SFB 1143

Solid State Theory (SS2020)

Lecture 15: Semiclassical electron transport theory

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§ 4.1 Drude theory

- Assumptions of the classical theory:

$$\begin{cases} \text{electrons as classical particles} \\ \text{collisions with a relaxation time } \tau \end{cases}$$

DC conductivity:

$$\vec{J} = \sigma \vec{E} \quad , \quad \sigma = \frac{n e^2 \tau}{m}$$

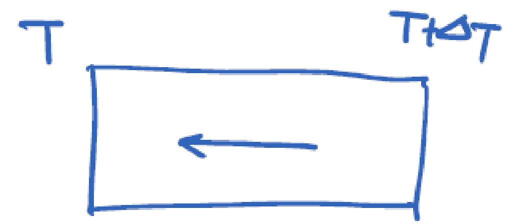
§ 4.1 Drude theory

- Thermal conductivity:

Fourier's law:

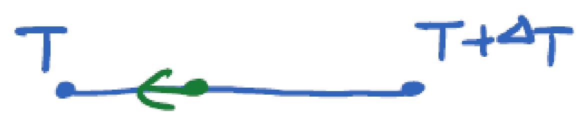
$$\vec{J}^q = -\kappa \vec{\nabla} T$$

thermal conductivity



1D case:

$$J^q = -\kappa \frac{dT}{dx}$$



Warmer region: larger electron (average) speed

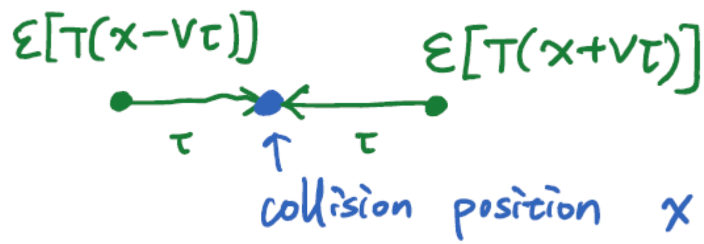
§ 4.1 Drude theory

thermal energy per electron (1D):

$$\varepsilon(T) = \frac{1}{2} m v^2 = \frac{1}{2} k_B T \qquad \left(3D: \frac{1}{2} m v^2 = \frac{3}{2} k_B T \right)$$

$\rightarrow$ T is now position dependent!

§ 4.1 Drude theory



Energy flow per electron:

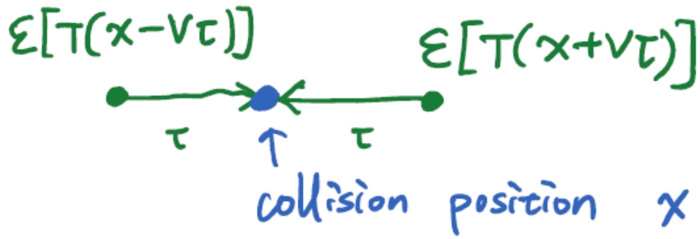
$$\mathcal{E}[T(x-v\tau)] - \mathcal{E}[T(x+v\tau)]$$

length: $v\tau$ $\quad$ $v\tau$

# of electrons: $\frac{1}{2}n\,v\tau$ (from left) $\quad$ $\frac{1}{2}nv\tau$ (from right)

electron density: $n = \frac{N_e}{L}$

§ 4.1 Drude theory



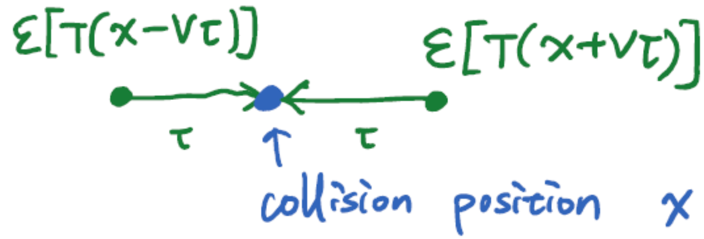
Energy flow per electron:

$$\mathcal{E}[T(x-v\tau)] - \mathcal{E}[T(x+v\tau)]$$

$\Rightarrow$ energy transport within time τ:

$$E^q = \frac{n}{2} v\tau \Big(\mathcal{E}[T(x-v\tau)] - \mathcal{E}[T(x+v\tau)] \Big)$$

§ 4.1 Drude theory



Energy flow per electron:

$$\varepsilon[T(x-v\tau)] - \varepsilon[T(x+v\tau)]$$

$\Rightarrow$ thermal current (energy transport per unit time):

$$J^q = \frac{E^q}{\tau} = \frac{n}{2} v \left(\varepsilon[T(x-v\tau)] - \varepsilon[T(x+v\tau)] \right)$$

