phi_1\rangle,|\phi_2\rangle} = -(q_x^2 - q_y^2)\tilde{\sigma}_x - 2\nu q_x q_y \tilde{\sigma}_y + \Delta\tilde{\sigma}_z \tag{7.3}$$

Now we can employ the formula in Eq. 7.2, and find, $\boxed{\mathbf{\Omega}(\boldsymbol{q}) = \frac{2\nu\Delta(q_x^2 + q_y^2)}{((q_x^2 + q_y^2)^2 + \Delta^2)^{\frac{3}{2}}}\hat{z}}$. Its integral

over the BZ is 0, because the two valleys $\boldsymbol{K}$ and $\boldsymbol{K}'$ have opposite signs of ν. This is expected, because the model has time reversal symmetry, and the overall band Chern number is 0.

However, if we can selectively fill one of the valleys (this can be done with circularly polarized light), then we can get a non-zero anomalous Hall response. The Berry curvature falls off very

quickly as a function of q, and to estimate the Chern number of a single valley, we can integrate from $q = 0$ to ∞.

The Chern number of a single valley is then, $\boxed{\mathcal{C}_\nu \approx \dfrac{1}{2\pi} \int_0^\infty \dfrac{2\nu \Delta q^2}{(q^4 + \Delta^2)^{\frac{3}{2}}} 2\pi q \, dq = \nu = \pm 1}$.

7.4 Fractional Chern Numbers?

7.4.1 Argument why Chern number should be an integer
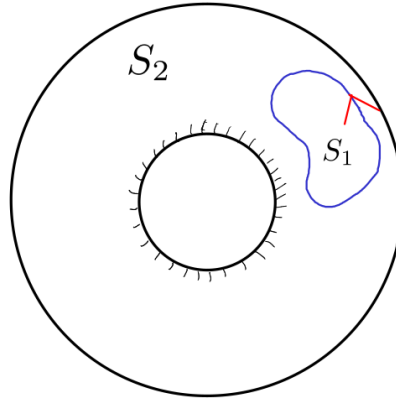
Figure 7.5: The Brillouin Zone is a Torus.

The Brillouin Zone is periodic in k_x and k_y, and can be mapped to a torus. Suppose a Bloch wavepacket moves along the blue curve, and returns to its initial position (see Fig. 7.5). Then, the geometric phase acquired by the electron would be, $\oint \boldsymbol{A}(\boldsymbol{k}) \cdot d\boldsymbol{k}$. Using Stokes' theorem, we can rewrite this as, $\int_{S_1} \nabla \times \boldsymbol{A}(\boldsymbol{k}) d^2 k$, and the phase factor is, $e^{i \int_{S_1} \nabla \times \boldsymbol{A}(\boldsymbol{k}) d^2 k}$. But, we could apply Stokes' theorem on the other surface, S_2, and rewrite the phase factor as, $e^{-i \int_{S_2} \nabla \times \boldsymbol{A}(\boldsymbol{k}) d^2 k}$. The negative sign appears due to the opposite orientation. However, since the overall phase factor has to be unique (because it can be found with interference experiments), we must have, $e^{i \int_{S_1} \nabla \times \boldsymbol{A}(\boldsymbol{k}) d^2 k} = e^{-i \int_{S_2} \nabla \times \boldsymbol{A}(\boldsymbol{k}) d^2 k}$, which implies, $e^{i \int_{BZ} \nabla \times \boldsymbol{A}(\boldsymbol{k}) d^2 k} = 1$.

Then, we must have, $\int_{BZ} \nabla \times \boldsymbol{A}(\boldsymbol{k}) d^2 k = 2n\pi$, with $n \in \mathbb{Z}$, implying that the Chern number $\mathcal{C} = \frac{1}{2\pi} \int_{BZ} \nabla \times \boldsymbol{A}(\boldsymbol{k}) d^2 k$ is an integer.

7.4.2 Possible explanation for half-integer Chern numbers

We see half integer Chern numbers when there is a band gap closing, which causes $\boldsymbol{\Omega}$ to diverge at the point of band gap closing. Our argument in the previous section does not anymore hold because we cannot apply the result of Stokes' theorem, as $\boldsymbol{\Omega}$ is not well defined at all points on the Brillouin Zone.

Chapter 8

New results

(needs to be updated with details)

1. Expression of electric and thermal Conductivity tensors when both Magnetic field and Berry Curvature are present (upto linear order in Magnetic field)

2. A condition on the energy magnetization that needs to hold for anomalous thermal current to satisfy the Einstein relation.

Appendix A

Time evolution of Crystal Momentum

text

Appendix B

Calculation of expectation value of the position of the wavepacket

We want to build a wavepacket centered about $\boldsymbol{r} = \boldsymbol{r}_0, \boldsymbol{k} = \boldsymbol{k}_0$. The calculation of this appendix is loosely based on Ref. [14].

Let $w(\boldsymbol{k} - \boldsymbol{k}_0)$ be a real weight function, sharply peaked at $\boldsymbol{k}_0$. If we take a wavepacket of the form $\int d\boldsymbol{k} w(\boldsymbol{k} - \boldsymbol{k}_0) e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_0} \left(e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{n,\boldsymbol{k}}(\boldsymbol{r}) \right)$, it may not be sharply peaked at $\boldsymbol{r} = \boldsymbol{r}_0$, because, although the functions $e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)}$ interfere constructively about $\boldsymbol{r} = \boldsymbol{r}_0$, the functions $u_{n,\boldsymbol{k}}(\boldsymbol{r}_0)$ may have different phases for different values of $\boldsymbol{k}$. To take account of this, let us consider the wavefunction,

$$\phi_{\boldsymbol{X}}(\boldsymbol{r}, t=0) = \int d\boldsymbol{k} w(\boldsymbol{k} - \boldsymbol{k}_0) e^{i\boldsymbol{X}(\boldsymbol{k_0})\cdot(\boldsymbol{k}-\boldsymbol{k}_0)} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_0} \left(e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{n,\boldsymbol{k}}(\boldsymbol{r}) \right) \tag{B.1}$$

B.1 Normalization

Let us choose the normalization of the individual Bloch wavefunctions such that

$$\int_{\text{unit cell}} d\boldsymbol{r} |u_{n,\boldsymbol{k}}(\boldsymbol{r})|^2 = 1 \tag{B.2}$$

Then, $\langle \phi_{\boldsymbol{X}}(\boldsymbol{r}, t=0) | \phi_{\boldsymbol{X}}(\boldsymbol{r}, t=0) \rangle$

$$= \int_{\text{all space}} d\boldsymbol{r} \int \int d\boldsymbol{k}_2 d\boldsymbol{k}_1 w(\boldsymbol{k}_1 - \boldsymbol{k}_0) w(\boldsymbol{k}_2 - \boldsymbol{k}_0) e^{i\boldsymbol{X}(\boldsymbol{k_0})\cdot(\boldsymbol{k}_1-\boldsymbol{k}_2)} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r}) u_{n,\boldsymbol{k}_1}(\boldsymbol{r})$$

Let us perform the $\boldsymbol{r}$ integral first. We can utilize the periodicity of $u_{n,\boldsymbol{k}_1}$ and rewrite,

$$\int_{\text{all space}} d\boldsymbol{r} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r}) u_{n,\boldsymbol{k}_1}(\boldsymbol{r})$$

$$= \sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{R}} \int_{\text{unit cell}} d\boldsymbol{r} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r}) u_{n,\boldsymbol{k}_1}(\boldsymbol{r})$$

where the index $\boldsymbol{R}$ runs over the coordinates of the unit cells, and the integral is over a single unit cell (and it is the same for every unit cell). The sum is zero unless $\boldsymbol{k}_1 - \boldsymbol{k}_2$ is a reciprocal lattice vector (because otherwise, the phase factors $e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{R}}$ would all cancel each other). Since both $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ belong to the first Brillouin zone, we must have $\boldsymbol{k}_1 = \boldsymbol{k}_2$. For a finite system with N unit cells, $\boldsymbol{k}$ can only take discrete values, and the sum is $N\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}$. When N is large, the points in reciprocal space are dense, and we can approximate, $\sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{R}} \to \frac{1}{V_c} \int d\boldsymbol{r} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}} =$

$\frac{(2\pi)^d}{V_c}\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2)$, where V_c is the volume of the d dimensional unit cell. We can further write $\frac{(2\pi)^d}{V_c} = V_{\text{BZ}}$, where V_{BZ} is the volume of the Brillouin zone.

