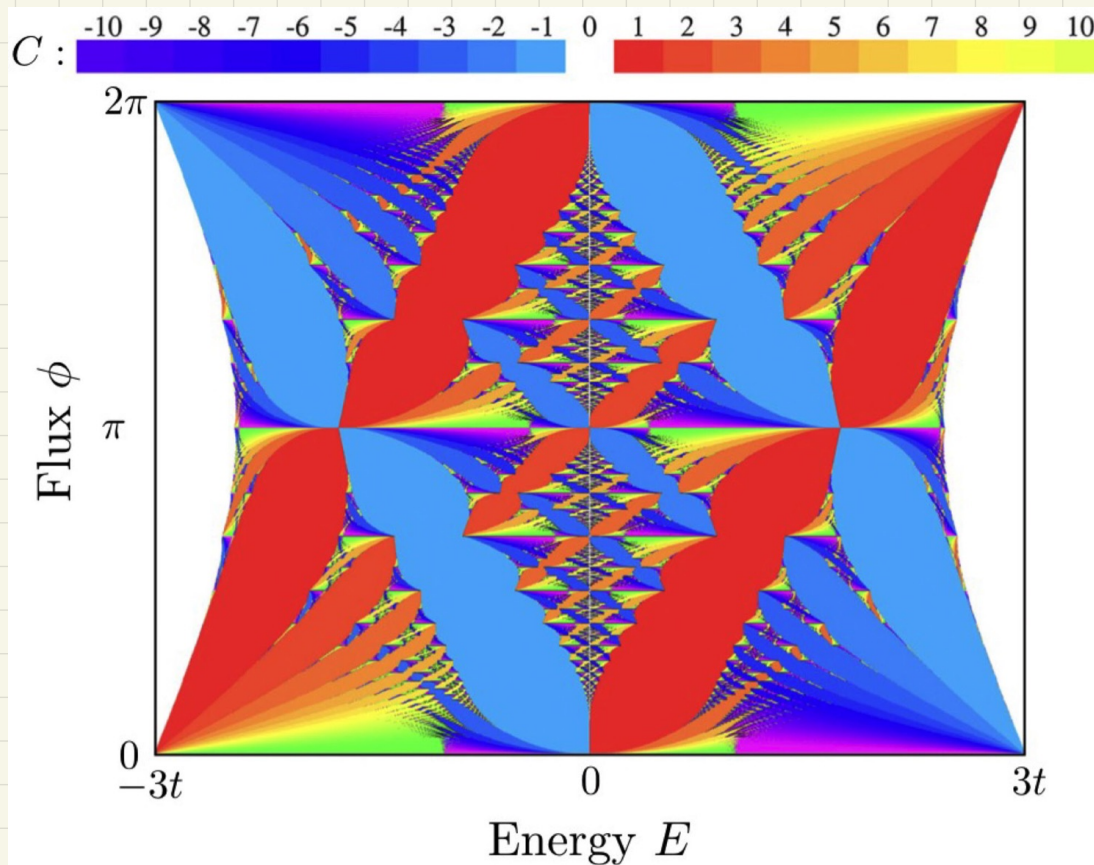Honeycomb lattice Avron–Hofstadter butterfly:

- **Lecture 5 (Jan. 19) : Transport theory** (§5.6)

  §5.5 : review

  Newton's law with friction :

  $$m^* \frac{d\vec{v}}{dt} = -e\vec{E} - \frac{e}{c}\vec{v} \times \vec{B} - \frac{m^*\vec{v}}{\tau}$$

  where m^* = effective mass and τ = momentum relaxation time. Current density : $\vec{j} = -ne\vec{v}$. With $\vec{B} = 0$, in steady state, $-e\vec{E} - \frac{1}{\tau}m^*\vec{v} = 0 \Rightarrow \vec{v} = -(e\tau/m^*)\vec{E}$ the drift velocity. The current density is

  $$\vec{j} = -ne\vec{v} = \frac{ne^2\tau}{m^*}\vec{E} = \sigma\vec{E}$$

Thus we obtain the Drude conductivity $\sigma = ne^2\tau/m^*$.
AC fields :

$$m^* \frac{d\vec{v}}{dt} = -e\vec{E}(\omega)e^{-i\omega t} - \frac{1}{\tau}m^*\vec{v}$$

$$\vec{v}(t) = \vec{v}(\omega)e^{-i\omega t} \implies \vec{v}(\omega) = -\frac{e\tau}{m^*}\frac{\vec{E}(\omega)}{1-i\omega\tau}$$