§ 4.1 Drude theory

Assumption: mean free path $l = v\tau$ small

$$J^q = \frac{1}{2} n v \Big(\mathcal{E}[T(x - v\tau)] - \mathcal{E}[T(x + v\tau)] \Big)$$

$$= \frac{1}{2} n v \cdot (-2v\tau) \frac{d\mathcal{E}}{dx}$$

$$= -n v^2 \tau \frac{d\mathcal{E}}{dT} \cdot \frac{dT}{dx} \leftarrow n \frac{d\mathcal{E}}{dT} = \frac{N}{L} \frac{d\mathcal{E}}{dT} = \frac{1}{L} \frac{d\mathcal{E}}{dT}$$

$= C_v$ (heat capacity)

§ 4.1 Drude theory

From 1D to 3D:

$$\frac{dT}{dx} \rightarrow \vec{\nabla} T$$

$$\langle V_x^2 \rangle + \langle V_y^2 \rangle + \langle V_z^2 \rangle = \frac{1}{3} v^2$$

$$\Rightarrow J^q = \frac{1}{3} v^2 \tau \underbrace{n \frac{d\varepsilon}{dT}}_{\parallel} \cdot (-\vec{\nabla} T)$$

$$\frac{N}{V}\frac{d\varepsilon}{dT} = \frac{1}{V}\frac{dE}{dV} = C_V$$

$E = N\varepsilon$: total internal energy

$$\Rightarrow J^q = k(-\vec{\nabla} T) \quad \text{with} \quad k = \frac{1}{3} v^2 \tau C_V$$

§ 4.1 Drude theory

- Wiedemann-Franz law:

$$\frac{k}{\sigma} = \frac{\frac{1}{3}v^2\cancel{\tau}C_v}{\frac{ne^2\cancel{\tau}}{m}} = \frac{\frac{1}{3}mv^2C_v}{ne^2}$$

$C_v = \frac{3}{2}nk_B$, $\frac{1}{2}mv^2 = \frac{3}{2}k_BT$

classical !

$$= \frac{3}{2}\left(\frac{k_B}{e}\right)^2 T$$

universal !

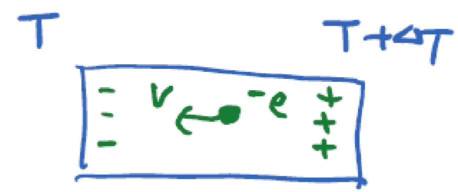
§ 4.1 Drude theory

- Thermoelectric effect:

Heat flow generates electric field !

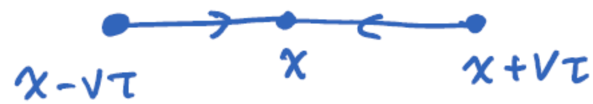
$$\vec{E} = Q \vec{\nabla} T$$

thermopower



§ 4.1 Drude theory

- “Net” velocity at position x (due to the temperature gradient):



$$
\begin{aligned}
v^q &= \frac{1}{2}\left[v(x-v\tau) - v(x+v\tau) \right] \\
&= \frac{1}{2}\cdot(-2v\tau)\frac{dv}{dx} \\
&= -v\tau\frac{dv^2}{dx} \\
&= -\frac{1}{2}\tau\frac{dv^2}{dT}\cdot\underbrace{\frac{dT}{dx}}_{\text{constant}}
\end{aligned}
$$

§ 4.1 Drude theory

From 1D to 3D: $v_x^2 = v_y^2 = v_z^2 = \frac{1}{3} v^2$

$$\Rightarrow \quad \vec{v}^{\,Q} = -\frac{1}{6} \tau \frac{dv^2}{dT} (\vec{\nabla} T)$$

$$\vec{v}^{\,E} = -\frac{e\vec{E}\tau}{m}$$

Due to the acceleration from the thermally generated electric field $\vec{E}$

§ 4.1 Drude theory

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Due to the acceleration from the thermally generated electric field $\vec{E}$

Steady state: $\quad \vec{v}^{Q} + \vec{v}^{E} = 0$

$$\frac{e\vec{E}\tau}{m} = -\frac{\tau}{6} \frac{dv^2}{dT} (\vec{\nabla} T)$$

§ 4.1 Drude theory

$$\vec{E} = -\frac{1}{6}\frac{m}{e}\frac{dv^2}{dT}(\vec{\nabla}T)$$

use $\frac{1}{2}mv^2 = \frac{3}{2}k_BT$

$$= -\frac{1}{3e}\frac{d}{dT}\left(\frac{3}{2}k_BT\right)(\vec{\nabla}T)$$

$C_v = \frac{3}{2}nk_B$

$$= -\frac{C_v}{3ne}(\vec{\nabla}T)$$

thermopower $Q = -\frac{C_v}{3ne}$

$$C_v = \frac{3}{2}nk_B \quad \Rightarrow Q = -\frac{k_B}{2e} \sim 10^{-4}\ \text{volt}/K$$

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10^2 times larger compared to experiments!

