In equilibrium, we have ....

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<td>$\vec{k}$, $n$ ($\hbar \vec{k}$ is the crystal momentum)</td>
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<td>For each $n$, $\vec{k}$ runs through all vectors in a single Brillouin zone, consistent with PBC</td>
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<td>Wave Function</td>
<td>$\psi_f(r) = \psi(r) e^{i \cdot r}$</td>
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How do we calculate the non-equilibrium response of Bloch’s electrons to external fields?

Semiclassical Model of Electron Dynamics: Between collisions, electrons move from equilibrium (field-free) eigenstate to eigenstate.

Semiclassical Model of Electron Dynamics

Our eigenstates have definite wave vectors but have no spatial confinement (PBC). How do we relate these wave functions to electron motion in real space (crystals)? We think of electrons as wave packets. The construction of wave packets from eigenfunctions automatically satisfies Heisenberg’s uncertainty principle, as the spatial extent of a wave packet and its spread in wave vector (momentum) are related.

For free electrons

$$\psi(r, t) = \sum_{\vec{k}'} g(\vec{k}') \exp \left[ i (\vec{k}' \cdot \vec{r} - \frac{\hbar \vec{k}'^2 t}{2m}) \right]$$

$$g(\vec{k}') \approx 0, \quad |\vec{k}' - \vec{k}| > \Delta k$$

common choice

$$g(\vec{k}') = C \exp \left[ - \frac{(\vec{k}' - \vec{k}_0)^2}{(\Delta k)^2} \right]$$

The central position of the wave packet can be obtained by setting $\nabla |\psi|^2 = 0$
Wave Packets Out Of Plane Waves

For a wave packet with wave vectors confined to a region $\Delta k$ about a point in reciprocal space, the spatial spread of the wave packet is of the order

$$\Delta r \approx |\Delta \vec{k}|^{-1}$$

To show this we construct a specific wave packet at $t=0$ in one dimension, using Gaussian distribution

$$\psi(x) = \frac{1}{\sqrt{\pi(\Delta x)^2}} \exp \left[ -\frac{(x-x_0)^2}{(\Delta x)^2} \right] \exp[ik_0(x-x_0)]$$

The Fourier transform of this wave packet also has the Gaussian form:

Integrate by parts to get

$$\psi(k) = \frac{(\Delta x)^2}{2\pi} \exp \left[ -\frac{(\Delta x)^2}{4} (k-k_0)^2 \right] \exp[-i(k-k_0)x_0]$$

Spreads In Real- and k-Space

To analyze the spread of this wave packet at $t=0$, we first remember that

$$\rho(x) = |\psi(x)|^2 \quad \rho(k) = |\psi(k)|^2$$

Since we are using free electrons, the integration goes over entire space and k-space, respectively.

$$<x^2> = x_0^2 + \frac{(\Delta x)^2}{4}; \quad \sigma_x = \frac{\Delta x}{2}$$

$$<k^2> = k_0^2 + \frac{1}{(\Delta x)^2}; \quad \sigma_k = \frac{1}{\Delta x}$$

As expected,

$$\sigma_x \cdot (\hbar \sigma_k) = \frac{\hbar}{2}$$
Wave Packets

At \( t=0 \), a Gaussian wave packet centered at \( x_0 \) is expressed as

\[
\psi(x,0) = \int \frac{2}{\sqrt{\pi(\Delta x)^2}} \exp \left( -\frac{(x-x_0)^2}{(\Delta x)^2} \right) \exp[i k_0(x-x_0)]
\]

\[
= \int \frac{(\Delta x)^2}{2\pi} \int dk \exp \left[ -\frac{(\Delta x)^2}{4} (k-k_0)^2 \right] \exp[-i(k-k_0)x_0] \exp(i k x)
\]

Since each \( k \) component is an eigenstate of the free electron Hamiltonian, with the eigenvalue \( \hbar^2 k^2 / 2m \), the time dependence of the mixed state as specified by the above initial boundary condition can be written down, in the absence of external field, as

\[
\psi(x,t) = \int \frac{\Delta x^2}{2\pi} \int dk \exp \left[ -\frac{(\Delta x)^2}{4} (k-k_0)^2 \right] \exp[-i(k-k_0)x_0] \exp(i k x - \frac{i\hbar k^2}{2m} t)
\]
Carrying out the integration in $k$-space, we get

$$\psi(x,t) = \frac{2}{\pi (\Delta x(t))^2} \exp \left( \frac{(x - [x_0 + \hbar k_0 / m])^2}{(\Delta x(t))^2} \right) \exp[i \hbar k_0 (x - x_0)]$$

$$\times \exp \left[ \frac{2it}{\Delta x(0)^2} (x - [x_0 + \hbar k_0 / m])^2 \right] \times \exp \left( - \frac{i}{2} \arg \Delta x(t) \right) \times \exp[- \frac{i \hbar^2 k_0^2 t}{2m}]$$

Once we constructed a wave packet, the motion of the wave packet under the influence of external disturbances can be regarded as how electrons would react. This allows us to think of electrons with somewhat defined $r$ and $k$ coordinates. The dynamics of electrons (between collisions) can then be predicted to follow the time dependence of states in both of these coordinates.

Generalized Plane Waves

$$\psi(\vec{r}, t) = \sum_{\tilde{k}} g(\tilde{k}) \exp \left[ i(\tilde{k} \cdot \vec{r} - \hbar^{-1} \varepsilon(\tilde{k}) t) \right]$$

\(\text{centered at } k_0\)
\(g(\tilde{k}) \approx 0, |\tilde{k} - \tilde{k}_0| > \Delta k\)

Not necessarily $\hbar^2 k^2 / (2m)$

At $t=0$, wave packet is assumed to be peaked at $r_o$

$$0 = \sum_{\tilde{k}} g(\tilde{k}) \sum_{\tilde{k}'} g(\tilde{k}') i(\tilde{k}' - \tilde{k}^*) \exp \left[ i(\tilde{k}' - \tilde{k}^*) \cdot \vec{r}_0 \right]$$

At $t=t$, where is the wave packet centered?

$$\left| \psi(\vec{r}, t) \right|^2 = \sum_{\tilde{k}} \sum_{\tilde{k}'} g(\tilde{k}) g(\tilde{k}') \exp \left[ i(\tilde{k}' - \tilde{k}^*) \cdot \vec{r} - i\hbar^{-1} (\varepsilon(\tilde{k}') - \varepsilon(\tilde{k}^*)) t \right]$$