Drude result becomes

$$\sigma(\omega) = \frac{ne^2\tau}{m^*}\frac{1}{1-i\omega\tau} \equiv \sigma'(\omega) + i\sigma''(\omega)$$

Add uniform magnetic field :

$$\left(\left(\frac{1}{\tau}-i\omega\right)\delta_{\alpha\beta} + \frac{e}{m^*c}\epsilon_{\alpha\beta\gamma}B^\gamma\right)v^\beta = -\frac{e}{m^*}E^\alpha(\omega)$$

so again with $J^\alpha = -ne\,v^\alpha$,

$$E^\alpha(\omega) = \underbrace{\frac{m^*}{ne^2}\left(\left(\frac{1}{\tau}-i\omega\right)\delta_{\alpha\beta} + \frac{e}{m^*c}\epsilon_{\alpha\beta\gamma}B^\gamma\right)}_{\text{resistivity } \rho_{\alpha\beta}(\omega)}J^\beta(\omega)$$

Read on in §5.5 of the lecture notes. Some issues with the simple Drude treatment :
- what do we mean by n ?
- how to treat multiple bands? Fermi surfaces?
- almost filled bands and "holes" ?
- how do we obtain τ ?

• Boltzmann Equation

Semiclassical dynamics of Bloch wavepackets (§ 4.5):

← geometric curvature

$$\frac{d\vec{r}}{dt} = \frac{1}{\hbar} \frac{\partial \mathcal{E}_n(\vec{k})}{\partial \vec{k}} - \frac{d\vec{k}}{dt} \times \vec{\Omega}_n(\vec{k})$$

$$\frac{d\vec{k}}{dt} = -\frac{e}{\hbar} \vec{E}(\vec{r}, t) - \frac{e}{\hbar c} \frac{d\vec{r}}{dt} \times \vec{B}(\vec{r}, t)$$

with

$$A_n^\mu(\vec{k}) = i \langle u_n(\vec{k}) | \frac{\partial}{\partial k^\mu} | u_n(\vec{k}) \rangle$$

$$\Omega_n^\mu(\vec{k}) = \epsilon^{\mu\nu\lambda} \frac{\partial}{\partial k^\nu} A_n^\lambda(\vec{k})$$

Caveats: see Eqns. 5.150 and 5.151 (orbital moments).

Phase space distribution:

$$f_{n\sigma}(\vec{r}, \vec{k}, t) \frac{d^3r \, d^3k}{(2\pi)^3} = \begin{array}{l} \text{\# of electrons in band } n \text{ and spin } \sigma \\ \text{within } d^3r \text{ of } \vec{r} \text{ and within } d^3k \text{ of } \vec{k} \\ \text{at time } t \end{array}$$

Note that the distribution function is dimensionless.

The **electrical current density** is (for $\vec{\Omega}_n(\vec{k}) = 0$ only!)

$$\vec{j}(\vec{r}, t) = -e \sum_{n, \sigma} \int_{\tilde{\Omega}} \frac{d^3k}{(2\pi)^3} f_{n\sigma}(\vec{r}, \vec{k}, t) \, \vec{v}_n(\vec{k})$$

← $\vec{k}$ integral is over Brillouin zone

The **heat current density** is

$$\vec{j}_q(\vec{r}, t) = -e \sum_{n, \sigma} \int_{\tilde{\Omega}} \frac{d^3k}{(2\pi)^3} f_{n\sigma}(\vec{r}, \vec{k}, t) \left(\mathcal{E}_n(\vec{k}) - \mu\right) \vec{v}_n(\vec{k})$$

Our goal is to compute the **linear response coefficients**

which relate the currents to forces $\vec{\mathcal{E}}$ and $\vec{\nabla}T$, e.g.

$$\vec{\mathcal{E}} = \rho\,\vec{j} + Q\,\vec{\nabla}T \quad , \quad \vec{j}_q = \Pi\vec{j} - K\vec{\nabla}T$$

where $\vec{\mathcal{E}} = \vec{E} + e^{-1}\vec{\nabla}\mu = -\vec{\nabla}\tilde{\phi}$ with $\tilde{\phi} = \phi - e^{-1}\mu$ the "electrochemical potential". The matrix coefficients ρ, Q, Π, K have names:

