

EFFECTS OF BERRY CURVATURE ON THERMOELECTRIC TRANSPORT IN BILAYER GRAPHENE AND OTHER MATERIALS

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Chapter 1

Introduction

intro

Chapter 2

Berry curvature in reciprocal space

2.1 Berry Curvature

When the Hamiltonian of a system has a parameter λ which evolves slowly (compared to the timescale $\frac{\hbar}{\varepsilon}$ of a state $|\varepsilon\rangle$), an eigenstate of the Hamiltonian evolves as ([2], see Appendix A for derivation),

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

where the geometric phase (also known as the *Pancharatnam–Berry phase*) $\gamma(t)$ is given by the expression

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

Its value depends on the trajectory in the parameter space λ , not just the endpoints. The real quantity $i \langle \varepsilon(\lambda) | \nabla_{\lambda} | \varepsilon(\lambda) \rangle = \mathbf{A}(\lambda)$ is known as the Berry connection¹, and its curl, $\mathbf{\Omega} = \nabla_{\lambda} \times \mathbf{A}$ 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.

2.2 Geometric phase of electrons in a lattice

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

The eigenfunctions of this Hamiltonian are of the form,

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

Here $u_{n,\mathbf{k}}(\mathbf{r})$ is a function with the same periodicity as $V(\mathbf{r})$ (e.g. in a lattice, it would be periodic in every unit cell). The quantity $\hbar\mathbf{k}$ 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

¹ $\langle \varepsilon(\lambda) | \nabla_{\lambda} | \varepsilon(\lambda) \rangle$ stands for $\int d\mathbf{r} \varepsilon_{\lambda}^*(\mathbf{r}) \nabla_{\lambda} \varepsilon_{\lambda}(\mathbf{r})$, where $\varepsilon_{\lambda}(\mathbf{r})$ is the suitably normalized position space wave-function of $|\varepsilon(\lambda)\rangle$.

lattice vector (times \hbar). Now, we can rewrite the eigenvalue equation $\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi_{n,\mathbf{k}}(\mathbf{r}) = \varepsilon_{n,\mathbf{k}}\psi_{n,\mathbf{k}}(\mathbf{r})$ as,

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

In this equation, \mathbf{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 B for derivation)

$$\boxed{\hbar\dot{\mathbf{k}} = -e(\mathbf{E} + \langle\dot{\mathbf{r}}\rangle \times \mathbf{B})} \quad (2.3)$$

As \mathbf{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 , \mathbf{k} would evolve to $\mathbf{k} + \dot{\mathbf{k}}\Delta t$ (we write $\dot{\mathbf{k}}\Delta t = \Delta\mathbf{k}$), and the periodic part of the Bloch wavefunction labeled with \mathbf{k} would evolve as

$$u_{n,\mathbf{k}} \rightarrow e^{i\gamma(\Delta t)} e^{-i\frac{\varepsilon_{\mathbf{k}}\Delta t}{\hbar}} u_{n,\mathbf{k}+\Delta\mathbf{k}}, \quad (2.4)$$

where $\gamma(\Delta t) = \mathbf{A}(\mathbf{k}) \cdot \Delta\mathbf{k}$, and $\mathbf{A}(\mathbf{k}) = i\langle u_{n,\mathbf{k}} | \nabla_{\mathbf{k}} | u_{n,\mathbf{k}} \rangle$ is the Berry connection² in the reciprocal space. Again, for a state labeled with a single \mathbf{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 \mathbf{k} , each of them would evolve with a different geometric phase $\gamma_n(\mathbf{k}) = \int_0^t dt' \mathbf{A}(\mathbf{k}) \cdot \frac{d\mathbf{k}}{dt'}$, and we would soon see that the interference of such phase factors would lead to many interesting effects.

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

Chapter 3

Effects of Berry Curvature

3.1 Modification of semiclassical equations of motion of a wavepacket

The probability density of the wavefunction $\psi_{n,\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n,\mathbf{k}}(\mathbf{r})$ is not localized anywhere, it is periodic over all unit cells (the blue curve in Fig. 3.1). We can construct a wave packet by forming a linear superposition of many such states, such that the wavepacket is localized at some point \mathbf{r}_0 in the real space (the red curve in 3.1), and its crystal momentum is also localized around a value of $\hbar\mathbf{k}_0$.

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, $\Delta\mathbf{r}\Delta\mathbf{k}$ is still greater than $\frac{1}{2}$. While the wavepacket is spread over many unit cells, its spatial variation $\Delta\mathbf{r}$ is much smaller than the dimensions of the system, and $\Delta\mathbf{k}$ 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.

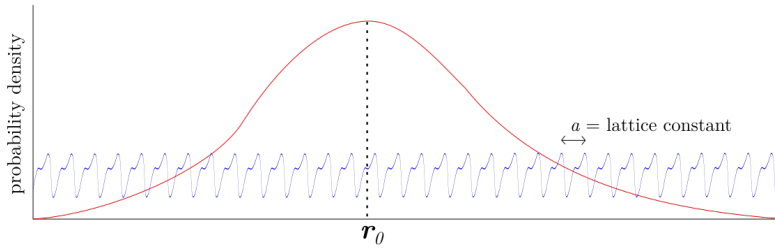


Figure 3.1: The blue curve shows the probability density of a Bloch wavefunction. It is periodic over unit cells. The red curve shows a wavepacket which is localized in real space (although it is spread over many unit cells, it is localized compared to the dimensions of the system), as well as in crystal momentum space.