For a small region near $k_0$ where $g$ is not zero, energy is given by

$$\varepsilon(\tilde{k}) = \varepsilon(\tilde{k}_0) + (\tilde{k} - \tilde{k}_0) \cdot \left[ \nabla \varepsilon(\tilde{k}) \right]_{\tilde{k}_0}$$
Generalized Plane Wave Packet

\[ |\psi(\vec{r}, t)|^2 = \sum_{k'} \sum_{k} g(\vec{k}') g(\vec{k}) \exp\left[ i (\vec{k}' - \vec{k}) \cdot \vec{r} - \frac{\hbar}{i} \left( \varepsilon(\vec{k}') - \varepsilon(\vec{k}) \right) t \right] \]

\[ = \sum_{k'} \sum_{k} g(\vec{k}') g(\vec{k}) \exp\left[ i (\vec{k}' - \vec{k}) \cdot \vec{r} - \frac{\hbar}{i} \left( \varepsilon(\vec{k}') - \varepsilon(\vec{k}) \right) \right] \nabla \cdot \vec{v} \]

\[ \nabla |\psi(\vec{r}, t)|^2 = \sum_{k'} \sum_{k} g(\vec{k}') g(\vec{k}) i (\vec{k}' - \vec{k}) \exp\left[ i (\vec{k}' - \vec{k}) \cdot \vec{r} - \frac{\hbar}{i} \left( \varepsilon(\vec{k}') - \varepsilon(\vec{k}) \right) \right] \nabla (\vec{k}' - \vec{k}) \cdot \vec{v} \]

If we can find an \( \vec{r} \) where the above gradient is zero, we have found where the wave packet is centered at \( t = t' \). Plug into the above equation

\[ \nabla |\psi(\vec{r}, t)|^2 = \sum_{k'} \sum_{k} g(\vec{k}') g(\vec{k}) i (\vec{k}' - \vec{k}) \exp\left[ i (\vec{k}' - \vec{k}) \cdot \vec{r} - \frac{\hbar}{i} \left( \varepsilon(\vec{k}') - \varepsilon(\vec{k}) \right) \right] \nabla \left[ i (\vec{k}' - \vec{k}) \cdot \vec{v} \right] = 0 \]

The wave packet has moved from \( \vec{r}_0 \) at \( t = 0 \) to \( \vec{r}_0 + \hbar^{-1} \nabla \varepsilon(\vec{k}_0) t \) at \( t = t' \). Its velocity is \( \hbar^{-1} \nabla \varepsilon(\vec{k}_0) \)

Wave Packets of Bloch Electrons

In crystals, we can still construct wave packets out of plane waves. However, this is cumbersome because plane waves are no longer eigenstates. It's more convenient to use equilibrium eigenstates as the basis set of the expansion. For Bloch electrons, we construct a wave packet for band \( n \) centered around \( \vec{k} \)

\[ \psi_n(\vec{r}, t; \vec{k}) = \sum_{\vec{k}} g(\vec{k}) \varphi_{\vec{k}n}(\vec{r}) \exp\left[ -i \varepsilon_n(\vec{k}) t / \hbar \right] \]

where the spread of the wave vector, \( \Delta k \), is small compared with the Brillouin zone. Can we estimate the spatial extent of this wave packet without knowing the exact crystal wave functions? Applying Bloch’s theorem, we get

\[ \psi_n(\vec{r}_0 + \vec{R}, t) = \sum_{\vec{k}} g(\vec{k}) \varphi_{\vec{k}n}(\vec{r}_0) \exp\left[ -i \varepsilon_n(\vec{k}) t / \hbar \right] \]

\[ = g(\vec{k}') \quad g(\vec{k}') \approx 0, \ |\vec{k}' - \vec{k}| > \Delta k \]
Wave Packets: Bloch Electrons

\[ \psi_a(\vec{r}_0 + \vec{R}, t) = \sum_{k'} \bar{g}(\vec{r}_0, \vec{k'}) \exp \left[ \left( \vec{k}' \cdot \vec{R} - \frac{\varepsilon_a(\vec{k'}) t}{\hbar} \right) \right] \]

The “envelope functions” behave like free electron wave functions. For a range of \( \Delta k \), the spatial spread is \( \Delta R \sim \Delta k^{-1} \). Therefore, a wave packet with wave vectors defined well within a Brillouin zone is spread out in real space over many primitive cells, just like in the case of plane waves in free space.

Since the periodic potential varies on a scale smaller than the primitive cell, its effect on the Bloch electrons cannot be treated classically. “Semi-classical” model means that the electrons react to the external fields classically, but they interact with the periodic lattice quantum mechanically.

Electronic Velocity

For FREE ELECTRONS,

\[ \hat{v} = \frac{\hbar \vec{k}}{2m} = \frac{\hbar^2}{m} \]

What about Bloch electrons?

\[ \psi_a(\vec{r}, \vec{k}_0, t) = \sum_{k'} g_{k_0}^{*}(\vec{k}') \psi_{ak}(\vec{r}) \exp \left[ -i \hbar (\varepsilon(\vec{k'}) \tau) \right] \]

\[ |\psi_a(\vec{r}, \vec{k}_0, 0)|^2 = \sum_{k'} g_{k_0}^{*}(\vec{k}') g_{k_0}^{*}(\vec{k}') \psi_{ak}(\vec{r}) \psi_{ak}(\vec{r}) \]

\[ \psi_{ak}(\vec{r}) = e^{i\vec{v} \cdot \vec{r}} u_{ak}(\vec{r}) \]

|\psi_a(\vec{r}, \vec{k}_0, 0)|^2 = \sum_{k'} \sum_{k''} g_{k_0}^{*}(\vec{k}') g_{k_0}^{*}(\vec{k}'') u_{ak}(\vec{r}) u_{ak}(\vec{r}) e^{i(\vec{v} - \vec{v}^{*}) \cdot \vec{r}} \]
**Bloch Wave Packet**

At $t=0$, wave packet is centered around $r_0$,

$$\nabla |\psi_\alpha(\vec{r}, \vec{k}_0, 0)|^2 \bigg|_{\vec{r}=\vec{r}_0} = 0$$

non-zero only near $k_0$

$$0 = \sum_{k} \sum_{l} g^* (\vec{k}) g(\vec{k}) \exp\left[i(\vec{k}' - \vec{k}) \cdot \vec{r}_0\right] \times i(\vec{k}' - \vec{k}) u_{\alpha l}(\vec{r}_0) u_{\text{ad} l}(\vec{r}_0) + \nabla\left[u_{\alpha l}^*(\vec{r}) u_{\text{ad} l}(\vec{r})\right]_{\vec{r}=\vec{r}_0}$$