ρ = electrical resistivity $\quad (\sigma = \rho^{-1} = $ conductivity$)$

Q = thermopower

Π = Peltier coefficient

K = thermal conductivity

To accomplish this, we need to know how the distribution functions $f_{n\sigma}(\vec{k}, t)$ evolve in time, and what their fixed point distributions are. To simplify matters, we'll assume that only one band is partially filled, and we'll consider only one spin polarization. You should know that filled and empty bands carry no current (in the absence of curvature):

$$\vec{J}_{filled} = -2e \int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3} \vec{v}(\vec{k}) = -\frac{2e}{\hbar}\int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3} \frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}} = 0$$

↗ spin degeneracy

↪ $f(\vec{k}) = 1$ (filled band)

↑ integrate total derivative over closed domain

So how does $f(\vec{r}, \vec{k}, t)$ evolve? If each quantum state or wavepacket were to evolve according to the semiclassical

equations of motion, we would have

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

where $\dot{\vec{r}} = \hbar^{-1} \vec{\nabla}_{\vec{k}} \, \varepsilon(\vec{k})$ and $\dot{\vec{k}} = -\hbar^{-1} e \, \vec{E}(\vec{r}, t) - \frac{e}{\hbar c} \dot{\vec{r}} \times \vec{B}(\vec{r}, t)$. This is the continuity equation. Here we've assumed zero geometric curvature, i.e. $\vec{\Omega}_n(\vec{k}) = 0$. When the geometric curvature is finite, we have $\dot{\vec{r}} = \hbar^{-1} \vec{\nabla}_{\vec{k}} \varepsilon(\vec{k}) - \dot{\vec{k}} \times \vec{\Omega}(\vec{k})$ and we must replace $f_n(\vec{r}, \vec{k}, t)$ with $\rho_n(\vec{r}, \vec{k}, t) = D_n(\vec{r}, \vec{k}, t) f_n(\vec{r}, \vec{k}, t)$, where

$$D_n(\vec{r}, \vec{k}, t) = 1 + \frac{e}{\hbar c} \vec{B}(\vec{r}, t) \cdot \vec{\Omega}_n(\vec{k})$$

The reason is that the phase flow, defined by the dynamical system

$$\frac{d\vec{\varphi}}{dt} = \vec{u}(\vec{\varphi}) \qquad ; \qquad \vec{\varphi} = \begin{pmatrix} \vec{r} \\ \vec{k} \end{pmatrix} \leftarrow 6\text{-component vector}$$

is not incompressible when $\vec{\Omega}_n(\vec{k}) \neq 0$. Rather (see §4.5.2),

$$\vec{\nabla} \cdot \vec{u} = \frac{\partial \dot{\vec{r}}}{\partial \vec{r}} + \frac{\partial \dot{\vec{k}}}{\partial \vec{k}} = -\frac{d \ln D_n}{dt}$$

This means that phase space volumes vary in time! To cancel this effect, we redefine the phase space probability density as $\rho_n(\vec{r}, \vec{k}, t)$. One then has

$$\vec{J}_n(\vec{r}, t) = \int\limits_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3} \, \rho_n(\vec{r}, \vec{k}, t) \, (-e\dot{\vec{r}})$$

However, $\dot{\vec{r}}$ is no longer given by $\vec{v}_n(\vec{k})$. Rather, from

$$\dot{x}^\alpha + \epsilon_{\alpha\beta\gamma}\, \dot{k}^\beta \Omega_n^\gamma = v_n^\alpha$$

$$\dot{k}^\alpha + \frac{e}{\hbar c}\, \epsilon_{\alpha\beta\gamma}\, \dot{x}^\beta B^\gamma = -\frac{e}{\hbar} E^\alpha$$

we invert to obtain

$$\dot{x}^\alpha = \left(1 + \frac{e}{\hbar c} \vec{B}\cdot\vec{\Omega}_n\right)^{-1}\left\{v_n^\alpha + \frac{e}{\hbar c}(\vec{v}_n\cdot\vec{\Omega}_n)B^\alpha + \frac{e}{\hbar}\epsilon_{\alpha\beta\gamma}E^\beta\Omega^\gamma\right\}$$