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

$$\langle \dot{\mathbf{r}} \rangle = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}} - \langle \dot{\mathbf{k}} \rangle \times \mathbf{\Omega}(\mathbf{k}) \quad (3.1)$$

Here, $\mathbf{\Omega}(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}(\mathbf{k}) = i \langle \nabla_{\mathbf{k}} u_{n,\mathbf{k}} | \times | \nabla_{\mathbf{k}} u_{n,\mathbf{k}} \rangle$ is the Berry curvature in the reciprocal space. Also, here the energy eigenvalues are modified due to orbital magnetic moment $\mathbf{m}_{\mathbf{k}}$ of a wavepacket (more about it in Section 3.3) arising due to the Berry curvature, $\varepsilon_{\mathbf{k}} = \varepsilon_0(\mathbf{k}) - \mathbf{m}_{\mathbf{k}} \cdot \mathbf{B}$, where $\varepsilon_0(\mathbf{k})$ is the original bandstructure energy at zero magnetic field.

In popular Solid State Physics textbooks, the second term in the RHS of Eq. (3.1), 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 [3]. To make the wavepacket localized near \mathbf{k}_0 in the reciprocal space, consider a *real* weight function $w(\mathbf{k} - \mathbf{k}_0)$, which is sharply localized about $\mathbf{k} = \mathbf{k}_0$. Now consider a linear superposition of the Bloch wavefunctions, of the form, $\int d\mathbf{k} w(\mathbf{k} - \mathbf{k}_0) e^{-i\mathbf{k} \cdot \mathbf{r}_0} (e^{i\mathbf{k} \cdot \mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r}))$. The expectation value of \mathbf{k} of this wavefunction should be localized about \mathbf{k}_0 . Then, near $\mathbf{r} = \mathbf{r}_0$, the functions $e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}_0)}$ constructively interfere, and we would expect the wavepacket to have a high probability density at \mathbf{r}_0 . However, the functions $u_{n,\mathbf{k}}(\mathbf{r})$ may have different phases for different values of \mathbf{k} at the same $\mathbf{r} = \mathbf{r}_0$, and then the waves would not constructively interfere. After properly taking account of this (See Appendix C.2), the wavefunction that is localized around $\langle \mathbf{r} \rangle = \mathbf{r}_0$, and peaked at crystal momentum $\hbar \mathbf{k}_0$ is found to be,

$$\psi(\mathbf{r}, t = 0) = \int d\mathbf{k} w(\mathbf{k} - \mathbf{k}_0) e^{i\mathbf{A}(\mathbf{k}_0) \cdot (\mathbf{k} - \mathbf{k}_0)} e^{-i\mathbf{k} \cdot \mathbf{r}_0} (e^{i\mathbf{k} \cdot \mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r})).$$

Here \mathbf{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,

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

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

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

After dividing the shift in $\langle \mathbf{r} \rangle$ by Δt , Eq. (3.1) follows.

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

We now drop the notation $\langle \cdot \rangle$ of expectation values, and denote $\langle \mathbf{r} \rangle \equiv \mathbf{r}$ and $\langle \mathbf{k} \rangle \equiv \mathbf{k}$ for a wavepacket localized at \mathbf{r} and \mathbf{k} . Consider a point (\mathbf{r}, \mathbf{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,

$$\dot{\mathbf{r}} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}} - \dot{\mathbf{k}} \times \boldsymbol{\Omega}(\mathbf{k}) \quad (3.2)$$

$$\hbar \dot{\mathbf{k}} = -e(\mathbf{E} + \dot{\mathbf{r}} \times \mathbf{B}) \quad (3.3)$$

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

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

remains a constant of motion (See Appendix D).

Liouville's theorem states that the volume ΔV occupied by a fixed number of points in the phase space remains invariant as the point (\mathbf{r}, \mathbf{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 \mathbf{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 $(\mathbf{r}(t), \mathbf{k}(t))$, and does not depend on the trajectory.

Since the number of phase space points in the volume element $\Delta\mathbf{k}\Delta\mathbf{r} (1 + \frac{e}{\hbar} \mathbf{B}(\mathbf{r}(t)) \cdot \boldsymbol{\Omega}(\mathbf{k}(t)))$ 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 $\Delta\mathbf{k}\Delta\mathbf{r} (1 + \frac{e}{\hbar} \mathbf{B}(t) \cdot \boldsymbol{\Omega}(\mathbf{k}))$ would be equal to the number of states in the initial volume $\Delta\mathbf{k}\Delta\mathbf{r}$.

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 $(1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}(\mathbf{k}))$ in the integrand, to correctly take account of all the states.

$$\langle \mathcal{O} \rangle = \int \frac{d\mathbf{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}(\mathbf{k}) \right) \langle \mathcal{O} \rangle_{\mathbf{k}} \tilde{g}_{\mathbf{k}} \quad (3.4)$$

Here, $\tilde{g}_{\mathbf{k}}$, known as the distribution function, counts the occupation number of electrons in a state labeled with \mathbf{k} . When no external fields are applied, in thermodynamic equilibrium, it is the Fermi distribution function, $\tilde{g}_{\mathbf{k}} = f_{\mathbf{k}} = \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}} - \mu)} + 1}$. When an electromagnetic field is applied, this equilibrium is disturbed, and we write the distribution function as $\tilde{g}_{\mathbf{k}} = f_{\mathbf{k}} + g_{\mathbf{k}}$, where $g_{\mathbf{k}}$ is the non-equilibrium part of the distribution. We will see how to calculate it in Section 9.