At $t=t$, where is the wave packet centered?

$$\psi_\alpha(\vec{r}, \vec{k}_0, t) = \sum_{k} g^* (\vec{k}) u_{\alpha l}(\vec{r}) \exp\left[i(\vec{k}' - \vec{k}) \cdot \vec{r} - i\hbar^{-1} \frac{\partial}{\partial t} \mathcal{E}(\vec{k}) t\right]$$

Use the same trick (expand $\mathcal{E}$ around $k_0$)

$$\mathcal{E}(\vec{k}) = \mathcal{E}(\vec{k}_0) + (\vec{k} - \vec{k}_0) \cdot \left[ \nabla \mathcal{E}(\vec{k}) \right]_{\vec{k}=\vec{k}_0}$$

**Bloch Wave Packet**

$$|\psi(\vec{r}, t)|^2 = \sum_{k} \sum_{l} g^* (\vec{k}) g(\vec{k}) u_{\alpha l}^*(\vec{r}) u_{\text{ad} l}(\vec{r}) \exp\left[i(\vec{k}' - \vec{k}) \cdot (\vec{r} - \hbar^{-1} \nabla \mathcal{E}(\vec{k}) t)\right]$$

$$\nabla |\psi(\vec{r}, t)|^2 = \sum_{k} \sum_{l} g^* (\vec{k}) g(\vec{k}) \exp\left[i(\vec{k}' - \vec{k}) \cdot (\vec{r} - \hbar^{-1} \nabla \mathcal{E}(\vec{k}) t)\right] \times \left\{ i(\vec{k}' - \vec{k}) u_{\alpha l}^*(\vec{r}) u_{\text{ad} l}(\vec{r}) + \nabla\left[u_{\alpha l}^*(\vec{r}) u_{\text{ad} l}(\vec{r})\right]_{\vec{r}=\vec{r}_0} \right\}$$

Plug $\vec{v} = \vec{r}_0 + \hbar^{-1} \nabla \mathcal{E}(\vec{k}_0) t$ into the above equation

$$\nabla |\psi(\vec{r}, t)|^2 = \sum_{k} \sum_{l} g^* (\vec{k}) g(\vec{k}) \exp\left[i(\vec{k}' - \vec{k}) \cdot \vec{r}_0\right] \times \left\{ i(\vec{k}' - \vec{k}) u_{\alpha l}^*(\vec{r}_0) u_{\text{ad} l}(\vec{r}_0) + \hbar^{-1} \nabla \mathcal{E}(\vec{k}_0) t + \nabla\left[u_{\alpha l}^*(\vec{r}) u_{\text{ad} l}(\vec{r})\right]_{\vec{r}=\vec{r}_0} \right\} = 0$$

for $\hbar^{-1} \nabla \mathcal{E}(\vec{k}_0) t = nR$

If we take snapshots of the wave packet every $\Delta t = R/h\Delta E$, the wave packet will have maintained its shape and moved by a distance of $R$. 

**velocity is**

$$\hbar^{-1} \nabla \mathcal{E}(\vec{k}_0)$$
**Description of Semi-classical Model**

1. Band index $n$ is a constant of the motion. No interband transitions. (applied fields are weak)

2. Ignore scattering, or first consider electron dynamics in between scattering events. The equations of motion are

$$\dot{\vec{r}} = \vec{v}_n(\vec{k}) = \frac{1}{\hbar} \frac{\partial \varepsilon_n(\vec{k})}{\partial \vec{k}}$$

$$\hbar \dot{\vec{k}} = -e \left[ \vec{E}(\vec{r}, t) + \frac{1}{c} \vec{v}_n(\vec{k}) \times \vec{H}(\vec{r}, t) \right]$$

3. The wave vector of an electron is only defined to within an additive reciprocal lattice vector $\vec{K}$. In thermal equilibrium the contribution to the electronic density from those electrons in the $n$th band with wave vectors in the infinitesimal volume element $d\vec{k}$ of $k$-space is given by the Fermi distribution:

$$f(\varepsilon_n(\vec{k})) \frac{d\vec{k}}{4\pi^3} = \frac{d\vec{k}}{4\pi^3} \frac{\left. \frac{\partial}{\partial \varepsilon} \right|_{\mu = \varepsilon} \left. \frac{\partial}{\partial \varepsilon} \right|_{\mu = \varepsilon} \exp \left\{ \frac{\varepsilon_n(\vec{k}) - \mu}{k_B T} \right\} + 1$$

**Comments and Restrictions**

A many-carrier theory

Crystal momentum is not momentum

Limits of validity

$$eEa << \{E_{\text{gap}}(\vec{k})\}^2 / E_F$$

$$\hbar \omega << \{E_{\text{gap}}(\vec{k})\}^2 / E_F$$

$$\hbar \omega << \varepsilon_{\text{gap}}$$

$$a << \lambda$$

Basis for equations of motion

$$\varepsilon_n(\vec{k}(t)) - e\phi(\vec{r}(t)) = \text{const.}$$

$$\begin{align*}
\hbar \dot{k} &= -e \vec{E} + C \hat{\nabla} \\
\hbar \dot{k} &= -e \left( \vec{E} + \frac{\vec{v}(\vec{k})}{c} \times \vec{H} \right)
\end{align*}$$

Take time derivative for time-indep. fields

$$\dot{\vec{v}}_n(\vec{k}) \left[ \hbar \dot{\vec{k}} - e \nabla \phi \right] = 0$$
Migration of Eigenstate in Weak External Field

Assume weak electric field. At t=0, in eigen state with wave vector k.

$$|k(t)⟩ = e^{-i\omega t/\hbar} |k(0)⟩$$

$$= e^{-ie_{\alpha t}/\hbar} e^{ie\tilde{E} t/\hbar} |k(0)⟩$$

$$= \sum_{k'} |k'(0)⟩ e^{-ie_{\alpha t}/\hbar} <k'(0)| e^{ie\tilde{E} t/\hbar} |k(0)⟩$$

$$= \sum_{k'} |k'(0)⟩ e^{-ie_{\alpha t}/\hbar} \delta_{\vec{k'}, \vec{k} - \vec{E} t/\hbar}$$

$$= e^{-ie_{\alpha t}/\hbar} |(\vec{k} - e\tilde{E} t/\hbar)(0)⟩$$

$$\hat{k} = (\vec{k} - e\tilde{E} t/\hbar - \vec{k})/t = -e\tilde{E}/\hbar \quad \text{semiclassical dynamics}$$

T=0 Examples

1. Filled Bands Are Inert

A filled band is characterized by the fact that the density of electrons in a six-dimensional \(\sigma\)-phase space is 1/4\(\pi^3\). Liouville’s theorem: volume is conserved.