$$\dot{k}^\alpha = -\left(1 + \frac{e}{\hbar c}\vec{B}\cdot\vec{\Omega}_n\right)^{-1}\left\{E^\alpha + \frac{e}{\hbar c}(\vec{E}\cdot\vec{B})\Omega_n^\alpha + \frac{1}{c}\epsilon_{\alpha\beta\gamma}v_n^\beta B^\gamma\right\}$$

and we see that the prefactor is $D_n^{-1}(\vec{r},\vec{k},t)$, hence

$$\vec{J}_n(\vec{r},t) = -e\int_{\hat{\Omega}}\frac{d^3k}{(2\pi)^3}\left\{\vec{v}_n(\vec{k}) + \frac{e}{\hbar c}(\vec{v}_n(\vec{k})\cdot\vec{\Omega}_n(\vec{k}))\vec{B}(\vec{r},t) + \frac{e}{\hbar c}\vec{E}(\vec{r},t)\times\vec{\Omega}_n(\vec{k})\right\}f_n(\vec{r},\vec{k},t)$$

wavepacket occupation ↗

which reduces to the familiar expression when $\vec{\Omega}_n(\vec{k}) = 0$.
Note that with $\dot{\vec{B}} = 0$, and taking $f_n = 1$ (i.e. a filled band),

$$\vec{J}_n = -\frac{e^2}{\hbar}\vec{E}\times\int_{\hat{\Omega}}\frac{d^3k}{(2\pi)^3}\vec{\Omega}_n(\vec{k})$$

Thus, when there is nonzero geometric curvature, **a filled band may carry finite current.** Henceforth, we will assume $\vec{\Omega}_n(\vec{k}) = 0$.

The **collisionless Boltzmann equation** is then $(\vec{\nabla}\cdot\vec{u} = 0)$

$$\frac{\partial f}{\partial t} + \dot{\vec{r}}\cdot\frac{\partial f}{\partial\vec{r}} + \dot{\vec{k}}\cdot\frac{\partial f}{\partial\vec{k}} = 0$$

What we are missing are **collisions**, where the wavevector $\vec{k}$ of the wave packet suddenly changes due to **scattering** by an impurity, a phonon, or another electron. This introduces a **collision integral**, viz.

"collision integral"

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \dot{\vec{r}} \cdot \frac{\partial f}{\partial \vec{r}} + \dot{\vec{k}} \cdot \frac{\partial f}{\partial \vec{k}} = \left(\frac{\partial f}{\partial t}\right)_{coll} \equiv I_{\vec{k}}[f]$$

because LHS is $\frac{D}{Dt} f(\vec{r}, \vec{k}, t)$

Simplest model : **relaxation time approximation**

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\frac{f(\vec{r}, \vec{k}, t) - f^0(\vec{r}, \vec{k})}{\tau(\vec{k})}$$

where $f^0(\vec{r}, \vec{k})$ describes a static **local equilibrium** at $\vec{r}$. The relaxation time is $\tau(\vec{k}) = \tau(\varepsilon(\vec{k}))$.

- **Local equilibrium**

  Collisions act locally in space and on short time scales they establish a local equilibrium distribution

  $$f^0(\vec{r}, \vec{k}, t) = \left[\exp\left(\frac{\varepsilon(\vec{k}) - \mu(\vec{r}, t)}{k_B T(\vec{r}, t)}\right) + 1\right]^{-1}$$

  ← Fermi function

  We assume $\mu(\vec{r}, t)$ and $T(\vec{r}, t)$ vary only on time scales much longer than the microscopic collision time. Thus

  $$\left(\frac{\partial f^0}{\partial t}\right)_{coll} = 0$$

The local equilibrium distribution however is not annihilated by the "streaming terms" $\dot{\vec{r}} \cdot \partial_{\vec{r}} + \dot{\vec{k}} \cdot \partial_{\vec{k}}$, and to obtain a solution to the Boltzmann equation we write

$$f(\vec{r}, \vec{k}, t) = f^0(\vec{r}, \vec{k}, t) + \delta f(\vec{r}, \vec{k}, t)$$