Also, when $\boldsymbol{k}_1 = \boldsymbol{k}_2$, the periodic part of the sum, $\int_{\text{unit cell}} d\boldsymbol{r} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r}) u_{n,\boldsymbol{k}_1}(\boldsymbol{r}) = 1$, due to normalization of Bloch wavefunctions (Eq. (B.2)). Finally, we get,

$$\int_{\text{all space}} d\boldsymbol{r} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r}) u_{n,\boldsymbol{k}_1}(\boldsymbol{r}) = V_{\text{BZ}}\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2)$$

Then, $\langle \phi_{\boldsymbol{X}}(\boldsymbol{r}, t = 0)|\phi_{\boldsymbol{X}}(\boldsymbol{r}, t = 0)\rangle$

$$= V_{\text{BZ}} \int\int d\boldsymbol{k}_2 d\boldsymbol{k}_1 \delta(\boldsymbol{k}_1 - \boldsymbol{k}_2) w(\boldsymbol{k}_1 - \boldsymbol{k}_0) w(\boldsymbol{k}_2 - \boldsymbol{k}_0) e^{i\boldsymbol{X}(\boldsymbol{k_0})\cdot(\boldsymbol{k}_1 - \boldsymbol{k}_2)} = V_{\text{BZ}} \int d\boldsymbol{k}[w(\boldsymbol{k} - \boldsymbol{k}_0)]^2$$

Then, have to scale $w(\boldsymbol{k} - \boldsymbol{k}_0)$ such that

$$\int d\boldsymbol{k}[w(\boldsymbol{k} - \boldsymbol{k}_0)]^2 = \frac{1}{V_{\text{BZ}}} \tag{B.3}$$

B.2 Calculation of $\langle \boldsymbol{r} \rangle$

Result: For this wavefunction,

$$\langle \boldsymbol{r} \rangle_{\phi_{\boldsymbol{X}}} = \langle \phi_X(t=0)|\, \boldsymbol{r}\, |\phi_X(t=0)\rangle = \boldsymbol{r}_0 - \boldsymbol{X}(\boldsymbol{k}_0) + \boldsymbol{A}(\boldsymbol{k}_0) \tag{B.4}$$

where $\boldsymbol{A}(\boldsymbol{k}_0)$ is the Berry connection.

Proof: For convenience, let us calculate $\langle \phi_X(\boldsymbol{r}, t=0)|\, \boldsymbol{r} - \boldsymbol{r}_0\, |\phi_X(\boldsymbol{r}, t=0)\rangle$

$$= \int\int d\boldsymbol{k}_1 d\boldsymbol{k}_2 w(\boldsymbol{k}_2 - \boldsymbol{k}_0) w(\boldsymbol{k}_1 - \boldsymbol{k}_0) e^{-i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_2 - \boldsymbol{k}_0)} e^{-i\boldsymbol{k}_2\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r})(\boldsymbol{r}-\boldsymbol{r}_0) e^{i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1-\boldsymbol{k}_0)} e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_1}(\boldsymbol{r})$$

Let us rewrite, $(\boldsymbol{r} - \boldsymbol{r}_0) e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} = \frac{1}{i}\nabla_{\boldsymbol{k}_1} e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)}$.
Then, $w(\boldsymbol{k}_1 - \boldsymbol{k}_0)(\boldsymbol{r} - \boldsymbol{r}_0) e^{i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1-\boldsymbol{k}_0)} e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_1}(\boldsymbol{r})$

$$= \frac{1}{i}\left[\nabla_{\boldsymbol{k}_1} e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)}\right] w(\boldsymbol{k}_1 - \boldsymbol{k}_0) e^{i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1-\boldsymbol{k}_0)} u_{n,\boldsymbol{k}_1}(\boldsymbol{r})$$

$$= \frac{1}{i}\nabla_{\boldsymbol{k}_1}\left[e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} w(\boldsymbol{k}_1 - \boldsymbol{k}_0) e^{i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1-\boldsymbol{k}_0)} u_{n,\boldsymbol{k}_1}(\boldsymbol{r})\right] - \frac{1}{i} e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)}\nabla_{\boldsymbol{k}_1}\left[w(\boldsymbol{k}_1 - \boldsymbol{k}_0) e^{i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1-\boldsymbol{k}_0)} u_{n,\boldsymbol{k}_1}(\boldsymbol{r})\right].$$

The first term would be zero when integrated over $\boldsymbol{k}_1$, because the sharply peaked weight $w(\boldsymbol{k}_1 - \boldsymbol{k}_0) \to 0$, far away from $\boldsymbol{k}_0$. Let us then look at the second term, $-\frac{1}{i} e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)}\nabla_{\boldsymbol{k}_1}\left[w(\boldsymbol{k}_1 - \boldsymbol{k}_0) e^{i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1-\boldsymbol{k}_0)} u_{n,\boldsymbol{k}_1}(\boldsymbol{r})\right]$

$$= -\frac{1}{i} e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} e^{i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1-\boldsymbol{k}_0)}\left[\nabla_{\boldsymbol{k}_1} w(\boldsymbol{k}_1 - \boldsymbol{k}_0) u_{n,\boldsymbol{k}_1}(\boldsymbol{r}) + w(\boldsymbol{k}_1 - \boldsymbol{k}_0)\nabla_{\boldsymbol{k}_1} u_{n,\boldsymbol{k}_1}(\boldsymbol{r}) + i\boldsymbol{X}(\boldsymbol{k}_0) w(\boldsymbol{k}_1 - \boldsymbol{k}_0) u_{n,\boldsymbol{k}_1}(\boldsymbol{r})\right]$$

Let us first take the first of the three terms in the third bracket, and calculate its contribution to $\langle \boldsymbol{r} - \boldsymbol{r}_0\rangle_{\phi_{\boldsymbol{X}}}$, which we denote as $\langle \boldsymbol{r} - \boldsymbol{r}_0\rangle_1$

$$= -\int_{\boldsymbol{r}}\int_{\boldsymbol{k}_1}\int_{\boldsymbol{k}_2} w(\boldsymbol{k}_2 - \boldsymbol{k}_0) e^{-i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_2-\boldsymbol{k}_0)} e^{-i\boldsymbol{k}_2\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r})\left[e^{i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1-\boldsymbol{k}_0)} e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)}\nabla_{\boldsymbol{k}_1} w(\boldsymbol{k}_1 - \boldsymbol{k}_0) u_{n,\boldsymbol{k}_1}(\boldsymbol{r})\right]$$

Now, when we integrate over $\boldsymbol{r}$, we would get a factor of $\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2)$, which would force $k_1 = k_2$. Then, we would get a factor, $\int d\boldsymbol{k} w(\boldsymbol{k} - \boldsymbol{k}_0)\nabla_{\boldsymbol{k}} w(\boldsymbol{k} - \boldsymbol{k}_0)$. The first term being sharply peaked at $\boldsymbol{k}_0$ would pick out the second term at $\boldsymbol{k}_0 = \boldsymbol{k}$. But $\nabla_{\boldsymbol{k}} w(\boldsymbol{k} - \boldsymbol{k}_0)|_{(\boldsymbol{k} - \boldsymbol{k}_0)} = 0$, as $\boldsymbol{k}_0$ is a maxima of $w(\boldsymbol{k} - \boldsymbol{k}_0)$. As a result, this term is 0.

Now consider the second term, $\langle \boldsymbol{r} - \boldsymbol{r}_0\rangle_2$

$$= -\frac{1}{i}\int_{\boldsymbol{r}}\int_{\boldsymbol{k}_1}\int_{\boldsymbol{k}_2} w(\boldsymbol{k}_2 - \boldsymbol{k}_0) e^{-i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_2-\boldsymbol{k}_0)} e^{-i\boldsymbol{k}_2\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r})\left[e^{i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1-\boldsymbol{k}_0)} e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} w(\boldsymbol{k}_1 - \boldsymbol{k}_0)\nabla_{\boldsymbol{k}_1} u_{n,\boldsymbol{k}_1}(\boldsymbol{r})\right]$$

When we integrate over $\boldsymbol{r}$, we get,

$$\int_{\text{all space}} d\boldsymbol{r} e^{i(\boldsymbol{k}_1 - \boldsymbol{k}_2)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r}) \nabla_{\boldsymbol{k}_1} u_{n,\boldsymbol{k}_1}(\boldsymbol{r})$$

$$= \sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}_1 - \boldsymbol{k}_2)\cdot\boldsymbol{R}} \int_{\text{unit cell}} d\boldsymbol{r} e^{i(\boldsymbol{k}_1 - \boldsymbol{k}_2)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r}) \nabla_{\boldsymbol{k}_1} u_{n,\boldsymbol{k}_1}(\boldsymbol{r})$$

$$= V_{\text{BZ}}\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2) \int_{\text{unit cell}} d\boldsymbol{r} e^{i(\boldsymbol{k}_1 - \boldsymbol{k}_2)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r}) \nabla_{\boldsymbol{k}_1} u_{n,\boldsymbol{k}_1}(\boldsymbol{r})$$

$$= V_{\text{BZ}}\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2) \int_{\text{unit cell}} d\boldsymbol{r} u_{n,\boldsymbol{k}_1}^*(\boldsymbol{r}) \nabla_{\boldsymbol{k}_1} u_{n,\boldsymbol{k}_1}(\boldsymbol{r})$$

$$= V_{\text{BZ}}\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2) \frac{1}{i} \boldsymbol{A}(\boldsymbol{k}_1)$$

Putting this back in the expression of $\langle \boldsymbol{r} - \boldsymbol{r}_0 \rangle_2$, and carrying out the integral over the delta function, we get,

$$\langle \boldsymbol{r} - \boldsymbol{r}_0 \rangle_2 = -\frac{1}{i} \int_{\boldsymbol{k}_1} [w(\boldsymbol{k}_1 - \boldsymbol{k}_0)]^2 \frac{1}{i} \boldsymbol{A}(\boldsymbol{k}_1) V_{\text{BZ}} \approx \boldsymbol{A}(\boldsymbol{k}_0) \int_{\boldsymbol{k}_1} [w(\boldsymbol{k}_1 - \boldsymbol{k}_0)]^2 V_{\text{BZ}} = \boldsymbol{A}(\boldsymbol{k}_0),$$

using the normalization condition in Eq. (B.3).