The electric and thermal currents are

$$\vec{j} = -e \int \frac{d\vec{k}}{4\pi^3} \frac{\hat{c}E}{\hbar \vec{k}}$$

$$\hat{j}_x = \int \frac{d\vec{k}}{4\pi^3} \hat{c}(\vec{k}) \frac{\hat{c}E}{\hbar \vec{k}} = \int \frac{d\vec{k}}{8\pi^3} \frac{\hat{c}}{\hbar \vec{k}} [\hat{c}(\vec{k})]^2$$

Both currents vanish for a filled band.

(1) Conduction is due only to those electrons in partially filled bands.

(2) Insulator elements must have even number of electrons, or a lattice with an even number of atoms as basis.

APPENDIX I: If \(u\) has the periodicity of Bravais lattice,

$$\int \omega \nabla \omega = \int \omega \nabla^2 \omega = 0$$

$$1(\vec{r}) = \int \omega \nabla (\vec{r} + \vec{r}') = \text{const.}$$

$$\int \omega \nabla \omega (\vec{r} + \vec{r}') = \int \omega \nabla \omega (\vec{r} + \vec{r}') = 0$$
2. Semiclassical Motion in DC Electric Field

\[ \vec{k}(t) = \vec{k}(0) - \frac{eE_t}{\hbar} \]
\[ \overline{v}[\vec{k}(t)] = \overline{v}(\vec{k}(0) - \frac{eE_t}{\hbar}) \]

The time-dependence (k-dependence) of velocity is periodic. In the upper half of the band, electric field leads to acceleration of electrons OPPOSITE to the direction of electrostatic force!

This is due to forces exerted by the lattice.

Without scattering, should see a.c. current!

The concept of “HOLES”.

---

HOLES

1. Current carried by occupied electrons in a partially filled band can be thought of as being carried by positively charged holes

\[ \dot{j} = (-e) \int_{\text{occ}} \frac{d\vec{k}}{4\pi^2} \overline{v}(\vec{k}) = (+e) \int_{\text{unocc}} \frac{d\vec{k}}{4\pi^2} \overline{v}(\vec{k}) \]

Picture cannot be mixed within a given band.

2. The dynamics of holes follows the same equations as (-e) charged electrons, i.e.

\[ \hbar \dot{\vec{k}} = -e \left[ \vec{E}(\vec{r},t) + \frac{1}{c} \vec{v}(\vec{k}) \times \vec{H}(\vec{r},t) \right] \]

3. Effective mass: near an energy maximum \( \varepsilon(\vec{k}_0) \), define positive \( m^* \) with

\[ \varepsilon(\vec{k}) \approx \varepsilon(\vec{k}_0) - \frac{\hbar^2}{2m^*} (\vec{k} - \vec{k}_0)^2 \quad \overline{v}(\vec{k}) \approx -\frac{\hbar}{m^*} (\vec{k} - \vec{k}_0) \]

\[ \dot{\vec{a}}(\vec{k}) = \frac{d}{dt} \overline{v}(\vec{k}) = -\frac{h}{m^*} (\vec{E} + \frac{\overline{v}(\vec{k})}{c} \times \vec{H}) \]
Effective Mass Tensor

If in a region of k-space, the following holds for all directions of $\hat{\mathbf{k}}$

$$\hat{\mathbf{k}} \cdot \hat{\mathbf{a}} = \begin{cases} > 0, & \text{electron-like} \\ < 0, & \text{hole-like} \end{cases}$$

$$\hat{\mathbf{k}} = \frac{\mathbf{v}}{\mathbf{v}} = \frac{\mathbf{E}^2}{\hbar \mathbf{\varepsilon}_k} = \frac{1}{\hbar} \sum_{i,j} \delta^3 \mathbf{e}_j \varepsilon_{ij} k_j$$

$$\frac{d}{dt} \nabla \mathbf{v} = \sum_j \frac{\partial^2 \mathbf{e}_j}{\partial k_i k_j} \hat{\mathbf{k}}_j$$

Electrons: $\sum_i \Delta_i \frac{\partial^2 \mathbf{e}_i}{\partial \mathbf{k}_i} \Delta_j > 0$ for all $\lambda$

Holes: $\sum_i \Delta_i \frac{\partial^2 \mathbf{e}_i}{\partial \mathbf{k}_i} \Delta_j < 0$ for all $\lambda$

$$\hat{\mathbf{a}} = \frac{d \mathbf{v}}{dt} = \left( \mathbf{M}^{-1}(\tilde{\mathbf{k}}) \right) \cdot \hbar \mathbf{k} = \left( \mathbf{M}^{-1}(\tilde{\mathbf{k}}) \right) \cdot \left[ \frac{e \mathbf{E}}{c} + \mathbf{v} \times \mathbf{H} \right]$$

Electrons and Holes

![Diagrams showing wave vectors and band structures for electrons and holes, with a 3D visual representation of band structure at the top.](image-url)
Effective Mass Tensors and Ellipsoids

\[ \varepsilon(\vec{k}) = \varepsilon(\vec{k}_0) \pm \frac{\hbar^2}{2} (\vec{k} - \vec{k}_0) \cdot \mathbf{M}^{-1} \cdot (\vec{k} - \vec{k}_0) \]

For a region in k-space around \( k_0 \)

\[ [\mathbf{M}^{-1}(\vec{k})]_{ij} = \pm \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(\vec{k})}{\partial \vec{k}_i \cdot \partial \vec{k}_j} = \pm \frac{1}{\hbar} \frac{\partial \mathbf{v}}{\partial \vec{k}_j} \]

\[ \nabla \varepsilon |_{\vec{k}} - \nabla \varepsilon |_{\vec{k} + \Delta \vec{k}} = \pm \hbar^2 M^{-1} \cdot \Delta \vec{k} \]

\[ \mathbf{v}(\vec{k}) - \mathbf{v}(\vec{k} + \Delta \vec{k}) = \mathbf{v}(\vec{k}') - \mathbf{v}(\vec{k}' + \Delta \vec{k}) = \pm \mathbf{M}^{-1} \cdot \hbar \Delta \vec{k} \]

Constant energy surfaces form ellipsoids.

Cross section of an ellipsoid with a plane is an ellipse.

Principal axes of ellipsoid have length a, b, c.