§ 4.2 Semiclassical approach

- Classical theory:

Electron velocity distribution in Drude's theory:

$$f_B(\vec{v}) \propto e^{-\frac{1}{2}mv^2/k_BT}$$

Boltzmann distribution

(electrons treated as classical particles)

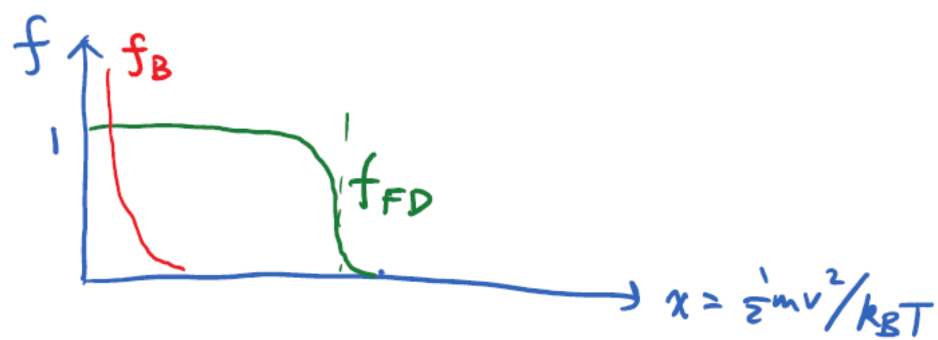
§ 4.2 Semiclassical approach

- Sommerfeld's theory:

free electron gas + Fermi-Dirac distribution

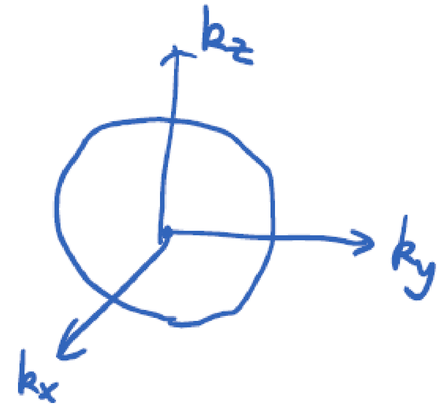
$$f_{FD}(\vec{v}) \propto \frac{1}{e^{(\frac{1}{2}m\vec{v}^2 - k_B T_0)/k_B T} + 1}$$

Fermi-Dirac distribution



§ 4.2 Semiclassical approach

$$E_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$$



$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

momentum: $\vec{p} = \frac{\hbar}{i}\vec{\nabla}$

$$\Rightarrow \vec{p}\,\psi_{\vec{k}}(\vec{r}) = \frac{\hbar}{i}\vec{\nabla}\psi_{\vec{k}}(\vec{r}) = \hbar\vec{k}\,\psi_{\vec{k}}(\vec{r})$$

velocity: $\vec{v} = \frac{\vec{p}}{m}$

$$\vec{v}\,\psi_{\vec{k}}(\vec{r}) = \frac{\hbar\vec{k}}{m}\psi_{\vec{k}}(\vec{r})$$

§ 4.2 Semiclassical approach

Work out $f(\vec{v})\,d\vec{v}$ (velocity distribution)

Each $\vec{k}$ point has volume $\dfrac{(2\pi)^3}{V}$

DOS in $\vec{k}$-space : $2 \times \dfrac{1}{(2\pi)^3/V}\, d\vec{k}$ $(T=0)$

Finite T : $2 \times \dfrac{V}{(2\pi)^3} f_{FD}(\varepsilon_{\vec{k}})\, d\vec{k}$

§ 4.2 Semiclassical approach

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Finite T : $2 \times \dfrac{V}{(2\pi)^3} f_{FD}(\varepsilon_{\vec{k}})\, d\vec{k}$

$\vec{v} = \dfrac{\hbar\vec{k}}{m} \Rightarrow d\vec{k} = \left(\dfrac{m}{\hbar}\right)^3 d\vec{v}$, $\varepsilon_{\vec{k}} = \dfrac{\hbar^2\vec{k}^2}{2m} = \dfrac{1}{2}m\vec{v}^2$

$$\Rightarrow \quad \underbrace{2 \times \frac{V}{(2\pi)^3} \frac{1}{e^{(\frac{1}{2}m\vec{v}^2-\mu)/k_BT}+1} \left(\frac{m}{\hbar}\right)^3 d\vec{v}}$$