Let us know take the final term inside the third bracket, $i\boldsymbol{X}(\boldsymbol{k}_0)w(\boldsymbol{k}_1 - \boldsymbol{k}_0)u_{n,\boldsymbol{k}_1}(\boldsymbol{r})$. Its contribution to $\langle \boldsymbol{r} - \boldsymbol{r}_0 \rangle$ is, $\langle \boldsymbol{r} - \boldsymbol{r}_0 \rangle_3$

$$= -\frac{1}{i} \int_{\boldsymbol{r}} \int_{\boldsymbol{k}_1} \int_{\boldsymbol{k}_2} w(\boldsymbol{k}_2 - \boldsymbol{k}_0) e^{-i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_2 - \boldsymbol{k}_0)} e^{-i\boldsymbol{k}_2\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} u_{n,\boldsymbol{k}_2}^*(\boldsymbol{r}) \left[e^{i\boldsymbol{X}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1 - \boldsymbol{k}_0)} e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} i\boldsymbol{X}(\boldsymbol{k}_0)w(\boldsymbol{k}_1 - \boldsymbol{k}_0)u_{n,\boldsymbol{k}_1}(\boldsymbol{r}) \right]$$

$$= -\boldsymbol{X}(\boldsymbol{k}_0) \langle \phi_{\boldsymbol{X}}(t=0)|\phi_{\boldsymbol{X}}(t=0) \rangle = -\boldsymbol{X}(\boldsymbol{k}_0)$$

Adding all the non-zero terms, we get, $\langle \boldsymbol{r} - \boldsymbol{r}_0 \rangle_{\phi_{\boldsymbol{X}}} = \boldsymbol{A}(\boldsymbol{k}_0) - \boldsymbol{X}(\boldsymbol{k}_0)$, from which Eq. (B.4) follows.

B.3   Wavepacket centered at $\boldsymbol{r}_0$

We found that the wavepacket in Eq. (B.1) is centered at $\boldsymbol{r}_0 - \boldsymbol{X}(\boldsymbol{k_0}) + \boldsymbol{A}(\boldsymbol{k_0})$. Then, to get a wavepacket centered at $\boldsymbol{r}_0$, we need to choose $\boldsymbol{X} = \boldsymbol{A}$, and the desired wavefunction is,

$$\phi_{\boldsymbol{X}}(\boldsymbol{r}, t=0) = \int d\boldsymbol{k}\, w(\boldsymbol{k} - \boldsymbol{k}_0) e^{i\boldsymbol{A}(\boldsymbol{k_0})\cdot(\boldsymbol{k}-\boldsymbol{k}_0)} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_0} \left(e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{n,\boldsymbol{k}}(\boldsymbol{r}) \right) \tag{B.5}$$

B.4   Calculation of the center of the time evolved wavepacket

Recall the the state $e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{\boldsymbol{k}}(\boldsymbol{r})$ evolves as, $e^{i\boldsymbol{k}+\Delta\boldsymbol{k}\cdot\boldsymbol{r}} e^{i\boldsymbol{A}(\boldsymbol{k})\cdot\Delta\boldsymbol{k}} e^{-\frac{i\varepsilon_{\boldsymbol{k}}\Delta t}{\hbar}} u_{\boldsymbol{k}+\Delta\boldsymbol{k}}(\boldsymbol{r})$. Then the wavefunction of the wavepacket is,

$$\psi(\boldsymbol{r}, \Delta t) = \int d\boldsymbol{k}\, w(\boldsymbol{k} - \boldsymbol{k}_0) e^{i\boldsymbol{A}(\boldsymbol{k_0})\cdot(\boldsymbol{k}-\boldsymbol{k}_0)} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_0} \left(e^{i(\boldsymbol{k}+\Delta\boldsymbol{k})\cdot\boldsymbol{r}} e^{i\boldsymbol{A}(\boldsymbol{k})\cdot\Delta\boldsymbol{k}} e^{-i\frac{\varepsilon_{\boldsymbol{k}}\Delta t}{\hbar}} u_{n,\boldsymbol{k}+\Delta\boldsymbol{k}} \right).$$

Let $\boldsymbol{k} + \Delta\boldsymbol{k} = \boldsymbol{k}'$. Note that upto linear order in Δt, $\Delta\boldsymbol{k} = \Delta\boldsymbol{k}'$. Then, after changing variables in the integral,

$$\psi(\boldsymbol{r}, \Delta t) = \int d\boldsymbol{k}'\, w(\boldsymbol{k}' - \Delta\boldsymbol{k} - \boldsymbol{k}_0) e^{i\boldsymbol{A}(\boldsymbol{k_0})\cdot(\boldsymbol{k}'-\Delta\boldsymbol{k}-\boldsymbol{k}_0)} e^{-i(\boldsymbol{k}'-\Delta\boldsymbol{k})\cdot\boldsymbol{r}_0} \left(e^{i\boldsymbol{k}'\cdot\boldsymbol{r}} e^{i\boldsymbol{A}(\boldsymbol{k}'-\Delta\boldsymbol{k})\cdot\Delta\boldsymbol{k}} e^{-i\frac{\varepsilon_{\boldsymbol{k}}\Delta t}{\hbar}} u_{n,\boldsymbol{k}'} \right)$$

$$= e^{i\left(\Delta\boldsymbol{k}_0\cdot\boldsymbol{r}_0 - \frac{\varepsilon_{\boldsymbol{k}}\Delta t}{\hbar}\right)} \int d\boldsymbol{k}'\, w(\boldsymbol{k}' - \Delta\boldsymbol{k} - \boldsymbol{k}_0) e^{i\boldsymbol{A}(\boldsymbol{k_0})\cdot(\boldsymbol{k}'-\boldsymbol{k}_0)} e^{i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} e^{i[\boldsymbol{A}(\boldsymbol{k}'-\Delta\boldsymbol{k})-\boldsymbol{A}(\boldsymbol{k_0})]\cdot\Delta\boldsymbol{k}} e^{-i\frac{\nabla\varepsilon_{\boldsymbol{k}}\cdot(\boldsymbol{k}'-\boldsymbol{k}_0)}{\hbar}} u_{n,\boldsymbol{k}'}$$

The weight function will force $\Delta\boldsymbol{k} = \Delta\boldsymbol{k}|_{\boldsymbol{k}=\boldsymbol{k}_0} \equiv \Delta\boldsymbol{k}_0$. We first simplify, $\boldsymbol{A}(\boldsymbol{k}' - \Delta\boldsymbol{k}) - \boldsymbol{A}(\boldsymbol{k}_0) = \left((\boldsymbol{k}' - \Delta\boldsymbol{k} - \boldsymbol{k}_0) \cdot \nabla_{\boldsymbol{k}}\right)\boldsymbol{A}(\boldsymbol{k}_0)$. Then,

$$
\begin{aligned}
\Delta\boldsymbol{k}_0 \cdot [\boldsymbol{A}(\boldsymbol{k}' - \Delta\boldsymbol{k}') - \boldsymbol{A}(\boldsymbol{k}_0)] &= \Delta\boldsymbol{k}_0 \cdot [((\boldsymbol{k}' - \Delta\boldsymbol{k} - \boldsymbol{k}_0) \cdot \nabla_{\boldsymbol{k}})\,\boldsymbol{A}(\boldsymbol{k}_0)] \\
&= \Delta k_{0\,\mu}(\boldsymbol{k}' - \Delta\boldsymbol{k} - \boldsymbol{k}_0)_\nu \partial_\nu A_\mu(\boldsymbol{k}_0) \\
&= (\boldsymbol{k}' - \Delta\boldsymbol{k} - \boldsymbol{k}_0) \cdot \nabla_{\boldsymbol{k}}\left(\boldsymbol{A}(\boldsymbol{k}) \cdot \Delta\boldsymbol{k}_0\right)|_{\boldsymbol{k}=\boldsymbol{k}_0}
\end{aligned}
$$

Using the result from Eq. (B.4),

$$
\begin{aligned}
\langle\boldsymbol{r} - \boldsymbol{r}_0\rangle(\Delta t) &= \boldsymbol{A}(\boldsymbol{k}_0 + \Delta\boldsymbol{k}_0) - \boldsymbol{A}(\boldsymbol{k}_0) - \nabla_{\boldsymbol{k}_0}(\boldsymbol{A}(\boldsymbol{k}_0) \cdot \Delta\boldsymbol{k}_0) + \frac{1}{\hbar}\nabla_{\boldsymbol{k}_0}\varepsilon_{\boldsymbol{k}_0}\Delta t \\
&= (\Delta\boldsymbol{k}_0 \cdot \nabla)\boldsymbol{A}(\boldsymbol{k}_0) - \nabla_{\boldsymbol{k}_0}(\boldsymbol{A}(\boldsymbol{k}_0) \cdot \Delta\boldsymbol{k}_0) + \frac{1}{\hbar}\nabla_{\boldsymbol{k}_0}\varepsilon_{\boldsymbol{k}_0}\Delta t \\
&= -\Delta\boldsymbol{k}_0 \times (\nabla \times \boldsymbol{A}(\boldsymbol{k}_0)) + \frac{1}{\hbar}\nabla_{\boldsymbol{k}_0}\varepsilon_{\boldsymbol{k}_0}\Delta t \\
&= -\Delta\boldsymbol{k}_0 \times \boldsymbol{\Omega} + \frac{1}{\hbar}\nabla_{\boldsymbol{k}_0}\varepsilon_{\boldsymbol{k}_0}\Delta t
\end{aligned}
$$

Then,

$$
\langle\dot{\boldsymbol{r}}\rangle = \frac{\langle\boldsymbol{r} - \boldsymbol{r}_0\rangle(\Delta t) - \langle\boldsymbol{r} - \boldsymbol{r}_0\rangle(0)}{\Delta t} = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} - \dot{\boldsymbol{k}} \times \boldsymbol{\Omega}.
$$

Appendix C

Evolution of phase space volume

A volume element ΔV in phase space evolves as, $\frac{1}{\Delta V}\frac{d\Delta V}{dt} = \nabla_{\boldsymbol{r}} \cdot \dot{\boldsymbol{r}} + \nabla_{\boldsymbol{k}} \cdot \dot{\boldsymbol{k}}$. We would show that $(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega})\Delta V$ is a constant of motion.