Volume of ellipsoid is \( \frac{4}{3} \pi abc \), area of ellipse is \( \pi ab \).

http://mathworld.wolfram.com/Ellipsoid.html

T=0 Examples

2. Semiclassical Motion in Uniform Magnetic Field

\[ \hbar \vec{k} = (-e) \frac{\mathbf{v}(\vec{k})}{c} \times \hat{\mathbf{H}} \]

\[ \dot{\vec{r}} = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \vec{k}} \]

The component of k along the magnetic field and the electronic energy are both constants of the motion.

In real space, the projection of orbit in a plane perpendicular to field:

\[ \vec{r}_\perp = \vec{r} - \hat{\mathbf{H}} \cdot \hat{\mathbf{r}} \]

\[ \hat{\mathbf{H}} = -\frac{eH}{c} (\hat{\mathbf{r}} - \hat{\mathbf{H}} \cdot \hat{\mathbf{r}}) = -\frac{eH}{c} \hat{\mathbf{r}} \]

\[ \vec{r}_\perp(t) - \vec{r}_\perp(0) = \frac{\hbar c}{eH} \hat{\mathbf{H}} \times (\vec{k}(t) - \vec{k}(0)) \]

The perpendicular orbit in real space is identical to, but rotated 90° from, the k-space orbit. \( k_\parallel \) is constant, however, \( v_\parallel \) need not be.
Constant Magnetic Field (Cont.)

\[
\hat{H} \times \hat{k} = -\frac{eH}{c} \hat{r}_\perp
\]

\[
t_2 - t_1 = \int_0^t dt = \int_0^k \frac{dk}{|k|} = \frac{\hbar^2 c}{eH} \int_0^k \frac{dk}{|\vec{\partial}\vec{E}/\vec{\partial}k)|} = \frac{\hbar^2 c}{eH} \Delta (\vec{k}) \int_0^k \Delta (\vec{k}) dk
\]

For closed (projected) orbits, \(A\) is the total area of the orbit.

\[
T(\varepsilon, k_z) = \frac{\hbar^2 c}{eH} \frac{\vec{\partial}}{\vec{\partial} \varepsilon} A(\varepsilon, k_z)
\]

In analogy with free electron cyclotron frequency, define cyclotron effective mass

\[
T = \frac{2mc}{eH}
\]

\[m^*(\varepsilon, k_z) = \frac{\hbar^2}{2\pi} \frac{\vec{\partial}A(\varepsilon, k_z)}{\vec{\partial} \varepsilon}
\]

T=0 Examples

3. Perpendicular Uniform Electric and Magnetic Fields

\[
\hat{r}_{\perp} = \vec{v}(\vec{k}) = \frac{1}{h} \frac{\vec{\partial} \varepsilon}{\vec{\partial} \vec{k}}
\]

Taking cross product with unit vector

\[
\hat{H} \times \hat{k} = -\frac{eE}{c} \hat{\vec{r}}_{\perp} = -\frac{eH}{c} \hat{\vec{r}}_{\perp}
\]

\[
\vec{r}_{\perp}(t) - \vec{r}_{\perp}(0) = -\frac{\hbar c}{eH} \hat{H} \times (\vec{k}(t) - \vec{k}(0)) + \vec{v}t
\]

\[
\vec{v} = \frac{eE}{H} (\vec{E} \times \hat{H})
\]

Motion in real space is a superposition of (1) motion under pure magnetic field plus (2) a uniform drift with velocity \(w\).
Crossed Magnetic and Electric Fields (Cont.)

What about motion in k-space?

\[ \hbar k' = -e \left( \vec{E} + \frac{\vec{v}(\vec{k}) \times \vec{H}}{c} \right) \]

\[ \vec{E}(\vec{k}) = \varepsilon(\vec{k}) - \hbar \vec{k} \cdot \vec{w} \]

for free electrons: kinetic energy viewed in reference frame moving with velocity of w.

k_\parallel is still conserved, \varepsilon is not. Electrons precess on constant \varepsilon surface with fixed k_\parallel. Closed orbits in k-space are still possible.

For closed orbits, why do the energies of the electrons oscillate back, rather than increase without bounds?

Why is the drift velocity perpendicular to the electric field?

Closed Cyclotron Orbits In Crossed E Field

\[ \frac{d\vec{v}}{dt} = -\frac{e}{c} \nabla \cdot (\vec{E} + \vec{v} \times \vec{H}) \]

\[ \dot{v}_x = \frac{eH}{c} (\mu_{yx} v_x - \mu_{xv} v_y) + eE_y \mu_{yx} \]

\[ \dot{v}_y = \frac{eH}{c} (\mu_{yx} v_x - \mu_{xv} v_y) + eE_y \mu_{yx} \]

\[ \dot{v}_z = \frac{eH}{c} (\mu_{zv} v_x - \mu_{zx} v_y) + eE_y \mu_{yz} \]

Assume magnetic field to lie in the z-direction and the electric field to lie in the y-direction.

Nearly free electrons:

\[ \dot{v}_x = -\frac{eH}{cm} v_y \]

\[ \dot{v}_y = \frac{eH}{cm} v_x + \frac{eE_y}{m} \]

\[ v_z = 0 \]

\[ v'_y = \frac{eH}{mc} v'_x \]

\[ v'_x = v_x \]

\[ v'_z = v_z \]
High-Field Hall Effect And Magnetoresistance

(1) large magnetic field ($\omega_c \tau >> 1$); (2) ε differs only slightly from ϵ.

**Case 1: All partially filled bands have closed orbits**

avg vel. perp. to H (since last collision)  \[
\lim_{\tau/\tau \to \infty} j_{\perp} = -n e \nu = \frac{-n e c}{\tau} (\vec{E} \times \vec{H}) + \nu \vec{w}
\]

**Holes**  \[
\frac{h c}{e H} \vec{H} \times \left( \vec{k}(\tau) - \vec{k}(0) \right) + \nu \vec{w}
\]

**Case 2: Some partially filled bands have open orbits**

**Electrons** can acquire energy from the electric field, magnetoresistance depends on the direction of the open orbits.

High field limit  \[
E(1) = 0
\]