$\parallel$

$$f(\vec{v}) = \frac{m^3 V}{4\pi^3\hbar^3} \frac{1}{e^{(\frac{1}{2}m\vec{v}^2-\mu)/k_BT}+1}$$

§ 4.2 Semiclassical approach

- Semiclassical approach: electrons treated as wave packets

$$v \simeq \frac{\hbar k_F}{m}$$

$$\Delta p \ll \hbar k_F$$

only those electrons close to the Fermi energy are important.

uncertainty principle:

$$\Delta x \cdot \Delta p \sim \hbar$$

$$\Rightarrow \Delta x \sim \frac{\hbar}{\Delta p} \gg \frac{1}{k_F} \simeq \underbrace{10^{-10}\,\mathrm{m}}_{\sim \text{ size of a unit cell}}$$

§ 4.2 Semiclassical approach

- Semiclassical approach: electrons treated as wave packets

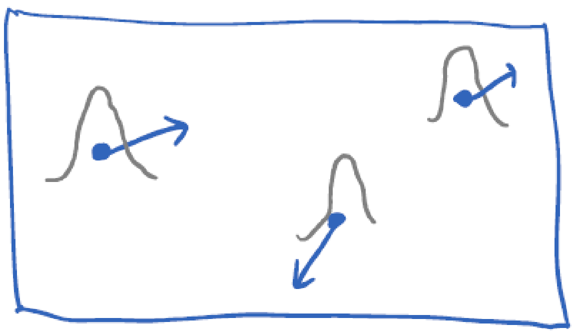
Mean free path:

$$\ell \simeq v_F \tau$$

$\tau \sim 10^{-14}\,s$

$\sim 10^{-8}\,m$

(room temperature)



§ 4.2 Semiclassical approach

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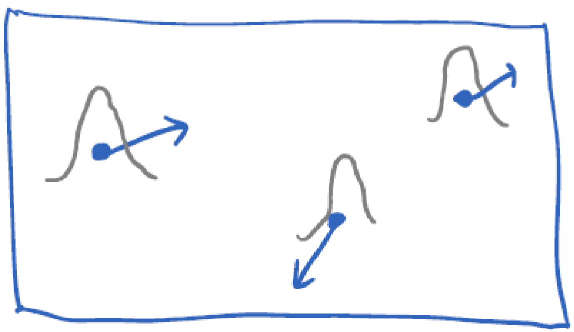

1) size of electron wave packet >> size of a unit cell

2) mean free path >> . . .

$\Downarrow$

Semiclassical treatment valid!

§ 4.2 Semiclassical approach

- Thermal conductivity:

$$\kappa = \frac{1}{3} v^2 \tau c_v$$

$$v_F^2 = \frac{2\varepsilon_F}{m}$$

$$\frac{\pi^2}{2} n k_B \left(\frac{k_B T}{\varepsilon_F}\right)$$

vs. Drude value $\frac{3}{2} n k_B$

vs. Drude value $v^2 = \frac{3 k_B T}{m}$

$$= \frac{\pi^2}{3} \frac{\tau}{m} n k_B^2 T$$

§ 4.2 Semiclassical approach

- Thermal conductivity:

$$\kappa = \frac{1}{3} v^2 \tau c_V$$

$$v_F^2 = \frac{2\varepsilon_F}{m}$$

vs. Drude value $v^2 = \frac{3k_BT}{m}$

$$c_V \rightarrow \frac{\pi^2}{2} n k_B \left(\frac{k_BT}{\varepsilon_F}\right)$$

vs. Drude value $\frac{3}{2} n k_B$

$$= \frac{\pi^2}{3} \frac{\tau}{m} n k_B^2 T$$

- Wiedemann-Franz law:

$$\sigma = \frac{ne^2\tau}{m}$$

$$\frac{\kappa}{\sigma} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 T$$

(Drude value: $\frac{3}{2}$)

more accurate now!

§ 4.2 Semiclassical approach

- Thermopower:

$$Q = -\frac{C_v}{3ne} \leftarrow C_v = \frac{\pi^2}{2} n k_B \left(\frac{k_B T}{\varepsilon_F}\right)$$

$$= -\frac{1}{6}\frac{k_B}{e}\left(\frac{k_B T}{\varepsilon_F}\right)$$

$$\sim -\left(\frac{\overset{\to 10^2 K}{T}}{\underset{\to 10^4 K}{T_F}}\right) \times 10^{-4}\ \text{volt}/K \quad \checkmark$$