This amounts to solving for the function $\delta f(\vec{r}, \vec{k}, t)$. The equation for δf is

$$\left(\frac{\partial}{\partial t} + \dot{\vec{r}} \cdot \frac{\partial}{\partial \vec{r}} + \dot{\vec{k}} \cdot \frac{\partial}{\partial \vec{k}} \right)(f^0 + \delta f) = I_{\vec{k}}[f^0 + \delta f]$$
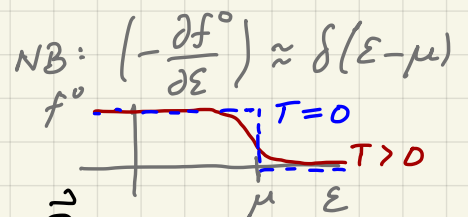
So now we need to roll up our sleeves and calculate:

$$df^0 = k_B T \frac{\partial f^0}{\partial \varepsilon} d\left(\frac{\varepsilon - \mu}{k_B T} \right)$$

$$= k_B T \frac{\partial f^0}{\partial \varepsilon} \left\{ -\frac{d\mu}{k_B T} - \frac{(\varepsilon - \mu) dT}{k_B T^2} + \frac{d\varepsilon}{k_B T} \right\}$$

$$= -\frac{\partial f^0}{\partial \varepsilon} \left\{ \frac{\partial \mu}{\partial \vec{r}} \cdot d\vec{r} + \frac{\varepsilon - \mu}{T} \frac{\partial T}{\partial \vec{r}} \cdot d\vec{r} - \frac{\partial \varepsilon}{\partial \vec{k}} \cdot d\vec{k} \right\}$$

Here we have assumed $\mu = \mu(\vec{r})$ and $T = T(\vec{r})$ are both time-independent. We now read off the partial derivatives

$$\frac{\partial f^0}{\partial \vec{r}} = \left\{ \frac{\partial \mu}{\partial \vec{r}} + \frac{\varepsilon - \mu}{T} \frac{\partial T}{\partial \vec{r}} \right\} \left(-\frac{\partial f^0}{\partial \varepsilon} \right)$$

$$\frac{\partial f^0}{\partial \vec{k}} = \frac{\partial \varepsilon}{\partial \vec{k}} \frac{\partial f^0}{\partial \varepsilon} = \hbar \vec{v} \frac{\partial f^0}{\partial \varepsilon}$$

NB: $\left(-\frac{\partial f^0}{\partial \varepsilon} \right) \approx \delta(\varepsilon - \mu)$

Thus, with $\dot{\vec{r}} = \vec{v}$ and $\dot{\vec{k}} = -\frac{e}{\hbar} \vec{E} - \frac{e}{\hbar c} \vec{v} \times \vec{B}$,

$$\frac{\partial \delta f}{\partial t} + \vec{v} \cdot \vec{\nabla} \delta f - \frac{e}{\hbar} \left[\vec{E} + \frac{1}{c} \vec{v} \times \vec{B} \right] \cdot \frac{\partial \delta f}{\partial \vec{k}}$$

$$+ \vec{v} \cdot \left[e \vec{\mathcal{E}} + \frac{\varepsilon - \mu}{T} \vec{\nabla} T \right] \left(-\frac{\partial f^0}{\partial \varepsilon} \right) = I_{\vec{k}} [f^0 + \delta f]$$

where $\vec{\mathcal{E}} = \vec{E} + e^{-1} \vec{\nabla} \mu = -\vec{\nabla}(\phi - e^{-1}\mu) \equiv -\vec{\nabla}\tilde{\phi}$ is minus the gradient of the "electrochemical potential" $\tilde{\phi} \equiv \phi - e^{-1}\mu$. The inhomogeneous term, in purple, is proportional to the notionally small quantities $\vec{\mathcal{E}} = -\vec{\nabla}\tilde{\phi}$ and $\vec{\nabla} T$. This means that δf is of this order in smallness, so we may drop the terms containing $\vec{\nabla} \delta f$ (extra spatial derivative) and $\vec{E} \cdot \partial \delta f / \partial \vec{k}$. We also have

$$\frac{\partial f^0}{\partial t} = -\frac{\partial f^0}{\partial \varepsilon} \frac{\partial \mu}{\partial t} - \frac{\varepsilon - \mu}{T} \frac{\partial f^0}{\partial \varepsilon} \frac{\partial T}{\partial t}$$