Also, since Liouville's theorem does not hold anymore, we cannot obtain the equations of motion (3.2) and (3.3) from any effective Hamiltonian.

3.3 Orbital Magnetic moment

Chapter 4

When do we get a non-zero Berry Curvature?

4.0.1 Spatial Inversion Symmetry

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

Then, if we apply the spatial inversion operator, the LHS of Eq. (3.1) changes sign, and then the RHS must change sign too. Then, $\dot{\mathbf{k}} \times \boldsymbol{\Omega}(\mathbf{k})$ must also change overall sign. But, under spatial inversion, $\dot{\mathbf{k}} \times \boldsymbol{\Omega}(\mathbf{k}) \rightarrow (-\dot{\mathbf{k}}) \times \boldsymbol{\Omega}(-\mathbf{k})$, and this must be equal to $-\dot{\mathbf{k}} \times \boldsymbol{\Omega}(\mathbf{k})$, and we must have,

$$\boldsymbol{\Omega}(-\mathbf{k}) = \boldsymbol{\Omega}(\mathbf{k}), \quad (4.1)$$

when spatial inversion symmetry is present.

4.0.2 Time Reversal Symmetry

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

If we apply the time reversal operator, the LHS of Eq. (3.1) changes sign, and then $\dot{\mathbf{k}} \times \boldsymbol{\Omega}(\mathbf{k})$ 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,

$$\boldsymbol{\Omega}_{n,\sigma}(-\mathbf{k}) = -\boldsymbol{\Omega}_{n,-\sigma}(\mathbf{k}). \quad (4.2)$$

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 $\boldsymbol{\Omega}(\mathbf{k}) = i \langle \nabla_{\mathbf{k}} u_{n,\mathbf{k}} | \times | \nabla_{\mathbf{k}} u_{n,\mathbf{k}} \rangle$ is a function of the spatial part of the wavefunction).

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

$$\boldsymbol{\Omega}_{n,\sigma}(-\mathbf{k}) = -\boldsymbol{\Omega}_{n,\sigma}(\mathbf{k}). \quad (4.3)$$

4.0.3 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. (4.1) and Eq. (4.3) $\boldsymbol{\Omega}_{n,\sigma}(-\mathbf{k}) = \boldsymbol{\Omega}_{n,\sigma}(\mathbf{k}) = -\boldsymbol{\Omega}_{n,\sigma}(\mathbf{k})$, i.e. $\boldsymbol{\Omega} \equiv 0$ for any \mathbf{k} .

Then, to get a non-zero Berry curvature [3], 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.

4.0.4 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 7.2) of the additional term in Eq. (3.2) 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.

Chapter 5

Validity of the argument when the effective Hamiltonian does not commute with itself at different times

The effective Hamiltonian $\left[\frac{\hbar^2}{2m}(\mathbf{k} - i\nabla)^2 + V(\mathbf{r}) \right]$ does not commute with itself for different values of the parameter \mathbf{k} . It can be easily verified that the commutator

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

Then, the phase factor in Eq. (2.1) is not completely correct, as we need to take the time ordered integral of the Hamiltonian. However, the contribution of the non-zero commutator to the time evolution in Eq. (2.4) is $\mathcal{O}(\Delta t^2)$ ¹, and it does not affect the semiclassical equations of motion, because in its derivation, we calculated the change in $\langle \mathbf{r} \rangle$ upto linear order in time Δt , and took the limit $\Delta t \rightarrow 0$.

¹follows by applying the Baker-Campbell-Hausdorff relation on the equation of time evolution,

$$e^{-\frac{i}{\hbar}H_1\Delta t_1}e^{-\frac{i}{\hbar}H_2\Delta t_2} = e^{-\frac{i}{\hbar}(H_1\Delta t_1+H_2\Delta t_2)+\frac{1}{2\hbar^2}[-iH_1,-iH_2]\Delta t_1\Delta t_2+\dots}$$

Chapter 6

Decoupling of the equations of motion and their simplification

The differential equations of motion for $\dot{\mathbf{r}}$ and $\dot{\mathbf{k}}$ (Eq. 3.2 and Eq. 3.3) can be easily decoupled (See Appendix E), and the resulting decoupled equations are,

$$\dot{\mathbf{r}} = \frac{\frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} + \frac{e}{\hbar} (\mathbf{E} \times \boldsymbol{\Omega}) + \frac{e}{\hbar^2} (\boldsymbol{\Omega} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}}) \mathbf{B}}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \quad (6.1)$$

$$\dot{\mathbf{k}} = - \frac{\frac{e}{\hbar} \mathbf{E} + \frac{e}{\hbar^2} \frac{\partial \varepsilon}{\partial \mathbf{k}} \times \mathbf{B} + \frac{e^2}{\hbar^2} (\mathbf{E} \cdot \mathbf{B}) \boldsymbol{\Omega}}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \quad (6.2)$$