C.0.1 Result: $\nabla_{\boldsymbol{k}} \cdot \boldsymbol{\Omega}(\boldsymbol{k}) = 0$

Since $\boldsymbol{\Omega} = i\int_{\text{unit cell}} d\boldsymbol{r}\nabla_{\boldsymbol{k}}u_{\boldsymbol{k}}^* \times \nabla_{\boldsymbol{k}}u_{\boldsymbol{k}}$,

$$\nabla_{\boldsymbol{k}} \cdot \boldsymbol{\Omega} = i\int_{\text{unit cell}} d\boldsymbol{r}\,\underbrace{(\nabla_{\boldsymbol{k}} \times \nabla_{\boldsymbol{k}}u_{\boldsymbol{k}}^*)}_{0} \cdot \nabla_{\boldsymbol{k}}u_{\boldsymbol{k}} - \underbrace{(\nabla_{\boldsymbol{k}} \times \nabla_{\boldsymbol{k}}u_{\boldsymbol{k}})}_{0} \cdot \nabla_{\boldsymbol{k}}u_{\boldsymbol{k}}^* = 0$$

Alternatively, $\nabla_{\boldsymbol{k}} \cdot \boldsymbol{\Omega} = \nabla_{\boldsymbol{k}} \cdot (\nabla_{\boldsymbol{k}} \times \boldsymbol{A}(\boldsymbol{k})) = 0$.

C.1 Calculation of evolution of volume element

We would also use that the magnetic field is divergenceless, $\nabla_{\boldsymbol{r}} \cdot \boldsymbol{B} = 0$. From Eq. (??),

$$\dot{\boldsymbol{r}} = \frac{\frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} + \frac{e}{\hbar}\boldsymbol{E} \times \boldsymbol{\Omega} + \frac{e}{\hbar^2}(\boldsymbol{\Omega} \cdot \nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}})\boldsymbol{B}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}$$

Only derivative of the denominator would contribute when we calculate its divergence. It follows that,

$$\nabla_{\boldsymbol{r}} \cdot \dot{\boldsymbol{r}} = -\frac{\nabla_{\boldsymbol{r}}(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega})}{(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega})} \cdot \dot{\boldsymbol{r}} = -\nabla_{\boldsymbol{r}}\log\left(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}\right) \cdot \dot{\boldsymbol{r}}$$

From Eq. 2.8,

$$\dot{\boldsymbol{k}} = -\frac{\frac{e}{\hbar}\boldsymbol{E} + \frac{e}{\hbar^2}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} \times \boldsymbol{B} + \frac{e^2}{\hbar^2}(\boldsymbol{E} \cdot \boldsymbol{B})\boldsymbol{\Omega}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}.$$

When we calculate its divergence, only the denominator contributes (the divergence of the numerator is 0), as Ω is divergenceless, and $\nabla_k \cdot (\varepsilon_{\boldsymbol{k}} \times \boldsymbol{B}) = (\nabla_k \times \varepsilon_{\boldsymbol{k}}) \cdot \boldsymbol{B} = 0$.

Then,

$$\nabla_{\boldsymbol{k}} \cdot \dot{\boldsymbol{k}} = -\frac{\nabla_{\boldsymbol{r}}(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega})}{(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega})} \cdot \dot{\boldsymbol{k}} = -\nabla_{\boldsymbol{k}}\log\left(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}\right) \cdot \dot{\boldsymbol{k}}$$

Then,

$$\nabla_{\boldsymbol{r}} \cdot \dot{\boldsymbol{r}} + \nabla_{\boldsymbol{k}} \cdot \dot{\boldsymbol{k}} = -\nabla_{\boldsymbol{k}}\log\left(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}\right) \cdot \dot{\boldsymbol{k}} - \nabla_{\boldsymbol{r}}\log\left(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}\right) \cdot \dot{\boldsymbol{r}}$$

$$= -\frac{d}{dt}\log\left(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}\right)$$

Therefore, $\frac{d}{dt}\log(\Delta V) = -\frac{d}{dt}\log\left(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}\right)$, i.e. $\frac{d}{dt}\log[\Delta V(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega})] = 0$. It follows that $(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega})\Delta V$ is a constant of motion.

Appendix D

Decoupling of equations of motion

Recall the coupled equations of motion,

$$\dot{\boldsymbol{r}} = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} - \dot{\boldsymbol{k}} \times \boldsymbol{\Omega} \tag{D.1}$$

$$\hbar\dot{\boldsymbol{k}} = -e\left(\boldsymbol{E} + \dot{\boldsymbol{r}} \times \boldsymbol{B}\right) \tag{D.2}$$

Dotting (D.2) with $\boldsymbol{B}$, we get $\boldsymbol{B} \cdot \dot{\boldsymbol{k}} = -\frac{e}{\hbar}\boldsymbol{E} \cdot \boldsymbol{B}$. Substituting the expression of $\dot{\boldsymbol{r}}$ from (D.1) into (D.2), we get,

$$\hbar\dot{\boldsymbol{k}} = -e\boldsymbol{E} + e\boldsymbol{B} \times \left(\frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} - \dot{\boldsymbol{k}} \times \boldsymbol{\Omega}\right)$$

$$= -e\boldsymbol{E} + \frac{e}{\hbar}\boldsymbol{B} \times \nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} - e(\boldsymbol{B} \cdot \boldsymbol{\Omega})\dot{\boldsymbol{k}} + e(\boldsymbol{B} \cdot \dot{\boldsymbol{k}})\boldsymbol{\Omega}$$

Substituting the expression of $\boldsymbol{B} \cdot \dot{\boldsymbol{k}}$ into the above expression,

$$\hbar\dot{\boldsymbol{k}} = -e\boldsymbol{E} + \frac{e}{\hbar}\boldsymbol{B} \times \nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} - e(\boldsymbol{B} \cdot \boldsymbol{\Omega})\dot{\boldsymbol{k}} - \frac{e^2}{\hbar}(\boldsymbol{E} \cdot \boldsymbol{B})\boldsymbol{\Omega}$$

Collecting the terms containing $\dot{\boldsymbol{k}}$,

$$\hbar\dot{\boldsymbol{k}}\left(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}\right) = -e\boldsymbol{E} - \frac{e}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} \times \boldsymbol{B} - \frac{e^2}{\hbar}(\boldsymbol{E} \cdot \boldsymbol{B})\boldsymbol{\Omega}$$

Finally,

$$\boxed{\dot{\boldsymbol{k}} = -\frac{\frac{e}{\hbar}\boldsymbol{E} + \frac{e}{\hbar^2}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} \times \boldsymbol{B} + \frac{e^2}{\hbar^2}(\boldsymbol{E} \cdot \boldsymbol{B})\boldsymbol{\Omega}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}} \tag{D.3}$$

Substituting the expression of $\dot{\boldsymbol{k}}$ from Eq. (D.3) to (D.1), we get,

$$\dot{\boldsymbol{r}} = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} + \frac{\left(\frac{e}{\hbar}\boldsymbol{E} + \frac{e}{\hbar^2}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} \times \boldsymbol{B}\right) \times \boldsymbol{\Omega}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}$$

$$= \frac{\frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}}(1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}) + \frac{e}{\hbar}\boldsymbol{E} \times \boldsymbol{\Omega} + \frac{e}{\hbar^2}(\boldsymbol{\Omega} \cdot \nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}})\boldsymbol{B} - \frac{e}{\hbar^2}(\boldsymbol{\Omega} \cdot \boldsymbol{B})\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}$$

Simplifying,

$$\boxed{\dot{\boldsymbol{r}} = \frac{\frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}} + \frac{e}{\hbar}\boldsymbol{E} \times \boldsymbol{\Omega} + \frac{e}{\hbar^2}(\boldsymbol{\Omega} \cdot \nabla_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}})\boldsymbol{B}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}} \tag{D.4}$$

Appendix E

Calculations for the Boltzmann Transport Equation

E.1 Simplification of RHS of Eq. (4.1)

Since $f = \frac{1}{e^{\beta(\varepsilon_{\boldsymbol{k}} - \mu)} + 1}$, it follows that $\frac{\partial f}{\partial \boldsymbol{r}} = \frac{\partial f}{\partial \varepsilon}\left[-\frac{\nabla T}{T}(\varepsilon_{\boldsymbol{k}} - \mu) - \nabla\mu\right]$, and $\frac{\partial f}{\partial \boldsymbol{k}} = \frac{\partial f}{\partial \varepsilon}\frac{\partial \varepsilon}{\partial \boldsymbol{k}}$. Using $\dot{\boldsymbol{r}} = \frac{\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} + \frac{e}{\hbar}(\boldsymbol{E} \times \boldsymbol{\Omega})}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}$, and $\dot{\boldsymbol{k}} = -\frac{\frac{e}{\hbar}\boldsymbol{E} + \frac{e}{\hbar^2}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \times \boldsymbol{B}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}$, we now calculate $\dot{\boldsymbol{r}} \cdot \frac{\partial}{\partial \boldsymbol{r}} f + \dot{\boldsymbol{k}} \cdot \frac{\partial}{\partial \boldsymbol{k}} f$. Here, $\frac{\partial f}{\partial \boldsymbol{r}}$ is linear in external fields, and $\dot{\boldsymbol{r}}$ has a term $\boldsymbol{E} \times \boldsymbol{\Omega}$, and we neglect their second order product.