**High-Field Magnetoresistance**

Assume open orbits along $\hat{n}$ direction in real space

**Hall bar measurement**

\[
\vec{E} = E^{(0)} \hat{n}' + E^{(1)} \hat{n}
\]

magnetoresistance  \[
\rho = \frac{\vec{E} \cdot \vec{j}}{\vec{j}} = \frac{E^{(0)} \cdot \hat{n}'}{E^{(0)} \cdot \hat{n}'}
\]

substitute $E$  \[
\vec{j} = \hat{n}' \cdot \vec{E}^{(0)} + \hat{n}' \cdot \vec{E}^{(1)}
\]

\[
\hat{n}' \cdot \vec{j} = E^{(0)} \hat{n}' \cdot \vec{E}^{(0)} + E^{(1)} \hat{n}' \cdot \vec{E}^{(1)}
\]

\[
\rho = \frac{(\hat{n}' \cdot \vec{j})^2}{\hat{n}' \cdot \vec{E}^{(0)} + \hat{n}' \cdot \vec{E}^{(1)}}
\]

ρ does not saturate at high field
13. Semiclassical Theory Of Conduction

Number of electrons of the n-th band, in dr and dk, at time t is

\[ dN = g_n(\vec{r}, \vec{k}, t) d\vec{r} \, d\vec{k} \]

Relaxation-Time Approximation

1. Probability that electron suffer a collision is \( dt/\tau \). \( \tau \) may depend on \( n \), \( r \), and \( k \).

2. The distribution of electrons emerging from the collisions at any time does not depend on the distribution prior to the collision.

3. When electrons have equilibrium distribution, collisions will not alter this distribution.

\[ g_n^0(\vec{r}, \vec{k}) = \frac{1}{1 + \exp \left\{ (\varepsilon_n(\vec{k}) - \mu(\vec{r})) / k_B T \right\}} \]

The distribution of electrons that emerge from collisions in \( dt \) is

\[ dg(\vec{r}, \vec{k}, t) = \frac{dt}{\tau_n(\vec{r}, \vec{k})} g_n^0(\vec{r}, \vec{k}) \]
Calculation of Nonequilibrium Distri. Fn.

Group electrons at time \( t = t' \) according to when they had their last collision. Follow a small phase space \( dr \, dk \) through time according to semiclassical model of dynamics (product \( dr^* \, dk \) is constant in time; Liouville theorem). At (an earlier) time \( t' \), this phase space volume is centered at \( r(t') \) and \( k(t') \).

The number of electrons emerging from collisions at \( r_n(t'), k_n(t') \) into the volume element \( dr' \, dk' \) is

\[
\frac{dt'}{\tau_n(r_n(t'), k(t'))} g_n^0(r_n(t'), k(t')) \frac{d\vec{r} \, d\vec{k}}{4\pi^3}
\]

Of this number, only a fraction \( P_n(r, k, t; t') \) survive from \( t' \) to \( t \).

\[
dN = g_n(\vec{r}, \vec{k}, t) \frac{d\vec{r} \, d\vec{k}}{4\pi^3} = \frac{d\vec{r} \, d\vec{k}}{4\pi^3} \int_{-\infty}^{\infty} \frac{dt' g_n^0(\vec{r}_n(t'), \vec{k}(t')) P_n(\vec{r}, \vec{k}, t; t')}{\tau_n(\vec{r}_n(t'), \vec{k}(t'))}
\]

In simplified notations,

\[
g(t) = \int_{-\infty}^{\infty} \frac{dt' g_n^0(\vec{r}(t')) P(t, t')}{\tau(t')}
\]

Relaxation Time Equations

Computation of \( P_n(r, k, t; t) \)

\[
P(t, t') = P(t, t' + dt') \left[ 1 - \frac{dt'}{\tau(t')} \right]
\]

\[
\frac{\partial}{\partial t'} P(t, t') = \frac{P(t, t')}{\tau(t')}
\]

\[
P(t, t') = \exp \left\{ - \int_{t'}^{t} \frac{dt''}{\tau(t'')} \right\}
\]

\[
P(t, t) = 1
\]

\[
g(t) = \int_{-\infty}^{\infty} \frac{dt' g^0(\vec{r}(t')) P(t, t')}{\tau(t')}
\]

Integrate by parts,

\[
g(t) = g^0(t) - \int_{-\infty}^{t} dt' P(t, t') \frac{d}{dt'} g^0(t')
\]
Relaxation Time Approximation

\[ g(t) = g^0(t) - \int_{-\infty}^{t} dt' P(t,t') \frac{d}{dt'} g^0(t') \]

\[ \text{time derivative of } g^0 \]

\[ g^0 \text{ can change with } \varepsilon \text{ through } k \text{ and with } \mu \text{ and } T \text{ through } r. \]

\[ \frac{d g^0(t')}{dt'} = \frac{\partial g^0}{\partial \varepsilon} \frac{\partial \varepsilon}{\partial t} + \frac{\partial g^0}{\partial T} \frac{\partial T}{\partial t} + \frac{\partial g^0}{\partial \mu} \frac{\partial \mu}{\partial t} + \frac{\partial g^0}{\partial r} \frac{\partial r}{\partial t} \]

\[ \frac{\partial g^0}{\partial \varepsilon} = \frac{\partial g^0}{\partial \varepsilon} \left( \frac{\varepsilon - \mu}{T} \right) \frac{\partial g^0}{\partial \varepsilon} \]

\[ g(t) = g^0 + \int_{-\infty}^{t} dt' P(t,t') \left[ - \frac{\partial f}{\partial \varepsilon} \nu \left( -eE - \nabla \mu - \frac{\varepsilon - \mu}{T} \nabla T \right) \right] \]

\[ \text{while evolving at } t', r(t'), \text{ and } k(t'). \]

No explicit dependence on magnetic field?

Comments On Non-Equilibrium Distribution

\[ g(t) = g^0 + \int_{-\infty}^{t} dt' P(t,t') \left[ - \frac{\partial f}{\partial \varepsilon} \nu \left( -eE - \nabla \mu - \frac{\varepsilon - \mu}{T} \nabla T \right) \right] \]