In a *2D sample*, $\boldsymbol{\Omega}$ is along the z axis, while $\frac{\partial \varepsilon}{\partial \mathbf{k}}$ is in the xy plane, then $\boldsymbol{\Omega} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}} = 0$. Also, in *2D*, $\boldsymbol{\Omega}$ is along the z axis, whereas \mathbf{k} is restricted to the xy plane. Then we can neglect the term $(\mathbf{E} \cdot \mathbf{B}) \boldsymbol{\Omega}$ in the expression of $\dot{\mathbf{k}}$. Then the equations (6.1) and (6.2) simplify to,

$$\boxed{\dot{\mathbf{r}} = \frac{\frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} + \frac{e}{\hbar} (\mathbf{E} \times \boldsymbol{\Omega})}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}}} \quad (6.3)$$

$$\boxed{\dot{\mathbf{k}} = - \frac{\frac{e}{\hbar} \mathbf{E} + \frac{e}{\hbar^2} \frac{\partial \varepsilon}{\partial \mathbf{k}} \times \mathbf{B}}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}}} \quad (6.4)$$

Chapter 7

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, $\hat{\mathbf{j}}_e = -e\hat{\mathbf{r}}$ over all states, and we substitute $\langle \hat{\mathbf{r}} \rangle_{\mathbf{k}}$ with its value in Eq. (6.3).

$$\langle \hat{\mathbf{j}}_e \rangle = \int \frac{d\mathbf{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}(\mathbf{k}) \right) (-e\dot{\mathbf{r}})_{\mathbf{k}} (f_{\mathbf{k}} + g_{\mathbf{k}}) \quad (7.1)$$

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 $\mathbf{j}_Q = \mathbf{j}_E - \mu \mathbf{j}_N$, where \mathbf{j}_Q , \mathbf{j}_E , and \mathbf{j}_N are the heat current density, energy current density, and number current density, respectively. Now we promote the current densities to their respective operators, and obtain the relation,

$$\langle \hat{\mathbf{j}}_Q \rangle_{\mathbf{k}} = \langle \hat{\mathbf{j}}_E \rangle_{\mathbf{k}} - \mu \langle \hat{\mathbf{j}}_N \rangle_{\mathbf{k}} = \varepsilon_{\mathbf{k}} \langle \dot{\mathbf{r}} \rangle_{\mathbf{k}} - \mu \langle \dot{\mathbf{r}} \rangle_{\mathbf{k}} \quad (7.2)$$

The total heat current is then given by,

$$\langle \hat{\mathbf{j}}_Q \rangle = \int \frac{d\mathbf{k}}{(2\pi)^d} \left(1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}(\mathbf{k}) \right) (\varepsilon_{\mathbf{k}} - \mu) \dot{\mathbf{r}}_{\mathbf{k}} (f_{\mathbf{k}} + g_{\mathbf{k}}) \quad (7.3)$$

We can now put $d = 2$ and use the expression of $\dot{\mathbf{r}}$ in Eq. (6.3) to further simplify Eq. (7.1) and Eq. (7.3), and obtain,

$$\boxed{\langle \hat{\mathbf{j}}_e \rangle = -e \int \frac{d\mathbf{k}}{(2\pi)^2} (f_{\mathbf{k}} + g_{\mathbf{k}}) \left[\frac{1}{\hbar} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} + \frac{e}{\hbar} (\mathbf{E} \times \boldsymbol{\Omega}(\mathbf{k})) \right]} \quad (7.4)$$

$$\boxed{\langle \hat{\mathbf{j}}_Q \rangle = \int \frac{d\mathbf{k}}{(2\pi)^2} (\varepsilon_{\mathbf{k}} - \mu) (f_{\mathbf{k}} + g_{\mathbf{k}}) \left[\frac{1}{\hbar} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} + \frac{e}{\hbar} (\mathbf{E} \times \boldsymbol{\Omega}(\mathbf{k})) \right]} \quad (7.5)$$

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

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

$\varepsilon_{\mathbf{k}}$ is usually an even function of \mathbf{k} . (CHECK: Why/When?) Then the Fermi distribution $f_{\mathbf{k}} = \frac{1}{1+e^{\beta(\varepsilon_{\mathbf{k}}-\mu)}}$ is also an even function, and the band structure part of the velocity, $\frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}}$ is an odd function of \mathbf{k} . Then, the integrals $\int d\mathbf{k} f_{\mathbf{k}} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}}$ and $\int d\mathbf{k} f_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}}$ in the expressions of the electric and heat currents are zero, because the overall integrand is an odd function.

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

In Eq. (9.3) and Eq. (9.0.2) it has been shown that upto leading order, the non-equilibrium part of the distribution function, $g_{\mathbf{k}}$ is a linear function of the electromagnetic field and the gradients of chemical potential and temperature. Then, the term $g_{\mathbf{k}}(\mathbf{E} \times \boldsymbol{\Omega}(\mathbf{k}))$ is a quadratic function of the externally applied fields, and we neglect its contribution in the expressions of electric and heat current densities.

7.1.3 Terms contributing to linear order in external fields

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

7.2 An illustration of the above procedure: the anomalous Hall effect

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 $\mathbf{B} = 0$. There are no temperature gradient or chemical potential gradient.