Then we get, $-\dot{\boldsymbol{r}} \cdot \frac{\partial}{\partial \boldsymbol{r}} f - \dot{\boldsymbol{k}} \cdot \frac{\partial}{\partial \boldsymbol{k}} f = \frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \cdot \left[e\nabla\boldsymbol{E} + \nabla\mu + \frac{\nabla T}{T}(\varepsilon_{\boldsymbol{k}} - \mu)\right]\frac{\partial \varepsilon_{\boldsymbol{k}}}{\partial \boldsymbol{k}}$.

E.2 Solution of the BTE for $\boldsymbol{E} \neq 0$, $\nabla\mu = \nabla T = 0$

In this limit, the equation becomes,

$$\frac{g}{\tau} - \frac{\frac{e}{\hbar^2}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \times \boldsymbol{B} \cdot \frac{\partial}{\partial \boldsymbol{k}} g = \frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \cdot e\boldsymbol{E} \tag{E.1}$$

We solve this equation, treating the second term in LHS as a perturbation (See Appendix F for justification). We write $g = g_0 + g_1$, such that $\frac{g_0}{\tau} = \frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \cdot e\boldsymbol{E}$, and $\frac{g_1}{\tau} - \frac{\frac{e}{\hbar^2}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \times \boldsymbol{B} \cdot \frac{\partial}{\partial \boldsymbol{k}} g_0 = 0$. Then, g_1 is a linear function of $\boldsymbol{B}$, and it is justified to discard the term $\frac{\frac{e}{\hbar^2}}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \times \boldsymbol{B} \cdot \frac{\partial}{\partial \boldsymbol{k}} g_1$, as it would be quadratic in $\boldsymbol{B}$

Then, $g_0 = \frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{e\tau}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \cdot \boldsymbol{E}$. To find g_1, we need to calculate $\frac{\partial g_0}{\partial \boldsymbol{k}}$, i.e., the quantity $\frac{\partial}{\partial \boldsymbol{k}}\left[\frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{e\tau}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \cdot \boldsymbol{E}\right]$.

To calculate it, let us first calculate $\nabla\left[\phi\boldsymbol{A} \cdot \boldsymbol{C}\right]$, where ϕ is a scalar function, $\boldsymbol{A}$ is a vector function, and $\boldsymbol{C}$ is a constant vector.

$\nabla\left[\phi\boldsymbol{A} \cdot \boldsymbol{C}\right] = (\nabla\phi)(\boldsymbol{A} \cdot \boldsymbol{C}) + \phi(\boldsymbol{C} \cdot \nabla)A + \phi(\boldsymbol{C} \times (\nabla \times \boldsymbol{A}))$. In our calculation, $\phi \sim \frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{e\tau}{\hbar}$, $\boldsymbol{A} \sim \frac{\partial \varepsilon}{\partial \boldsymbol{k}}$, and $\boldsymbol{C} \sim \boldsymbol{E}$.

Then,

$$\frac{\partial}{\partial \boldsymbol{k}}\left[\frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\frac{e\tau}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} \cdot \boldsymbol{E}\right] = \frac{\partial}{\partial \boldsymbol{k}}\left[\frac{\frac{\partial f}{\partial \varepsilon}\tau}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\right]\frac{e\boldsymbol{E}}{\hbar} \cdot \frac{\partial \varepsilon}{\partial \boldsymbol{k}} + \frac{\frac{\partial f}{\partial \varepsilon}\tau}{1 + \frac{e}{\hbar}\boldsymbol{B} \cdot \boldsymbol{\Omega}}\left[(\frac{e}{\hbar}\boldsymbol{E} \cdot \frac{\partial}{\partial \boldsymbol{k}})\frac{\partial \varepsilon}{\partial \boldsymbol{k}} + \frac{e}{\hbar}\boldsymbol{E} \times (\frac{\partial}{\partial \boldsymbol{k}} \times \frac{\partial \varepsilon}{\partial \boldsymbol{k}})\right].$$

The last term is zero because it is the curl of a gradient, $\frac{\partial}{\partial \boldsymbol{k}} \times \frac{\partial \varepsilon}{\partial \boldsymbol{k}} = \nabla_{\boldsymbol{k}} \times (\nabla_{\boldsymbol{k}}\varepsilon) = 0$.

Finally, the solution is, obtained by adding g_0 and g_1,

$$g = \frac{\partial f}{\partial \varepsilon} \frac{1}{1 + \frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}} \frac{\tau}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}}\cdot e\boldsymbol{E} + \frac{\frac{e\tau}{\hbar^2}}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\cdot\boldsymbol{B}\times\left[\frac{\partial}{\partial\boldsymbol{k}}\left[\frac{\frac{\partial f}{\partial\varepsilon}\tau}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}\right]\frac{e\boldsymbol{E}}{\hbar}\cdot\frac{\partial\varepsilon}{\partial\boldsymbol{k}} + \frac{\frac{\partial f}{\partial\varepsilon}\tau}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}\left[(\frac{e}{\hbar}\boldsymbol{E}\cdot\frac{\partial}{\partial\boldsymbol{k}})\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\right]\right]$$

(E.2)

E.3   Solution of the BTE for $\boldsymbol{E} = 0$, $\nabla\mu \neq 0$, $\nabla T \neq 0$

Under these conditions, the equation becomes,

$$\frac{g}{\tau} - \frac{\frac{e}{\hbar^2}\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\times\boldsymbol{B}}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}\cdot\frac{\partial}{\partial\boldsymbol{k}}g = \frac{\partial f}{\partial\varepsilon}\frac{1}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}\frac{1}{\hbar}\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\cdot\left[\nabla\mu + \nabla T\frac{\varepsilon-\mu}{T}\right]$$

Let $g = g_0 + g_1$, with $g_0 = \frac{\partial f}{\partial\varepsilon}\frac{1}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}\frac{\tau}{\hbar}\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\cdot\left[\nabla\mu + \nabla T\frac{\varepsilon-\mu}{T}\right]$ and $\frac{g_1}{\tau} - \frac{\frac{e}{\hbar^2}\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\times\boldsymbol{B}}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}\cdot\frac{\partial}{\partial\boldsymbol{k}}g_0 = 0$.

The form is otherwise similar to the form of the equations in Appendix E.2, but here we have a factor of $(\varepsilon - \mu)$ with ∇T. As a result, we would get *additional factors* like $\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\cdot\nabla T$ when we calculate $\frac{\partial g_0}{\partial\boldsymbol{k}}$ in order to calculate g_1. We may think that such additional factors may violate the Onsager relation. But such factors would cancel beautifully due to a vector triple product being zero, and the Onsager relation continues to hold.

Then,

$$\frac{\partial g_0}{\partial\boldsymbol{k}} = \frac{\partial}{\partial\boldsymbol{k}}\left[\frac{\frac{\partial f}{\partial\varepsilon}\tau}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}\right]\frac{\nabla\mu+\frac{\varepsilon-\mu}{T}}{\hbar}\cdot\frac{\partial\varepsilon}{\partial\boldsymbol{k}} + \frac{\frac{\partial f}{\partial\varepsilon}\tau}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}\left[\left(\frac{\nabla\mu+\frac{\varepsilon-\mu}{T}}{\hbar}\cdot\frac{\partial}{\partial\boldsymbol{k}}\right)\frac{\partial\varepsilon}{\partial\boldsymbol{k}} + \frac{1}{\hbar}(\nabla\mu+\frac{\varepsilon-\mu}{T})\times\underbrace{(\frac{\partial}{\partial\boldsymbol{k}}\times\frac{\partial\varepsilon}{\partial\boldsymbol{k}})}_{0}\right]$$

$$+ \frac{\frac{\partial f}{\partial\varepsilon}\tau}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}\left[\frac{1}{\hbar}(\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\cdot\frac{\partial}{\partial\boldsymbol{k}})(\frac{\varepsilon\nabla T}{T}) + \frac{1}{\hbar}\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\times\left(\frac{\partial}{\partial\boldsymbol{k}}\times\left(\frac{\varepsilon\nabla T}{T}\right)\right)\right]$$

The term inside the final third bracket can be further simplified.

$$(\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\cdot\frac{\partial}{\partial\boldsymbol{k}})(\frac{\varepsilon\nabla T}{T}) + \frac{\partial\varepsilon}{\partial\boldsymbol{k}}\times\left(\frac{\partial}{\partial\boldsymbol{k}}\times\left(\frac{\varepsilon\nabla T}{T}\right)\right) = (\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\cdot\frac{\partial\varepsilon}{\partial\boldsymbol{k}})(\frac{\nabla T}{T}) + \frac{\partial\varepsilon}{\partial\boldsymbol{k}}\times\left(\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\times\left(\frac{\nabla T}{T}\right)\right)$$

$$= (\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\cdot\frac{\partial\varepsilon}{\partial\boldsymbol{k}})(\frac{\nabla T}{T}) + \left(\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\cdot\frac{\nabla T}{T}\right)\frac{\partial\varepsilon}{\partial\boldsymbol{k}} - (\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\cdot\frac{\partial\varepsilon}{\partial\boldsymbol{k}})(\frac{\nabla T}{T})$$

$$= \left(\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\cdot\frac{\nabla T}{T}\right)\frac{\partial\varepsilon}{\partial\boldsymbol{k}}.$$

When we calculate $g_1 = \tau\frac{\frac{e}{\hbar^2}\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\times\boldsymbol{B}}{1+\frac{e}{\hbar}\boldsymbol{B}\cdot\boldsymbol{\Omega}}\cdot\frac{\partial}{\partial\boldsymbol{k}}g_0$, this term cancels because $\frac{\partial\varepsilon}{\partial\boldsymbol{k}}\times\boldsymbol{B}\frac{\partial\varepsilon}{\partial\boldsymbol{k}} = 0$.

