

§4. Transport properties of solids

* Boltzmann equation

Semiclassical wave-packet picture:



$$\Delta x \sim \frac{\hbar}{\Delta p} \gg \frac{1}{k_F} \sim 10^{-10} \text{ m (unit cell size)}$$

$$\text{mean free path: } l \approx v_F \tau \sim 10^{-8} \text{ m}$$

- Distribution function

Thermal equilibrium (without external perturbation)

$$f_0(\vec{k}) = \frac{1}{e^{(\epsilon_{\vec{k}} - \mu)/k_B T} + 1} \quad \text{Fermi-Dirac}$$

With external perturbation (\vec{E} , \vec{B} , $\vec{\nabla}T \dots$):

$$H' = -e\vec{E} \cdot \vec{r} \theta(t-t_0)$$

$$f(\vec{r}, \vec{k}, t) = ?$$

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②

of electrons in phase-space volume $d\vec{r} \frac{d\vec{k}}{(2\pi)^3}$ at time t :

$$2 \int f(\vec{r}, \vec{k}, t) d\vec{r} \frac{d\vec{k}}{(2\pi)^3}$$

↑
Spin

$$N_e = \int 2 f(\vec{r}, \vec{k}, t) d\vec{r} \frac{d\vec{k}}{(2\pi)^3}$$

Wave packets move in phase space:
(semiclassical picture)

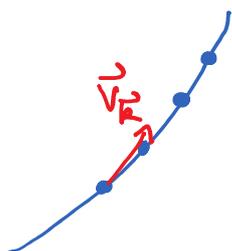


$$(\vec{r}, \vec{k}) \xrightarrow{dt} \left(\vec{r} + \vec{v}_R dt, \vec{k} + \frac{\vec{F}}{\hbar} dt \right)$$

$$\vec{v}_R = \frac{1}{\hbar} \frac{\partial \mathcal{E}_R}{\partial \vec{k}}$$

$$\frac{d(\hbar \vec{k})}{dt} = \vec{F} \quad (\text{external force})$$

↑
band information encoded



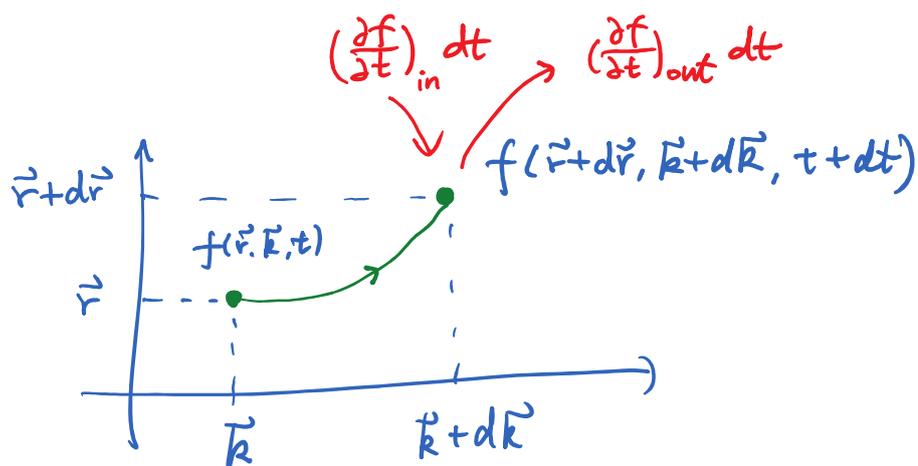
$$\mathcal{E}_R \approx \frac{\hbar^2 |\vec{k}|^2}{2m^*}$$

$$\Rightarrow \frac{1}{\hbar} \frac{\partial \mathcal{E}_R}{\partial \vec{k}} = \frac{\hbar \vec{k}}{m^*} = \vec{v}_R$$

(velocity of single-particle states)

04.06.19

③



$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} dt = \left(\frac{\partial f}{\partial t}\right)_{\text{in}} dt - \left(\frac{\partial f}{\partial t}\right)_{\text{out}} dt$$

due to collisions

$$f(\vec{r}+d\vec{r}, \vec{k} + \frac{1}{\hbar} \vec{F} dt, t+dt) = f(\vec{r}, \vec{k}, t) + \left(\frac{\partial f}{\partial t}\right)_{\text{coll}} dt$$

detailed balance

$$\begin{aligned} \text{LHS} &\simeq f(\vec{r}, \vec{k}, t) + \frac{\partial f}{\partial \vec{r}} \cdot d\vec{r} + \frac{\partial f}{\partial \vec{k}} \cdot d\vec{k} + \frac{\partial f}{\partial t} dt \\ &= \text{RHS} \end{aligned}$$

\downarrow $v_{\vec{k}} dt$ \downarrow $\frac{1}{\hbar} \vec{F} dt$

$$\Rightarrow \frac{\partial f}{\partial \vec{r}} \cdot v_{\vec{k}} + \frac{\partial f}{\partial \vec{k}} \cdot \frac{1}{\hbar} \vec{F} + \frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}$$

↑
How to model it?