It can be shown that $g_{\mathbf{k}} = \frac{\partial f}{\partial \varepsilon} \frac{\tau}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot e\mathbf{E}$, upto linear order in \mathbf{E} (this is a special case of Eq. (9.3), with $\mathbf{B} = 0$). Ignoring the terms with quadratic and zero contribution, (See section 7.1.2 and 7.1.1), the electric current $\langle \hat{\mathbf{j}}_e \rangle = -e \int \frac{d\mathbf{k}}{(2\pi)^2} [f_{\mathbf{k}} \frac{e}{\hbar} (\mathbf{E} \times \boldsymbol{\Omega}(\mathbf{k})) + g_{\mathbf{k}} \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}}]$. The second term contributes to σ_{xx} , and it is nothing but a regular Ohmic response (analyzed in section 9.1). The first term ¹ leads to a current perpendicular to the applied electric field,

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

For a fully filled band, the integral of $\frac{1}{2\pi} \boldsymbol{\Omega}(\mathbf{k})$ over the first Brillouin zone is an integer [cite:something], and it is called the first Chern Number (see Chapter 12), which we denote as \mathcal{C} . Then, the off-diagonal part of the conductivity tensor is *quantized*²,

$$\sigma_{xy} = \frac{j_y}{E_x} = \frac{e^2}{2\pi\hbar} \mathcal{C}.$$

¹It 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, $g_{\mathbf{k}}$).

²The factor of $(1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega})$ gets canceled in the numerator (from the phase space connection) and the denominator (from the expression of $\mathbf{r}_{\mathbf{k}}$), as seen in Eq. (7.4) and Eq. (7.5), and the fact that the ‘‘Anomalous Hall response is quantized’’ holds true even when there is a non-zero magnetic field.

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.

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

When time reversal symmetry is present, the Berry curvature is an odd function, $\mathbf{\Omega}(\mathbf{k}) = -\mathbf{\Omega}(-\mathbf{k})$, 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.

7.3 Einstein and Onsager relations

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

$$\begin{aligned}\langle \hat{j}_e \rangle &= \overset{\leftrightarrow}{L}_{11} \cdot \left(\mathbf{E} + \nabla \frac{\mu}{e} \right) + \overset{\leftrightarrow}{L}_{12} \cdot \nabla T \\ \langle \hat{j}_Q \rangle &= \overset{\leftrightarrow}{L}_{21} \cdot \left(\mathbf{E} + \nabla \frac{\mu}{e} \right) + \overset{\leftrightarrow}{L}_{22} \cdot \nabla T\end{aligned}\tag{7.6}$$

Here $\overset{\leftrightarrow}{L}_{ij}$ ($i, j \in 1, 2$) are tensors, they act on a vector to give a vector.

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

Experimentally, it is found that $\overset{\leftrightarrow}{L}_{12} = T \overset{\leftrightarrow}{L}_{21}$. Relations like this are known as *Onsager relations*. In this particular case, the Onsager relation is equivalent to the relation between the Seebeck and Peltier coefficients (See chapter 10).

7.3.1 (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 [5] 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 ($\mathbf{E} \times \mathbf{\Omega}$) of the velocity of the electron wavepacket. However, there are no terms like $\nabla \mu \times \mathbf{\Omega}$ or $\nabla T \times \mathbf{\Omega}$. As a result, apparently, there are no off-diagonal thermoelectric response when $\mathbf{E} = 0$ (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 8), i.e., the electron density is circulating about its center of mass (more specifically, the local value of the momentum, $\psi^*(\mathbf{r})(-i\hbar\nabla_{\mathbf{r}})\psi(\mathbf{r})$ circulates about the center \mathbf{r}_0). This circulating current is known as the magnetization current, $\mathbf{j}_M = \nabla \times \mathbf{M}$, 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, $\mathbf{j}_{tr} = \mathbf{j} - \mathbf{j}_M$. It can be shown that the Onsager and the Einstein relations are valid for the transport electric current and the transport heat current.

Chapter 8

Orbital magnetization

Chapter 9

Boltzmann Transport Equation and its solution

In equilibrium, the electron distribution function reduces to the Fermi distribution, $f_{\mathbf{k}} = \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} - \mu)} + 1}$. 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 modified from the Fermi distribution, $\tilde{g}_{\mathbf{k}} = f_{\mathbf{k}} + g_{\mathbf{k}}$. To calculate $g_{\mathbf{k}}$, we employ the following idea. Consider an electron wavepacket in the phase space point (\mathbf{r}, \mathbf{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, $\left[\frac{\partial}{\partial t} + \dot{\mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}} + \dot{\mathbf{r}} \cdot \frac{\partial}{\partial \mathbf{r}} \right] \tilde{g}_{\mathbf{k}}$. 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 $\tau_{\mathbf{k}}$, 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, $\left[\frac{\partial}{\partial t} + \dot{\mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}} + \dot{\mathbf{r}} \cdot \frac{\partial}{\partial \mathbf{r}} \right] \tilde{g}_{\mathbf{k}} = -\frac{g_{\mathbf{k}}}{\tau}$. The scattering timescale can in general depend on \mathbf{k} . We would soon see that only the values of \mathbf{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 [5], 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 (BTE) can be cast into the form,

$$\frac{g}{\tau} + \dot{\mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}} g + \dot{\mathbf{r}} \cdot \frac{\partial}{\partial \mathbf{r}} g = -\dot{\mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}} f - \dot{\mathbf{r}} \cdot \frac{\partial}{\partial \mathbf{r}} f. \quad (9.1)$$

Using the decoupled equations of motion, right hand side of Eq. (9.1) simplifies to (*Need to show the steps*),

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

When the fields are constant in space and time, we drop the term containing $\frac{\partial g}{\partial \mathbf{r}}$.