1. For small \( T \), \( g \) deviates from \( g^0 \) only near the Fermi level
2. The effect of magnetic field is only implicit, since it does not change \( \varepsilon \).
3. Usually, the spatial dependence of electric field and temperature gradient are weak and only need to be kept to linear order, i.e. \( t' \) dependence can be evaluated at zero field and gradient.
4. For uniform electromagnetic fields, constant \( T \) gradients, and position-independent relaxation times: integrand taken out of \( t' \) integral.
5. If \( \tau \) depends on \( k \) only through \( \varepsilon \), then

\[ P(t,t') = e^{-r(t')/\tau(k)} \]

\[ g(k,t) = g^0(k) + \int_{-\infty}^{t} dt' e^{-r(t')/\tau(k)} \left( - \frac{\partial f}{\partial \varepsilon} \nu(k(t')) \left( -eE(t') - \nabla \mu(t') - \frac{\varepsilon - \mu}{T} \nabla T(t') \right) \right) \]
DC Electrical Conductivity

\[ g(k, t) = g^0(k) + \int d^3r e^{-i(k \cdot r + i\tau)} \left( \frac{\partial f}{\partial \varepsilon} \right) (\varepsilon(k(t)) - e\bar{E}(t) - \nabla \mu(t) - \frac{\bar{g}}{T} \nabla T(t)) \]

\[ g(k) = g^0(k) - e\bar{E} \cdot \vec{v}(k(t)) \left( - \frac{\partial f}{\partial \varepsilon} \right) \]

\[ \vec{j}_n = -e \int \frac{d^3k}{4\pi^3} \vec{v}_n(k) g_s(k) \]

total current: sum all bands

\[ \bar{\sigma} = \sum_n \bar{\sigma}^{(n)} \]

\[ \bar{\sigma}^{(n)} = e^2 \int \frac{d^3k}{4\pi^3} \tau_n(\varepsilon_n(k)) \vec{v}_n(k) \vec{v}_n(k) \left( - \frac{\partial f}{\partial \varepsilon} \right)_{\varepsilon = \varepsilon_n(k)} \]

This is why bands completely filled or completely empty conduct no electricity.

1. Conductivity is in general anisotropic. However, isotropic for cubic systems.

2. Filled bands (and empty bands) contribute nothing.

3. Equivalence of particle and hole pictures in metals.

Since only a narrow range of energy contributes to the conductivity, \( \tau \) can be regarded as constant.

\[ \vec{v}_n(k) \left( - \frac{\partial f}{\partial \varepsilon} \right)_{\varepsilon = \varepsilon_n(k)} = -\frac{\hbar}{\varepsilon} \frac{\partial}{\partial \varepsilon} f(\varepsilon(k)) \]

\[ \bar{\sigma}^{(n)} = e^2 \tau(\varepsilon_F) \int \frac{d^3k}{4\pi^3} \vec{v}_n(k) \frac{\partial f(\varepsilon_n(k))}{\partial k} = e^2 \tau(\varepsilon_F) \int \frac{d^3k}{4\pi^3} f(\varepsilon_n(k)) \frac{\partial}{\partial k} \vec{v}_n(k) \]

\[ \bar{\sigma} = e^2 \tau(\varepsilon_F) \int_{\text{occupied}} \frac{d^3k}{4\pi^3} [M^{-1}(\bar{k})] \]

\[ \bar{\sigma} = e^2 \tau(\varepsilon_F) \int_{\text{unoccupied}} \frac{d^3k}{4\pi^3} [-M^{-1}(\bar{k})] \]

4. Recovery of the free electron result, if \( M^{-1} \) is constant (near band minimum or maximum)

\[ [M^{-1}(\bar{k})] = \pm \left( \frac{1}{m^*} \right) \delta_{ij} \]

\[ \sigma = ne^2 \tau / m^* \]
Conductivity ↔ Effective Mass

\[ \vec{\sigma} \cdot \vec{\dot{x}} = e^2 \tau_n(\epsilon_F) \int \frac{dk}{4\pi} v_n(k) \dot{v}(k) \left( -\frac{\partial f}{\partial \epsilon} \right) = e^2 \tau_n(\epsilon_F) \int \frac{dk}{4\pi} \frac{\partial \epsilon}{\hbar^2 k} \frac{1}{\hbar} \nabla f \left( -\frac{\partial f}{\partial \epsilon} \right) \]

\[ \vec{\sigma} \cdot \vec{\dot{x}} = -e^2 \tau_n(\epsilon_F) \int \frac{dk}{4\pi} \frac{f}{h^2 k} \nabla \frac{\partial \epsilon}{\partial k_x} \]

\[ \vec{\sigma}_o = e^2 \tau_n(\epsilon_F) \int \frac{dk}{4\pi} f \frac{\partial \epsilon^2}{h^2 \partial k \partial k_j} \]

\[ \vec{\sigma}_{ij} = e^2 \tau_n(\epsilon_F) \int \frac{dk}{4\pi} f \left[ M^{-1}(k) \right]_{ij} \]

AC Electrical Conductivity

\[ \vec{E}(t) = \text{Re} \left[ \vec{E}(\omega) e^{-i\omega t} \right] \]

\[ \vec{j}(t) = \text{Re} \left[ \vec{j}(\omega) e^{-i\omega t} \right] \]

\[ \vec{j}(\omega) = \vec{\sigma}(\omega) \cdot \vec{E}(\omega) \]

\[ \vec{\sigma}(\omega) = \sum_n \vec{\sigma}^{(n)}(\omega) \]

\[ \vec{\sigma}^{(n)}(\omega) = e^2 \int \frac{dk}{4\pi^2 h} \frac{\tilde{v}_n(k) \tilde{v}_n(k) (-\partial f / \partial \epsilon)}{\left[ 1 / \tau(\epsilon_n(k)) \right] - i\omega} \]

Drude result:
\[ \sigma(\omega) = \frac{ne^2 \tau / m}{1 - i\omega \tau} = \frac{\sigma_d}{1 - i\omega \tau} \]

In the limit \( \omega \tau \gg 1 \).

\[ \vec{\sigma}^{(n)}(\omega) = -\frac{e^2}{i\omega} \int \frac{dk}{4\pi^2 h} \tilde{v}_n(k) \tilde{v}_n(k) (-\partial f / \partial \epsilon) \]

\[ \vec{\sigma} = -\frac{e^2}{i\omega} \int_{\text{occupied}} \frac{dk}{4\pi^2} \left[ M^{-1}(k) \right] \]

Independent of \( \tau \).
Thermal Conductivity (Electronic)

\[ dQ = T \ dS \quad \text{thermal current density} \]

\[ j^q = T \ j^S \quad \text{entropy current density} \]

since volume is fixed

\[ T \ dS = dU - \mu \ dN \]

\[ T \ j^S = j^e - \mu \ j^N \]

\[ \left\{ \begin{array}{l} j^e \\ j^N \end{array} \right\} = \sum_n \int \frac{d\vec{k}}{4\pi^3} \left[ \varepsilon_n(\vec{k}) \right] \hat{v}_n(\vec{k}) g_n(\vec{k}) \]

\[ j^q = \sum_n \int \frac{d\vec{k}}{4\pi^3} \left[ \varepsilon_n(\vec{k}) - \mu \right] \hat{v}_n(\vec{k}) g_n(\vec{k}) \]