However, we will assume that the uniform ($\vec{k} = 0$) components of $\mu(\vec{r}, t)$ and $T(\vec{r}, t)$ are constant. We then obtain the **linearized Boltzmann equation,**

$$\boxed{\frac{\partial \delta f}{\partial t} - \frac{e}{\hbar c} \vec{v} \times \vec{B} \cdot \frac{\partial \delta f}{\partial \vec{k}} + \vec{v} \cdot \left(e \vec{\mathcal{E}} + \frac{\varepsilon - \mu}{T} \vec{\nabla} T \right) \left(-\frac{\partial f^0}{\partial \varepsilon} \right) = \mathcal{L} \, \delta f}$$

where $\mathcal{L}$ is the **linearized collision integral.** Note that we have not assumed that $\vec{B}$ is small here. Now let us apply this formalism to something useful.

Conductivity of normal metals

Assume $\vec{B} = \vec{\nabla}T = 0$ to begin. Then

$$\frac{\partial \delta f}{\partial t} - \frac{\partial f^0}{\partial \varepsilon} e \vec{v} \cdot \vec{E} = \mathcal{L}\delta f$$

In the relaxation time approximation, $\mathcal{L} = -\frac{1}{\tau}$.

When $\vec{E} = 0$, then, $\delta f(t) = \delta f(0) e^{-t/\tau}$ relaxes to zero, and we recover the equilibrium Fermi distribution.
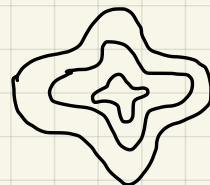
With $\vec{E}(t) = \vec{E} e^{-i\omega t}$, we obtain

$$\delta f(\vec{k}, t) = \frac{e\vec{E} \cdot \vec{v}(\vec{k}) \tau(\vec{k})}{1 - i\omega\tau(\vec{k})} \frac{\partial f^0}{\partial \varepsilon} e^{-i\omega t}$$

Typically $\tau(\vec{k}) = \tau(\varepsilon(\vec{k}))$ gets its $\vec{k}$-dependence through the dispersion $\varepsilon(\vec{k})$. The current density is

$$j^\alpha(\vec{r}, t) = -2e \int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3} \delta f \, v^\alpha(\vec{k})$$

$$= 2e^2 \int_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3} \underbrace{\frac{\tau(\vec{k}) \, v^\alpha(\vec{k}) v^\beta(\vec{k})}{1 - i\omega\tau(\vec{k})} \left(-\frac{\partial f^0}{\partial \varepsilon}\right) \mathcal{E}^\beta e^{-i\omega t}}$$

$$\sigma_{\alpha\beta}(\omega) = \text{conductivity}$$

For $k_B T \ll \varepsilon_F$, we have $\frac{\partial f^0}{\partial \varepsilon} \approx -\delta(\varepsilon - \varepsilon_F)$ and we can express $\sigma_{\alpha\beta}(\omega)$ as an integral over the Fermi surface:

$$d^3k = \frac{d\varepsilon \, dS_\varepsilon}{|\partial\varepsilon/\partial\vec{k}|} = \frac{d\varepsilon \, dS_\varepsilon}{|\hbar\vec{v}|}$$

S_ε for three values of ε

Thus, for $T \ll T_F$,

$$\sigma_{\alpha\beta}(\omega) = \frac{e^2}{4\pi^3 \hbar} \frac{\tau(\varepsilon_F)}{1 - i\omega\tau(\varepsilon_F)} \int dS_F \frac{v^\alpha(\vec{k}) v^\beta(\vec{k})}{|\vec{v}(\vec{k})|}$$

For ballistic electrons with $\varepsilon(\vec{k}) = \hbar^2 k^2 / 2m^*$, find

$$\sigma_{\alpha\beta}(\omega) = \frac{ne^2\tau}{m^*} \frac{\delta_{\alpha\beta}}{1 - i\omega\tau} \quad , \quad n = \int d\varepsilon \, g(\varepsilon) f^0(\varepsilon)$$

Thus we recover the Drude result. But note that in general our expression for $\sigma_{\alpha\beta}(\omega)$ does depend on details of the Fermi surface.