Appendix F

Validity of the perturbation theory on Boltzmann Transport Equation

Classically, $\dot{\boldsymbol{k}} \cdot \frac{\partial}{\partial \boldsymbol{k}} g \sim \dot{\boldsymbol{p}} \cdot \frac{\partial}{\partial \boldsymbol{p}} g \sim e(\boldsymbol{v} \times B) \cdot \frac{\partial}{m\partial \boldsymbol{v}} g \sim \boldsymbol{\omega} \times \boldsymbol{v} \cdot \frac{\partial g}{\partial \boldsymbol{v}} \sim \omega g$.

When $\omega \ll \frac{1}{\tau}$ (in the limit of low magnetic field), it is justified to treat ωg as a perturbation over $\frac{g}{\tau}$, in the LHS of Eq. (4.1).

F.1   How low magnetic is 'low'?

For $\omega = \frac{1}{\tau}$, $B_{crit} = \frac{m^*}{\tau e}$, and a magnetic field much lower than this qualifies as a "low" magnetic field. If we take $m^* = m_e$ and $\tau \sim 10^{-14}s$ (chapter 3 of [16]), $B_{crit} \sim 570T$ (which is found in a typical metal), which is order of magnitudes above the magnetic field accessible in labs. In typical metals, $m^* > m_e$, the bare electron mass, and the critical magnetic field is even higher.

In very clean samples, τ can be as high as $10^{-12}s$, and even there, the critical magnetic field would be $5.7T$, which too is hard to achieve in most labs. In less clean samples, the critical magnetic field is much more.

Conclusion: Unless the sample is very clean, the magnetic fields produced in labs qualify as "low", and in this regime, this perturbation theory remains valid.

Appendix G

Mass of the Bloch wavepackets

The Heisenberg equation of motion for the expectation value of the velocity is, $\frac{d}{dt}\langle\hat{\boldsymbol{r}}\rangle = \frac{i}{\hbar}\langle[H,\boldsymbol{r}]\rangle$.

For the Hamiltonian $H = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(r)$ (under zero magnetic field), this is just $\frac{\langle\hat{\boldsymbol{p}}\rangle}{m}$, where m is the bare electron mass (not the effective mass). And this relation between the velocity and the momentum is valid for the Bloch wavepackets.

This is why, we can write $\hat{\boldsymbol{j}}_e = -e\frac{\hat{\boldsymbol{p}}}{m}$ while calculating the electric current density, with m being the bare electron mass.

G.1   Where does the effective mass appear, then?

The effective mass tensor appears in the quantum analog of Newton's second law,

$\boldsymbol{F}_{\text{external}} = \overset{\leftrightarrow}{M}{}^* \cdot \frac{d^2}{dt^2}\langle\hat{\boldsymbol{r}}\rangle$. See chapter 12 of Ashcroft and Mermin ([1]) for more details.

Appendix H

Derivations of properties of Magnetic moments

H.1 $\mathcal{M}_{ij} = \langle \psi_{\boldsymbol{k}, \boldsymbol{r}_1} | \frac{1}{2} \{ -e\frac{\hat{p}_j}{m}, (\hat{\boldsymbol{r}} - \boldsymbol{r}_1)_i \} | \psi_{\boldsymbol{k}, \boldsymbol{r}_1} \rangle$ is a totally antisymmetric tensor

Recall that the effective Hamiltonian acting on $u_{n,\boldsymbol{k}}$ is, $H(\boldsymbol{k}) = \left[\frac{\hbar^2}{2m}(\boldsymbol{k} - i\nabla)^2 + V(\boldsymbol{r}) \right] = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \hat{H} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$, with $\hat{H}$ being the original Hamiltonian.

Let us define $\tilde{\boldsymbol{P}}(\boldsymbol{k}) = \frac{m}{\hbar}\frac{\partial H(\boldsymbol{k})}{\partial \boldsymbol{k}} = \hbar(\boldsymbol{k} - i\nabla) = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \hat{\boldsymbol{P}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$. We would first prove some preliminary results which we would need later on.

H.1.1 Calculation of $\langle u_{\boldsymbol{k}} | \tilde{\boldsymbol{P}}(\boldsymbol{k}) | u_{\boldsymbol{k}} \rangle$

The idea of this calculation is based on [6].

$$
\begin{aligned}
\left\langle \tilde{\boldsymbol{P}}(\boldsymbol{k}) \right\rangle = \langle u_{\boldsymbol{k}} | \tilde{\boldsymbol{P}}(\boldsymbol{k}) | u_{\boldsymbol{k}} \rangle &= \frac{m}{\hbar} \langle u_{\boldsymbol{k}} | \frac{\partial H(\boldsymbol{k})}{\partial \boldsymbol{k}} | u_{\boldsymbol{k}} \rangle \\
&= \frac{m}{\hbar} \left[\langle u | \frac{\partial}{\partial \boldsymbol{k}} \left(H(\boldsymbol{k}) | u \rangle \right) - \langle u | H(\boldsymbol{k}) \left| \frac{\partial}{\partial \boldsymbol{k}} u \right\rangle \right] \\
&= \frac{m}{\hbar} \left[\langle u | \frac{\partial}{\partial \boldsymbol{k}} \left(\varepsilon_{\boldsymbol{k}} | u \rangle \right) - \varepsilon_{\boldsymbol{k}} \left\langle u \left| \frac{\partial}{\partial \boldsymbol{k}} u \right\rangle \right] \\
&= \frac{m}{\hbar} \left[\langle u | \left(\varepsilon_{\boldsymbol{k}} \left| \frac{\partial}{\partial \boldsymbol{k}} u \right\rangle \right) + \langle u | \left(\frac{\partial \varepsilon_{\boldsymbol{k}}}{\partial \boldsymbol{k}} | u \rangle \right) - \varepsilon_{\boldsymbol{k}} \left\langle u \left| \frac{\partial}{\partial \boldsymbol{k}} u \right\rangle \right] \\
&= \frac{m}{\hbar} \frac{\partial \varepsilon_{\boldsymbol{k}}}{\partial \boldsymbol{k}}
\end{aligned}
$$

which is just the (bare) electron mass times its velocity. Note that the Berry curvature term does not appear here because we took a single Bloch eigenstate, not an wavepacket. A method to find $\left\langle \tilde{\boldsymbol{P}}(\boldsymbol{k}) \right\rangle$ using operator algebra for a wavepacket (for which there will be a Berry curvature term) has been outlined in appendices of [14] (we instead analyzed how to wavepacket evolves to find that expression, in section 2.1.1).

H.1.2 Calculation of $\left\langle \frac{\partial}{\partial \boldsymbol{k}} u_{\boldsymbol{k}} \right| \tilde{\boldsymbol{P}}(\boldsymbol{k}) | u_{\boldsymbol{k}} \rangle$

This calculation is based on [6].

$$
\left\langle \frac{\partial}{\partial k_\mu} u_{\boldsymbol{k}} \right| \tilde{P}_\nu(\boldsymbol{k}) \left| u_{\boldsymbol{k}} \right\rangle = \frac{m}{\hbar} \left\langle \frac{\partial}{\partial k_\mu} u_{\boldsymbol{k}} \right| \frac{\partial H(\boldsymbol{k})}{\partial k_\nu} \left| u_{\boldsymbol{k}} \right\rangle
$$

$$
= \frac{m}{\hbar} \left[\left\langle \frac{\partial}{\partial k_\mu} u \right| \frac{\partial}{\partial k_\nu} \left(H(\boldsymbol{k}) \left| u \right\rangle \right) - \left\langle \frac{\partial}{\partial k_\mu} u \right| H(\boldsymbol{k}) \left| \frac{\partial}{\partial k_\nu} u \right\rangle \right]
$$

$$
= \frac{m}{\hbar} \left[\left\langle \frac{\partial}{\partial k_\mu} u \right| \frac{\partial}{\partial k_\nu} \left(\varepsilon_{\boldsymbol{k}} \left| u \right\rangle \right) - \left\langle \frac{\partial}{\partial k_\mu} u \right| H(\boldsymbol{k}) \left| \frac{\partial}{\partial k_\nu} u \right\rangle \right]
$$

$$
= \frac{m}{\hbar} \left[\left\langle \frac{\partial}{\partial k_\mu} u \right| \left(\varepsilon_{\boldsymbol{k}} \left| \frac{\partial}{\partial k_\nu} u \right\rangle \right) + \left\langle \frac{\partial}{\partial k_\mu} u \right| \left(\frac{\partial \varepsilon_{\boldsymbol{k}}}{\partial k_\nu} \left| u \right\rangle \right) - \varepsilon_{\boldsymbol{k}} \left\langle \frac{\partial}{\partial k_\mu} u \right| \frac{\partial}{\partial k_\nu} u \right\rangle \right] '
$$

$$
= \frac{m}{\hbar} \left[\left\langle \frac{\partial}{\partial k_\mu} u \right| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k}) \left| \frac{\partial}{\partial k_\nu} u \right\rangle \right] + \frac{m}{\hbar} \frac{\partial \varepsilon_{\boldsymbol{k}}}{\partial k_\nu} \left\langle \frac{\partial}{\partial k_\mu} u \right| u \right\rangle
$$

$$
= \frac{m}{\hbar} \left[\left\langle \frac{\partial}{\partial k_\mu} u \right| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k}) \left| \frac{\partial}{\partial k_\nu} u \right\rangle \right] + i A_\mu(\boldsymbol{k}) \left\langle P_\nu(\boldsymbol{k}) \right\rangle
$$