For \( H=0, \ E=\text{const}, \) and \( \nabla T=\text{const}, \) and constant relaxation time,

\[ g(\vec{k}) = g^s(\vec{k}) + \tau(\epsilon(\vec{k})) \left( -\frac{\partial f}{\partial \epsilon} \right) \hat{v}(\vec{k}) \hat{v}(\vec{k})' \left( -eE - \nabla \mu - \frac{\epsilon(\vec{k}) - \mu}{T} \nabla T \right) \]

Thermal and Electric Currents

\[ j^s = \sum_n \int \frac{d\vec{k}}{4\pi^3} \left[ \varepsilon_n(\vec{k}) - \mu \right] \hat{v}_n(\vec{k}) g_n(\vec{k}) \]

\[ j^e = L^{(1)} \vec{E} + L^{(2)} \left( -\nabla T \right) \]

\[ j^q = L^{(1)} \vec{E} + L^{(2)} \left( -\nabla T \right) \]

\[ L^{(1)} = \frac{\tau(\epsilon(\vec{k}))}{4\pi^3} \hat{v}(\vec{k}) \hat{v}(\vec{k})' \left( \epsilon(\vec{k}) - \mu \right) \]

define

\[ \sigma(\epsilon) = e^2 \tau(\epsilon) \int \frac{d\vec{k}}{4\pi^3} \hat{v}(\vec{k}) \hat{v}(\vec{k})' \left( \epsilon(\vec{k}) - \mu \right) \]

\[ \tilde{\sigma}(\epsilon) = e^2 \tau(\epsilon) \int \frac{d\vec{k}}{4\pi^3} \hat{v}(\vec{k}) \hat{v}(\vec{k})' \left( \epsilon(\vec{k}) - \mu \right) \]

\[ \tilde{\sigma}(\epsilon) = e^2 \tau(\epsilon) \int \frac{d\vec{k}}{4\pi^3} \hat{v}(\vec{k}) \hat{v}(\vec{k})' \left( \epsilon(\vec{k}) - \mu \right) \]

\[ \tilde{\sigma}(\epsilon) = e^2 \tau(\epsilon) \int \frac{d\vec{k}}{4\pi^3} \hat{v}(\vec{k}) \hat{v}(\vec{k})' \left( \epsilon(\vec{k}) - \mu \right) \]
\( k_B T \ll \varepsilon_F \) Results

\[ \tilde{I}^{(e)} = \int d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) (\varepsilon - \mu)^{\prime} \bar{\sigma}(\varepsilon) \]

\[ \tilde{I}^{(o)} = \int d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) \tilde{\sigma}(\varepsilon) \approx \tilde{\sigma}(\varepsilon_F) \int d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) = \tilde{\sigma}(\varepsilon_F) \]

\[ \tilde{I}^{(0)} = \int d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) (\varepsilon - \mu) \tilde{\sigma}(\varepsilon) = \int d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) (\varepsilon - \mu) [\tilde{\sigma}(\varepsilon_F)(\varepsilon - \mu) + (\varepsilon - \mu) \tilde{\sigma}(\varepsilon_F) + \cdots] \]

\[ = \tilde{\sigma}(\varepsilon_F) \int d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) (\varepsilon - \mu)^{\prime} = \tilde{\sigma}(\varepsilon_F) 2a_1(k_B T)^2 \]

\[ a_1 = 1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \cdots = \pi^2 \]

\( k_B T \ll \varepsilon_F \) Thermal/Electric Currents

\[ \tilde{I}^{(2e)} = \int d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) (\varepsilon - \mu)^{\prime} \tilde{\sigma}(\varepsilon) \]

\[ = \int d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) (\varepsilon - \mu)^{\prime} [\tilde{\sigma}(\varepsilon_F)(\varepsilon - \mu) + (\varepsilon - \mu) \tilde{\sigma}(\varepsilon_F) + \cdots] \]

\[ = \tilde{\sigma}(\varepsilon_F) \int d\varepsilon \left( -\frac{\partial f}{\partial \varepsilon} \right) (\varepsilon - \mu)^{\prime} = \frac{\pi^2 k_B^2 T^2}{3} \tilde{\sigma}(\varepsilon_F) \]

\[ \tilde{L}^{11} = \tilde{\sigma}(\varepsilon_F) = \tilde{\sigma} \]

\[ \tilde{L}^{21} = \tilde{I}^{(2e)} = \frac{\pi^2 k_B^2 T^2}{3e} \tilde{\sigma}(\varepsilon_F) \]

\[ \tilde{L}^{22} = -\frac{\pi^2 k_B^2 T^2}{3e^2} \tilde{\sigma}(\varepsilon_F) \]
Thermal Conductivity

Thermal conductivity measured in the absence of steady-state electrical current.

When \( j = 0 \),

\[
\vec{e} = -(\bar{L}^1)^{-1} \bar{L}^2 (\nabla T)
\]

\[
\vec{j}^s = \vec{K} (\nabla T)
\]

\[
\vec{K} = \bar{L}^{22} - \bar{L}^{21}(\bar{L}^{11})^{-1} \bar{L}^{12}
\]

\[
\vec{K} \approx \frac{\pi^2}{3} \left( \frac{k_B}{e} \right)^2 T \bar{\sigma}
\]

Wiedemann-Franz Law

Other Properties

Thermoelectric Power, \( Q \), is defined as

\[
\int \vec{e} \cdot d\bar{L} = Q \Delta T \quad \vec{e} = -Q \nabla T
\]

\[
Q = \frac{L^{12}}{L^{11}} = -\frac{\pi^2}{3} \frac{k_B^2 T}{e} \frac{\sigma'}{\sigma}
\]

Uniform Magnetic Field

\[
\bar{\sigma}^{(\alpha)} = e^2 \int \frac{dk}{4\pi^3} r_s (c_s(k)) \bar{v}_s(k) \bar{v}_s(k) \left( -\frac{\partial f}{\partial \epsilon} \right)_{\ell \neq 0, \ell'}
\]

replaced with

\[
\bar{\sigma}^{(\alpha)} = e^2 \int \frac{dk}{4\pi^3} r_s (c_s(k)) \bar{v}_s(k) \bar{v}_s(k) \left( -\frac{\partial f}{\partial \epsilon} \right)_{s \neq 0, \ell'}
\]

\[
\bar{v}_s(k) = \int \frac{dt}{\tau_s(k)} e^{i\ell(k) \bar{V}_s(k)} (\bar{K}_s(t))
\]

average velocity (past history)