• Optical conductivity

When $\omega\tau \gg 1$, assuming cubic symmetry so $\sigma_{\alpha\beta}(\omega) = \sigma(\omega)\delta_{\alpha\beta}$,

$$\sigma(\omega) = \frac{ie^2}{12\pi^3 \hbar\omega} \int d\varepsilon \left(-\frac{\partial f^0}{\partial\varepsilon} \right) \int dS_\varepsilon |\vec{v}(\vec{k})| \equiv \frac{ine^2}{m_{opt}\omega}$$

where m_{opt} is the **optical mass**,

$$\frac{1}{m_{opt}} = \frac{1}{12\pi^3 \hbar n} \int d\varepsilon \left(-\frac{\partial f^0}{\partial\varepsilon} \right) \int dS_\varepsilon |\vec{v}(\vec{k})|$$

Note that $\sigma(\omega \gg \tau^{-1})$ is purely imaginary, which means that the current response is $90°$ out of phase with the electric field. Thus the power dissipated averaged over one cycle is $\langle \vec{j}(t) \cdot \vec{E}(t) \rangle = 0$.

When $T \ll T_F$, we have

$$\frac{1}{m_{opt}} = \frac{1}{12\pi^3 \hbar n} \int dS_F \, |\vec{v}(\vec{k})|$$

The DOS is (exercise!)

$$g(\varepsilon_F) = \frac{1}{4\pi^3 \hbar} \int dS_F \, |\vec{v}(\vec{k})|^{-1}$$

and the low-T specific heat is given by

$$C_V(T) = \frac{\pi^2}{3} k_B^2 T g(\varepsilon_F) \equiv \frac{m_{th}^*}{m_e} C_V^0(T)$$

where m_{th}^* is the **thermal mass**,

$$m_{th}^* = \frac{\hbar}{4\pi(3\pi^2 n)^{1/3}} \int dS_F \, |\vec{v}(\vec{k})|^{-1}$$

and

$$C_V^0(T) = \frac{m_e (3\pi^2 n)^{1/3}}{3\hbar^2} k_B^2 T$$

is the low-T specific heat of the free electron gas.

- **Calculation of the scattering time**

  Let's endeavor to do better than the phenomenological relaxation time approximation and use Fermi's Golden Rule to model the collision integral:

$$I_{\vec{k}}[f] = \frac{2\pi}{\hbar} \sum_{\vec{k}'} |\langle \vec{k}' | \mathcal{U} | \vec{k} \rangle|^2 \underbrace{(f_{\vec{k}'} - f_{\vec{k}})}_{f_{\vec{k}'}^0 - f_{\vec{k}}^0 + \delta f_{\vec{k}'} - \delta f_{\vec{k}}} \delta(\varepsilon(\vec{k}) - \delta(\varepsilon(\vec{k}')))$$

Here $U(\vec{r}) = \sum_{j=1}^{N_{imp}} U_j(\vec{r} - \vec{R}_j)$ is a sum over the impurity ion scatterers, where $\vec{R}_j$ is the location of the jth impurity ion. We then have, assuming $U_j(\vec{r}) = U(\vec{r})$, i.e. identical impurities,

$$|\langle \vec{k}' | U | \vec{k} \rangle|^2 = \frac{1}{V^2} |\hat{U}(\vec{k} - \vec{k}')|^2 \left| \sum_{j=1}^{N_{imp}} e^{i(\vec{k} - \vec{k}') \cdot \vec{R}_j} \right|^2$$

We assume the impurities are randomly distributed in space, and we replace $|\langle \vec{k}' | U | \vec{k} \rangle|^2$ by its average:

average over $\{\vec{R}_j\}$ $\nearrow$ $\overline{\left| \sum_{j=1}^{N_{imp}} e^{i(\vec{k} - \vec{k}') \cdot \vec{R}_j} \right|^2}$ $= N_{imp} + N_{imp}(N_{imp} - 1)\, \delta_{\vec{k}, \vec{k}'}$

↙ from diagonal terms in double sum
↖ from off-diagonal terms

$$= \sum_{j=1}^{N_{imp}} \sum_{\ell=1}^{N_{imp}} e^{i(\vec{k} - \vec{k}') \cdot (\vec{R}_j - \vec{R}_\ell)}$$