H.1.3 Calculation of $_{\text{all space}} \langle u_{\boldsymbol{k}_1} | e^{-i\boldsymbol{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)} (\boldsymbol{r}-\boldsymbol{r}_0)_\mu \hat{\boldsymbol{P}}_\nu e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} | u_{\boldsymbol{k}_2} \rangle_{\text{all space}}$

We use the relation, $\hat{\boldsymbol{P}}(e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} | u_{\boldsymbol{k}_2} \rangle) = e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} \tilde{\boldsymbol{P}}(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2} \rangle$. Then,

$$
_{\text{all space}} \langle u_{\boldsymbol{k}_1,n} | e^{-i\boldsymbol{k}\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)} (\boldsymbol{r}-\boldsymbol{r}_0)_\mu \hat{\boldsymbol{P}}_\nu e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} | u_{\boldsymbol{k}_2,n} \rangle_{\text{all space}}
$$

$$
= {}_{\text{all space}} \langle u_{\boldsymbol{k}_1,n} | e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)} (\boldsymbol{r}-\boldsymbol{r}_0)_\mu \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_{\text{all space}}
$$

Since $| u_{\boldsymbol{k}_2,n} \rangle$ for different values of n are eigenstates of $H(\boldsymbol{k}_2)$ for fixed value of $\boldsymbol{k}_2$, they form a complete set. $\mathcal{I} = \sum_n | u_{\boldsymbol{k}_2,n} \rangle_{\text{cell cell}} \langle u_{\boldsymbol{k}_2,n} |$, and we insert this in the expression above.

$$
_{\text{all space}} \langle u_{\boldsymbol{k}_1,n} | e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot(\hat{\boldsymbol{r}}-\boldsymbol{r}_0)} (\boldsymbol{r}-\boldsymbol{r}_0)_\mu \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_{\text{all space}}
$$

$$
= {}_{\text{all space}} \langle u_{\boldsymbol{k}_1,n} | i \left(\frac{\partial}{\partial k_{1\mu}} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} \right) \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_{\text{all space}}
$$

$$
= \sum_{n'} {}_{\text{all space}} \langle u_{\boldsymbol{k}_1,n} | i \left(\frac{\partial}{\partial k_{1\mu}} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} \right) | u_{\boldsymbol{k}_2,n'} \rangle_{\text{cell cell}} \langle u_{\boldsymbol{k}_2,n'} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_{\text{all space}}
$$

$$
= \sum_{n'} {}_{\text{all space}} \langle u_{\boldsymbol{k}_1,n} | i \left(\frac{\partial}{\partial k_{1\mu}} e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} \right) | u_{\boldsymbol{k}_2,n'} \rangle_{\text{all space cell}} \langle u_{\boldsymbol{k}_2,n'} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_{\text{cell}}
$$

where we used the periodicity of the Bloch wavefunctions to shift the normalization factor. Now we would manipulate the derivative with respect to $\boldsymbol{k}_{1\mu}$.

$$
= i \sum_{n'} \left(\frac{\partial}{\partial k_{1\mu}} {}_{\text{all space}} \langle u_{\boldsymbol{k}_1,n} | e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} \right) | u_{\boldsymbol{k}_2,n'} \rangle_{\text{all space cell}} \langle u_{\boldsymbol{k}_2,n'} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_{\text{cell}}
$$

$$
- i \sum_{n'} {}_{\text{all space}} \left\langle \frac{\partial}{\partial k_{1\mu}} u_{\boldsymbol{k}_1,n} \right| e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} | u_{\boldsymbol{k}_2,n'} \rangle_{\text{cell cell}} \langle u_{\boldsymbol{k}_2,n'} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_{\text{all space}}
$$

In the second term, we again use $\mathcal{I} = \sum_n | u_{\boldsymbol{k}_2,n} \rangle_{\text{cell cell}} \langle u_{\boldsymbol{k}_2,n} |$.

$$
= i \sum_{n'} \frac{\partial}{\partial k_{1\mu}} \left({}_{\text{all space}} \langle u_{\boldsymbol{k}_1,n} | e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} | u_{\boldsymbol{k}_2,n'} \rangle_{\text{all space}} \right)_{\text{cell}} \langle u_{\boldsymbol{k}_2,n'} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_{\text{cell}}
$$

$$
- i \, {}_{\text{all space}} \left\langle \frac{\partial}{\partial k_{1\mu}} u_{\boldsymbol{k}_1,n} \right| e^{i(\boldsymbol{k}_2-\boldsymbol{k}_1)\cdot(\boldsymbol{r}-\boldsymbol{r}_0)} \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_{\text{all space}}
$$

Now we apply the result in B.1, $\int_{\text{all space}} e^{-(\boldsymbol{k}_1-\boldsymbol{k}_2)} f(\text{periodic}) = V_{\text{BZ}} \delta(\boldsymbol{k}_1-\boldsymbol{k}_2) \int_{\text{unit cell}} f(\text{periodic})$. Now we choose units such that $V_{\text{BZ}} = 1$ for simplicity of subsequent calculation (anyway it would

be absorbed in the normalization, as in Eq. (B.3)). We get,

$$
= i \sum_{n'} \frac{\partial}{\partial k_{1_\mu}} \left(\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2)_\text{cell} \langle u_{\boldsymbol{k}_1,n} | u_{\boldsymbol{k}_2,n'} \rangle_\text{cell} \right)_\text{cell} \langle u_{\boldsymbol{k}_2,n'} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_\text{cell}
$$

$$
- i \delta(\boldsymbol{k}_1 - \boldsymbol{k}_2)_\text{cell} \left\langle \frac{\partial}{\partial k_{1_\mu}} u_{\boldsymbol{k}_1,n} \middle| \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_\text{cell}
$$

$$
= i \sum_{n'} \frac{\partial}{\partial k_{1_\mu}} \left(\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2) \right)_\text{cell} \langle u_{\boldsymbol{k}_1,n} | u_{\boldsymbol{k}_2,n'} \rangle_\text{cell} {}_\text{cell}\langle u_{\boldsymbol{k}_2,n'} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_\text{cell}
$$

$$
+ i \sum_{n'} \delta(\boldsymbol{k}_1 - \boldsymbol{k}_2)_\text{cell} \left\langle \frac{\partial}{\partial k_{1_\mu}} u_{\boldsymbol{k}_1,n} \middle| u_{\boldsymbol{k}_2,n'} \right\rangle_\text{cell} {}_\text{cell}\langle u_{\boldsymbol{k}_2,n'} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_\text{cell}
$$

$$
- i \delta(\boldsymbol{k}_1 - \boldsymbol{k}_2)_\text{cell} \left\langle \frac{\partial}{\partial k_{1_\mu}} u_{\boldsymbol{k}_1,n} \middle| \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_\text{cell}
$$

The second and the third term cancel after summing over n'.

$$
= i \sum_{n'} \left[\frac{\partial}{\partial k_{1_\mu}} \delta(\boldsymbol{k}_1 - \boldsymbol{k}_2) \right]_\text{cell} \langle u_{\boldsymbol{k}_1,n} | u_{\boldsymbol{k}_2,n'} \rangle_\text{cell} {}_\text{cell}\langle u_{\boldsymbol{k}_2,n'} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_\text{cell}
$$

$$
\boxed{ = i \left[\frac{\partial}{\partial k_{1_\mu}} \delta(\boldsymbol{k}_1 - \boldsymbol{k}_2) \right]_\text{cell} \langle u_{\boldsymbol{k}_1,n} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_\text{cell} }
$$

H.1.4 $\langle \psi_{\boldsymbol{k},\boldsymbol{r}_0} | \{ (\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\nu \} | \psi_{\boldsymbol{k},\boldsymbol{r}_0} \rangle$ is antisymmetric in μ, ν for a Bloch wavepacket $\psi_{\boldsymbol{k},\boldsymbol{r}_0}$, implying $\mathcal{M}_{ij}$ is totally antisymmetric

It is mentioned in [8] that $\mathcal{M}_{\mu\nu} = \langle \psi_{\boldsymbol{k},\boldsymbol{r}_0} | \frac{1}{2} \{ (\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\nu \} | \psi_{\boldsymbol{k},\boldsymbol{r}_0} \rangle$ is a completely antisymmetric tensor. Here we prove it. A similar calculation to find the orbital angular momentum of a wavepacket can be found at Appendix B of [6].