Validity of the assumption: When we solve the equation after discarding this term, we would find that (See Eq. (9.3)) this term is second order in the applied fields. Then upto linear order, we can discard this term.

$$\text{Then, the BTE becomes, } \frac{g}{\tau} - \frac{\frac{e}{\hbar} \mathbf{E} + \frac{e}{\hbar^2} \frac{\partial \epsilon}{\partial \mathbf{k}} \times \mathbf{B}}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \cdot \frac{\partial}{\partial \mathbf{k}} g = \frac{\partial f}{\partial \epsilon} \frac{1}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \frac{1}{\hbar} \frac{\partial \epsilon}{\partial \mathbf{k}} \cdot \left[e\mathbf{E} + \nabla\mu + \nabla T \frac{\epsilon - \mu}{T} \right]$$

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

In this limit, the equation becomes,

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

If we discard the term $\mathbf{E} \cdot \frac{\partial\varepsilon}{\partial\mathbf{k}}$ in the LHS, we would find that g is a linear function of \mathbf{E} . Then, $\mathbf{E} \cdot \frac{\partial\varepsilon}{\partial\mathbf{k}}$ would be quadratic in \mathbf{E} . This is why, we can discard this term. (This is not a circular argument. If we do this, everything remains self consistent upto linear order).

Then, the equation takes the form,

$$\frac{g}{\tau} - \frac{\frac{e}{\hbar^2}}{1 + \frac{e}{\hbar}\mathbf{B} \cdot \mathbf{\Omega}} \frac{\partial\varepsilon}{\partial\mathbf{k}} \times \mathbf{B} \cdot \frac{\partial}{\partial\mathbf{k}} g = \frac{\partial f}{\partial\varepsilon} \frac{1}{1 + \frac{e}{\hbar}\mathbf{B} \cdot \mathbf{\Omega}} \frac{1}{\hbar} \frac{\partial\varepsilon}{\partial\mathbf{k}} \cdot e\mathbf{E} \quad (9.2)$$

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

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

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

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

Then,

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

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

Finally,

$$g = \frac{\partial f}{\partial\varepsilon} \frac{1}{1 + \frac{e}{\hbar}\mathbf{B} \cdot \mathbf{\Omega}} \frac{\tau}{\hbar} \frac{\partial\varepsilon}{\partial\mathbf{k}} \cdot e\mathbf{E} + \frac{\frac{e\tau}{\hbar^2}}{1 + \frac{e}{\hbar}\mathbf{B} \cdot \mathbf{\Omega}} \frac{\partial\varepsilon}{\partial\mathbf{k}} \cdot \mathbf{B} \times \left[\frac{\partial}{\partial\mathbf{k}} \left[\frac{\frac{\partial f}{\partial\varepsilon}\tau}{1 + \frac{e}{\hbar}\mathbf{B} \cdot \mathbf{\Omega}} \right] \frac{e\mathbf{E}}{\hbar} \cdot \frac{\partial\varepsilon}{\partial\mathbf{k}} + \frac{\frac{\partial f}{\partial\varepsilon}\tau}{1 + \frac{e}{\hbar}\mathbf{B} \cdot \mathbf{\Omega}} \left[\left(\frac{e}{\hbar}\mathbf{E} \cdot \frac{\partial}{\partial\mathbf{k}} \right) \frac{\partial\varepsilon}{\partial\mathbf{k}} \right] \right] \quad (9.3)$$

Verification: When $\mathbf{\Omega} = 0$, and $\varepsilon = \frac{\hbar^2 k^2}{2m^*}$, this term produces $\sigma_{xy} = -\omega_c \tau \frac{ne^2\tau}{m^*}$. (Need to show the steps)

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

Here

$$\dot{\mathbf{r}} = \frac{\frac{1}{\hbar} \frac{\partial\varepsilon}{\partial\mathbf{k}}}{1 + \frac{e}{\hbar}\mathbf{B} \cdot \mathbf{\Omega}} \quad (9.4)$$

$$\dot{\mathbf{k}} = -\frac{\frac{e}{\hbar^2} \frac{\partial\varepsilon}{\partial\mathbf{k}} \times \mathbf{B}}{1 + \frac{e}{\hbar}\mathbf{B} \cdot \mathbf{\Omega}} \quad (9.5)$$

We again take $\frac{\partial g}{\partial\mathbf{k}} \sim 0$.

Under these circumstances, the equation becomes,

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

Let $g = g_0 + g_1$, with $g_0 = \frac{\partial f}{\partial \varepsilon} \frac{1}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \frac{\tau}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot [\nabla \mu + \nabla T \frac{\varepsilon - \mu}{T}]$ and $\frac{g_1}{\tau} - \frac{\frac{e}{\hbar^2} \frac{\partial \varepsilon}{\partial \mathbf{k}} \times \mathbf{B}}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \cdot \frac{\partial}{\partial \mathbf{k}} g_0 = 0$
 Then, (*Need to show the steps*)