Thus,

$$\overline{|\langle \vec{k}' | U | \vec{k} \rangle|^2} = \frac{N_{imp}}{V^2} |\hat{U}(\vec{k} - \vec{k}')|^2 + \frac{N_{imp}(N_{imp} - 1)}{V^2} |\hat{U}(0)|^2 \delta_{\vec{k}\vec{k}'}$$

NB: we have assumed $\psi_{n\vec{k}}(\vec{r}) = V^{-1/2} \exp(i\vec{k} \cdot \vec{r})$, approximating the true Bloch functions. The $\delta_{\vec{k}\vec{k}'}$ term will cancel out from our calculation since it describes purely forward scattering with no change in wavevector. Thus,

$$\mathcal{L}\delta f = I_{\vec{k}}[f^0 + \delta f] = \frac{2\pi n_{imp}}{\hbar} \int_{\hat{\Omega}} \frac{d^3 k'}{(2\pi)^3} |\hat{U}(\vec{k} - \vec{k}')|^2 \, \delta\left(\frac{\hbar^2 k^2}{2m^*} - \frac{\hbar^2 k'^2}{2m^*} \right) (\delta f_{\vec{k}'} - \delta f_{\vec{k}})$$

where $n_{imp} = N_{imp}/V$ is the density of impurities. We now make the Ansatz

$$\delta f_{\vec{k}} = \tau(\varepsilon(\vec{k}))\, e\, \vec{E} \cdot \vec{v}(\vec{k}) \left. \frac{\partial f^0}{\partial \varepsilon} \right|_{\varepsilon(\vec{k})}$$

Skipping the details (see Eqns. 5.208-209), we obtain

$$\frac{1}{\tau_F} = \frac{m^* k_F n_{imp}}{4\pi^2 \hbar^3} \int d\hat{k}' |\hat{U}(k_F \hat{k} - k_F \hat{k}')|^2 (1 - \hat{k} \cdot \hat{k}')$$

at $T = 0$, with $\varepsilon(k) = \hbar^2 k^2 / 2m^*$. Recalling the expression for differential scattering cross section in the Born approximation,

$$\sigma(\vartheta) = \left(\frac{m^*}{2\pi \hbar^2}\right)^2 |\hat{U}(k - k')|^2$$

we have

$$\frac{1}{\tau_F} = 2\pi n_{imp} v_F \int_0^\pi d\vartheta \ \sigma_F(\vartheta) (1 - \cos\vartheta) \sin\vartheta$$

where $v_F = \hbar k_F / m^*$. Note how the $(1 - \cos\vartheta)$ factor kills forward scattering. The LBE defines a hierarchy of relaxation times, viz. $(\vec{E} = 0)$

$$\frac{\partial \delta f_{\vec{k}}}{\partial t} = n_{imp} v_F \int d\hat{k}' \ \sigma(\vartheta_{\hat{k}\hat{k}'}) (\delta f_{\vec{k}'} - \delta f_{\vec{k}})$$

where $\vartheta_{\hat{k}\hat{k}'} = \cos^{-1}(\hat{k} \cdot \hat{k}')$. Spherical harmonic expansion:

$$\sigma(\vartheta_{\hat{k}\hat{k}'}) = \sigma_{tot} \sum_{L,M} v_L \ Y_{LM}(\hat{k}) \ Y_{LM}^*(\hat{k}')$$

where

$$\sigma_{tot} = 2\pi \int_0^\pi d\vartheta \ \sin\vartheta \ \sigma(\vartheta) = \text{total cross section}$$

Then writing

$$\delta f_{\underline{k}}(t) = \sum_{L,M}^{\cdot} A_{LM}(t)\, Y_{LM}(\hat{k})$$

we obtain

$$\frac{\partial A_{LM}}{\partial t} + (1-\nu_L)\, n_{imp}\, \nu_F\, \sigma_{tot}\, A_{LM} = 0$$

and

$$\tau_L^{-1} = (1-\nu_L)\, n_{imp}\, \nu_F\, \sigma_{tot}$$

Note $\tau_{transport} = \bar{\tau}_{L=1}$ and $\tau_{single\ particle} = \tau_{L=0}$. Th-1,

$$A_{LM}(t) = A_{LM}(0)\, e^{-t/\tau_L}$$