First we calculate the quantity without the anticommutator.

$$
\langle \psi_{\boldsymbol{k},\boldsymbol{r}_0} | (\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\nu | \psi_{\boldsymbol{k},\boldsymbol{r}_0} \rangle
$$

$$
= \int \int d\boldsymbol{k}_1 d\boldsymbol{k}_2 w(\boldsymbol{k}_1 - \boldsymbol{k}_0) w(\boldsymbol{k}_2 - \boldsymbol{k}_0) e^{-i\boldsymbol{A}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1 - \boldsymbol{k}_0)} e^{i\boldsymbol{A}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_2 - \boldsymbol{k}_0)}
$$

$$
{}_\text{all space}\langle u_{\boldsymbol{k}_1} | e^{-i\boldsymbol{k}\cdot(\hat{\boldsymbol{r}} - \boldsymbol{r}_0)} (\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{\boldsymbol{P}}_\nu e^{i\boldsymbol{k}\cdot(\boldsymbol{r} - \boldsymbol{r}_0)} | u_{\boldsymbol{k}_2} \rangle_\text{all space}
$$

Now we use the boxed result from the previous section,

$$
= \int \int d\boldsymbol{k}_1 d\boldsymbol{k}_2 w(\boldsymbol{k}_1 - \boldsymbol{k}_0) w(\boldsymbol{k}_2 - \boldsymbol{k}_0) e^{-i\boldsymbol{A}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1 - \boldsymbol{k}_0)} e^{i\boldsymbol{A}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_2 - \boldsymbol{k}_0)}
$$

$$
i \left[\frac{\partial}{\partial k_{1_\mu}} \delta(\boldsymbol{k}_1 - \boldsymbol{k}_2) \right]_\text{cell} \langle u_{\boldsymbol{k}_1,n} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_\text{cell}
$$

After integrating by parts to shift the derivative from the delta function to the other quantities,

$$
= \int \int d\boldsymbol{k}_1 d\boldsymbol{k}_2 w(\boldsymbol{k}_1 - \boldsymbol{k}_0) w(\boldsymbol{k}_2 - \boldsymbol{k}_0) e^{-i\boldsymbol{A}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1 - \boldsymbol{k}_0)} e^{i\boldsymbol{A}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_2 - \boldsymbol{k}_0)}
$$

$$
i \left[\frac{\partial}{\partial k_{1_\mu}} \delta(\boldsymbol{k}_1 - \boldsymbol{k}_2) \right]_\text{cell} \langle u_{\boldsymbol{k}_1,n} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_\text{cell}
$$

$$
= -i \int \int d\boldsymbol{k}_1 d\boldsymbol{k}_2 w(\boldsymbol{k}_1 - \boldsymbol{k}_0) w(\boldsymbol{k}_2 - \boldsymbol{k}_0) e^{-i\boldsymbol{A}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_1 - \boldsymbol{k}_0)} e^{i\boldsymbol{A}(\boldsymbol{k}_0)\cdot(\boldsymbol{k}_2 - \boldsymbol{k}_0)}
$$

$$
\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2) \left[{}_\text{cell}\left\langle \frac{\partial}{\partial k_{1_\mu}} u_{\boldsymbol{k}_1,n} \middle| \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_\text{cell} - i\boldsymbol{A}_\mu(\boldsymbol{k}_0) {}_\text{cell}\langle u_{\boldsymbol{k}_1,n} | \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) | u_{\boldsymbol{k}_2,n} \rangle_\text{cell} \right]
$$

Using the result $_\text{cell}\left\langle \frac{\partial}{\partial k_{1_\mu}} u_{\boldsymbol{k}_1,n}\right| \tilde{\boldsymbol{P}}_\nu(\boldsymbol{k}_2) \left| u_{\boldsymbol{k}_2,n}\right\rangle_\text{cell} = \frac{m}{\hbar}\left[\left\langle \frac{\partial}{\partial k_\mu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\nu} u\right\rangle\right] + iA_\mu(\boldsymbol{k})\left\langle P_\nu(\boldsymbol{k})\right\rangle$ from the previous section, and integrating over the delta function, we get,

$$-i\int d\boldsymbol{k}_1 [w(\boldsymbol{k}_1 - \boldsymbol{k}_0)]^2 \frac{m}{\hbar}\left[\left\langle \frac{\partial}{\partial k_\mu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\nu} u\right\rangle\right]$$

$$\boxed{= -i\frac{m}{\hbar}\left[\left\langle \frac{\partial}{\partial k_\mu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\nu} u\right\rangle\right]}$$

Case: $\mu \neq \nu$

In this case, $(\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\nu$ Hermitian (because $(\boldsymbol{r} - \boldsymbol{r}_0)_\mu$ and $\hat{P}_\nu$ commute, and they are individually Hermitian), and its expectation value must be real. Then, $\left\langle \frac{\partial}{\partial k_\mu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\nu} u\right\rangle$ must be purely imaginary.

Now, $\varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})$ is Hermitian. Then, $\left\langle \frac{\partial}{\partial k_\mu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\nu} u\right\rangle^* = \left\langle \frac{\partial}{\partial k_\nu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\mu} u\right\rangle$.

But since this is purely imaginary, $\left\langle \frac{\partial}{\partial k_\mu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\nu} u\right\rangle^* = -\left\langle \frac{\partial}{\partial k_\mu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\nu} u\right\rangle$.

Combining the two, we get, $\left\langle \frac{\partial}{\partial k_\mu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\nu} u\right\rangle = -\left\langle \frac{\partial}{\partial k_\nu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\mu} u\right\rangle$.

Also, since $(\boldsymbol{r} - \boldsymbol{r}_0)_\mu$ and $\hat{P}_\nu$ commute, $(\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\nu = \frac{1}{2}\{(\boldsymbol{r} - \boldsymbol{r}_0)_\mu, \hat{P}_\nu\}$.

Consequently, for $\mu \neq \nu$, $\boxed{\langle \psi_{\boldsymbol{k},\boldsymbol{r}_0}| \frac{1}{2}\{(\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\nu\} |\psi_{\boldsymbol{k},\boldsymbol{r}_0}\rangle = -\langle \psi_{\boldsymbol{k},\boldsymbol{r}_0}| \frac{1}{2}\{(\boldsymbol{r} - \boldsymbol{r}_0)_\nu \hat{P}_\mu\} |\psi_{\boldsymbol{k},\boldsymbol{r}_0}\rangle}$,

and $\boxed{\mathcal{M}_{\mu\nu} = -\mathcal{M}_{\nu\mu}}$.

Case: $\mu = \nu$

In this section, no sum is implied for repeated indices, In this case, $(\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\mu$ is not anymore Hermitian. However, $\left[\left\langle \frac{\partial}{\partial k_\mu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\mu} u\right\rangle\right]$ must be real. Consequently, $-i\frac{m}{\hbar}\left[\left\langle \frac{\partial}{\partial k_\mu} u\Big| \varepsilon_{\boldsymbol{k}} - H(\boldsymbol{k})\Big| \frac{\partial}{\partial k_\mu} u\right\rangle\right] = \left\langle (\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\mu\right\rangle$ is purely imaginary, say, iy. Then, $\left\langle \hat{P}_\mu(\boldsymbol{r} - \boldsymbol{r}_0)_\mu\right\rangle = -iy$, and

$$\left\langle (\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\mu + \hat{P}_\mu(\boldsymbol{r} - \boldsymbol{r}_0)_\mu\right\rangle = 0.$$

It follows that $\boxed{\mathcal{M}_{\mu\mu} = 0}$, for all μ.

Note: Since we know that $\left\langle (\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\mu\right\rangle$ is purely imaginary, and also, $[(\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\mu - \hat{P}_\mu(\boldsymbol{r} - \boldsymbol{r}_0)_\mu] = i\hbar$, it follows that $\left\langle (\boldsymbol{r} - \boldsymbol{r}_0)_\mu \hat{P}_\mu\right\rangle = \frac{i\hbar}{2}$.

Therefore, $\mathcal{M}$ is a completely antisymmetric tensor.

H.2 $m_i = \frac{1}{2}\mathcal{M}_{jk}\epsilon_{ijk}$ is the magnetic moment

Since only the $j \neq k$ terms contribute in $\mathcal{M}_{jk}\epsilon_{ijk}$, and $\hat{p}_k$ commutes with $\hat{r}_j$ for $j \neq k$, we can get rid of the anticommutator,

$$m_i = \frac{1}{2}\langle \psi_{\boldsymbol{k},\boldsymbol{r}_1}| \frac{1}{2}\{-e\frac{\hat{p}_k}{m}, (\hat{\boldsymbol{r}} - \boldsymbol{r}_1)_j\} |\psi_{\boldsymbol{k},\boldsymbol{r}_1}\rangle \epsilon_{ijk} = -\frac{e}{2m}\epsilon_{ijk}\langle \psi_{\boldsymbol{k},\boldsymbol{r}_1}| (\hat{\boldsymbol{r}} - \boldsymbol{r}_1)_j \hat{p}_k |\psi_{\boldsymbol{k},\boldsymbol{r}_1}\rangle$$
$$= -\frac{e}{2m}\langle \psi_{\boldsymbol{k},\boldsymbol{r}_1}| ((\hat{\boldsymbol{r}} - \boldsymbol{r}_1) \times \hat{\boldsymbol{p}})_i |\psi_{\boldsymbol{k},\boldsymbol{r}_1}\rangle$$

which is the i-th component of magnetic moment, defined in Eq. (5.1).

Appendix I

Calculation of Effective Hamiltonian

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