$$\begin{aligned} \frac{\partial g_0}{\partial \mathbf{k}} &= \frac{\partial}{\partial \mathbf{k}} \left[\frac{\frac{\partial f}{\partial \varepsilon} \tau}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \right] \frac{\nabla \mu + \frac{\varepsilon - \mu}{T}}{\hbar} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}} + \frac{\frac{\partial f}{\partial \varepsilon} \tau}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \left[\left(\frac{\nabla \mu + \frac{\varepsilon - \mu}{T}}{\hbar} \cdot \frac{\partial}{\partial \mathbf{k}} \right) \frac{\partial \varepsilon}{\partial \mathbf{k}} + \frac{1}{\hbar} (\nabla \mu + \frac{\varepsilon - \mu}{T}) \times \underbrace{\left(\frac{\partial}{\partial \mathbf{k}} \times \frac{\partial \varepsilon}{\partial \mathbf{k}} \right)}_0 \right] \\ &\quad + \frac{\frac{\partial f}{\partial \varepsilon} \tau}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \left[\frac{1}{\hbar} \left(\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}} \right) \left(\frac{\varepsilon \nabla T}{T} \right) + \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \times \left(\frac{\partial}{\partial \mathbf{k}} \times \left(\frac{\varepsilon \nabla T}{T} \right) \right) \right] \end{aligned}$$

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

$$\begin{aligned} \left(\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}} \right) \left(\frac{\varepsilon \nabla T}{T} \right) + \frac{\partial \varepsilon}{\partial \mathbf{k}} \times \left(\frac{\partial}{\partial \mathbf{k}} \times \left(\frac{\varepsilon \nabla T}{T} \right) \right) &= \left(\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}} \right) \left(\frac{\nabla T}{T} \right) + \frac{\partial \varepsilon}{\partial \mathbf{k}} \times \left(\frac{\partial \varepsilon}{\partial \mathbf{k}} \times \left(\frac{\nabla T}{T} \right) \right) \\ &= \left(\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}} \right) \left(\frac{\nabla T}{T} \right) + \left(\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\nabla T}{T} \right) \frac{\partial \varepsilon}{\partial \mathbf{k}} - \left(\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}} \right) \left(\frac{\nabla T}{T} \right) \\ &= \left(\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\nabla T}{T} \right) \frac{\partial \varepsilon}{\partial \mathbf{k}}. \end{aligned}$$

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

Finally we get,

$$g = \frac{\partial f}{\partial \varepsilon} \frac{1}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \frac{\tau}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \mathbf{S} + \frac{\frac{e \tau}{\hbar^2}}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \mathbf{B} \times \left[\frac{\partial}{\partial \mathbf{k}} \left[\frac{\frac{\partial f}{\partial \varepsilon} \tau}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \right] \frac{\mathbf{S}}{\hbar} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}} + \frac{\frac{\partial f}{\partial \varepsilon} \tau}{1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}} \left[\left(\frac{1}{\hbar} \mathbf{S} \cdot \frac{\partial}{\partial \mathbf{k}} \right) \frac{\partial \varepsilon}{\partial \mathbf{k}} \right] \right] \quad (9.6)$$

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

Einstein and Onsager relations are perfectly valid.

9.1 Special case, $\mathbf{E} \neq 0, \boldsymbol{\Omega} \neq 0, \mathbf{B} = \nabla T = \nabla \mu = 0$

Chapter 10

Seebeck and Peltier effects

Chapter 11

Nernst effect

Chapter 12

Chern Number in different Models

12.0.1 Monolayer and Bilayer Graphene

12.0.2 Selective Valley Population

12.0.3 Valley Chern Number

12.0.4 Calculation of Effective Hamiltonian and its Chern Number

Chapter 13

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

Calculation of Berry Phase

text

Appendix B

Time evolution of Crystal Momentum

text

Appendix C

Calculation of expectation value of the position of the wavepacket

We want to build a wavepacket centered about $\mathbf{r} = \mathbf{r}_0, \mathbf{k} = \mathbf{k}_0$. The calculation of this appendix is loosely based on Ref. [3].

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

$$\phi_{\mathbf{X}}(\mathbf{r}, t = 0) = \int d\mathbf{k} w(\mathbf{k} - \mathbf{k}_0) e^{i\mathbf{X}(\mathbf{k}_0) \cdot (\mathbf{k} - \mathbf{k}_0)} e^{-i\mathbf{k} \cdot \mathbf{r}_0} (e^{i\mathbf{k} \cdot \mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r})) \quad (\text{C.1})$$

C.1 Normalization

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

$$\int_{\text{unit cell}} d\mathbf{r} |u_{n,\mathbf{k}}(\mathbf{r})|^2 = 1 \quad (\text{C.2})$$

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

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

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

$$\begin{aligned} & \int_{\text{all space}} d\mathbf{r} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot (\mathbf{r} - \mathbf{r}_0)} u_{n,\mathbf{k}_2}^*(\mathbf{r}) u_{n,\mathbf{k}_1}(\mathbf{r}) \\ &= \sum_{\mathbf{R}} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{R}} \int_{\text{unit cell}} d\mathbf{r} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot (\mathbf{r} - \mathbf{r}_0)} u_{n,\mathbf{k}_2}^*(\mathbf{r}) u_{n,\mathbf{k}_1}(\mathbf{r}) \end{aligned}$$

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

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

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

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

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

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

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

C.2 Calculation of $\langle \mathbf{r} \rangle$

Claim: For this wavefunction,

$$\langle \mathbf{r} \rangle_{\phi_{\mathbf{X}}} = \langle \phi_{\mathbf{X}}(t=0) | \mathbf{r} | \phi_{\mathbf{X}}(t=0) \rangle = \mathbf{r}_0 - \mathbf{X}(\mathbf{k}_0) + \mathbf{A}(\mathbf{k}_0) \quad (\text{C.4})$$

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

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

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

Let us rewrite, $(\mathbf{r} - \mathbf{r}_0) e^{i\mathbf{k}_1 \cdot (\mathbf{r} - \mathbf{r}_0)} = \frac{1}{i} \nabla_{\mathbf{k}_1} e^{i\mathbf{k}_1 \cdot (\mathbf{r} - \mathbf{r}_0)}$.

Then, $w(\mathbf{k}_1 - \mathbf{k}_0) (\mathbf{r} - \mathbf{r}_0) e^{i\mathbf{X}(\mathbf{k}_0) \cdot (\mathbf{k}_1 - \mathbf{k}_0)} e^{i\mathbf{k}_1 \cdot (\mathbf{r} - \mathbf{r}_0)} u_{n, \mathbf{k}_1}(\mathbf{r})$

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

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

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

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

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

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

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

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

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

When we integrate over \mathbf{r} , we get,

$$\begin{aligned} & \int_{\text{all space}} d\mathbf{r} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot (\mathbf{r} - \mathbf{r}_0)} u_{n,\mathbf{k}_2}^*(\mathbf{r}) \nabla_{\mathbf{k}_1} u_{n,\mathbf{k}_1}(\mathbf{r}) \\ &= \sum_{\mathbf{R}} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{R}} \int_{\text{unit cell}} d\mathbf{r} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot (\mathbf{r} - \mathbf{r}_0)} u_{n,\mathbf{k}_2}^*(\mathbf{r}) \nabla_{\mathbf{k}_1} u_{n,\mathbf{k}_1}(\mathbf{r}) \\ &= V_{\text{BZ}} \delta(\mathbf{k}_1 - \mathbf{k}_2) \int_{\text{unit cell}} d\mathbf{r} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot (\mathbf{r} - \mathbf{r}_0)} u_{n,\mathbf{k}_2}^*(\mathbf{r}) \nabla_{\mathbf{k}_1} u_{n,\mathbf{k}_1}(\mathbf{r}) \\ &= V_{\text{BZ}} \delta(\mathbf{k}_1 - \mathbf{k}_2) \int_{\text{unit cell}} d\mathbf{r} u_{n,\mathbf{k}_1}^*(\mathbf{r}) \nabla_{\mathbf{k}_1} u_{n,\mathbf{k}_1}(\mathbf{r}) \\ &= V_{\text{BZ}} \delta(\mathbf{k}_1 - \mathbf{k}_2) \frac{1}{i} \mathbf{A}(\mathbf{k}_1) \end{aligned}$$

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

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

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

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

$$\begin{aligned} &= -\frac{1}{i} \int_{\mathbf{r}} \int_{\mathbf{k}_1} \int_{\mathbf{k}_2} w(\mathbf{k}_2 - \mathbf{k}_0) e^{-i\mathbf{X}(\mathbf{k}_0) \cdot (\mathbf{k}_2 - \mathbf{k}_0)} e^{-i\mathbf{k}_2 \cdot (\mathbf{r} - \mathbf{r}_0)} u_{n,\mathbf{k}_2}^*(\mathbf{r}) \left[e^{i\mathbf{X}(\mathbf{k}_0) \cdot (\mathbf{k}_1 - \mathbf{k}_0)} e^{i\mathbf{k}_1 \cdot (\mathbf{r} - \mathbf{r}_0)} i\mathbf{X}(\mathbf{k}_0) w(\mathbf{k}_1 - \mathbf{k}_0) u_{n,\mathbf{k}_1}(\mathbf{r}) \right] \\ &= -\mathbf{X}(\mathbf{k}_0) \langle \phi_{\mathbf{X}}(t=0) | \phi_{\mathbf{X}}(t=0) \rangle = -\mathbf{X}(\mathbf{k}_0) \end{aligned}$$

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

C.3 Wavepacket centered at \mathbf{r}_0

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

$$\phi_{\mathbf{X}}(\mathbf{r}, t=0) = \int d\mathbf{k} w(\mathbf{k} - \mathbf{k}_0) e^{i\mathbf{A}(\mathbf{k}_0) \cdot (\mathbf{k} - \mathbf{k}_0)} e^{-i\mathbf{k} \cdot \mathbf{r}_0} (e^{i\mathbf{k} \cdot \mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r})) \quad (\text{C.5})$$

C.4 Calculation of the position space center of the time evolved wavepacket

Appendix D

Evolution of phase space volume

Appendix E

Decoupling of equations of motion

Recall the coupled equations of motion,

$$\dot{\mathbf{r}} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \varepsilon_{\mathbf{k}} - \dot{\mathbf{k}} \times \boldsymbol{\Omega} \quad (\text{E.1})$$

$$\hbar \dot{\mathbf{k}} = -e(\mathbf{E} + \dot{\mathbf{r}} \times \mathbf{B}) \quad (\text{E.2})$$

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

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

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

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

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

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

Finally,

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

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

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

Simplifying,

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

Appendix F

Calculations for the Boltzmann Transport Equation

F.1 Simplification of RHS of Eq. (9.1)

Appendix G

Validity of the perturbation theory on Boltzmann Transport Equation

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

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. (9.1).

G.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 [4]), $B_{crit} \sim 570T$ (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.

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.

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