Relaxation time assumption:

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\frac{f-f_0}{\tau} \quad \leftarrow \text{relaxation time, } \tau = \tau(\vec{r}, \vec{k})$$

Boltzmann equation:

$$\frac{\partial f}{\partial \vec{r}} \cdot \vec{v}_k + \frac{1}{\hbar} \frac{\partial f}{\partial \vec{k}} \cdot \vec{F} + \frac{\partial f}{\partial t} = -\frac{f-f_0}{\tau}$$

Example: $\vec{F} = 0$ (sudden removal of external force at $t=0$)

$$\frac{\partial f}{\partial \vec{r}} = 0 \quad (\text{uniform system})$$

$$\Rightarrow \frac{\partial f}{\partial t} = -\frac{f-f_0}{\tau}$$

$$f(\vec{k}, t) = f_0 + [f(\vec{k}, t=0) - f_0] e^{-t/\tau}$$

$$f(\vec{k}, t) \simeq f_0 \quad \text{for } t \gg \tau$$

(τ justified as "relaxation time")

Transport quantities can be calculated with the distribution function f (obtained from the Boltzmann equation).

- DC conductivity of metal

Charge current density:

$$\vec{J} = 2 \int \frac{d\vec{k}}{(2\pi)^3} (-e) \vec{v}_{\vec{k}} f(\vec{k}) \quad (\text{c.f. } \vec{J} = -en\vec{v})$$

↑
average velocity

$$\underbrace{\frac{\partial f}{\partial \vec{r}}}_{=0 \text{ (uniform)}} \cdot \vec{v}_{\vec{k}} + \frac{1}{\hbar} \frac{\partial f}{\partial \vec{k}} \cdot \underbrace{\vec{F}}_{=-e\vec{E}} + \underbrace{\frac{\partial f}{\partial t}}_{=0 \text{ (steady state)}} = - \frac{f - f_0}{\tau}$$

$$\Rightarrow \frac{1}{\hbar} \frac{\partial f}{\partial \vec{k}} \cdot (-e)\vec{E} = - \frac{f - f_0}{\tau}$$

$$f \simeq f_0 + \frac{e\tau}{\hbar} \frac{\partial f_0}{\partial \vec{k}} \cdot \vec{E}$$

$e|\vec{E}| \ll \hbar k_F$
(electric field weak)

$$f_1 = f - f_0 = \frac{e\tau}{\hbar} \frac{\partial f_0}{\partial \vec{k}} \cdot \vec{E}$$

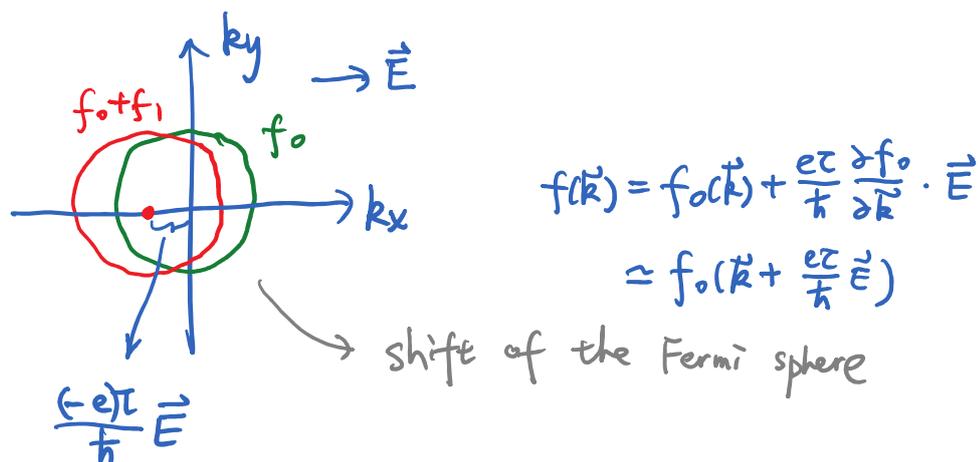
$$= \frac{e\tau}{\hbar} \frac{\partial f_0}{\partial \varepsilon_{\vec{k}}} \frac{\partial \varepsilon_{\vec{k}}}{\partial \vec{k}} \cdot \vec{E}$$

$$\left\langle \frac{1}{\hbar} \frac{\partial \varepsilon_{\vec{k}}}{\partial \vec{k}} = \vec{v}_{\vec{k}} \right\rangle$$

$$= e\tau \frac{\partial f_0}{\partial \varepsilon} \vec{v}_{\vec{k}} \cdot \vec{E}$$

04.06.19

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$$\vec{J} = 2 \int \frac{d\vec{k}}{(2\pi)^3} (-e) \vec{v}_{\vec{k}} f(\vec{k})$$

$$f_0(\vec{k}) + f_1(\vec{k})$$

no contribution since there is no DC current without \vec{E}

$$\vec{J} = \frac{1}{4\pi^3} \int d\vec{k} (-e) \vec{v}_{\vec{k}} e\tau_{\vec{k}} \frac{\partial f_0}{\partial \vec{E}} (\vec{v}_{\vec{k}} \cdot \vec{E})$$

$$= \frac{e^2}{4\pi^3} \int d\vec{k} \tau_{\vec{k}} \left(-\frac{\partial f_0}{\partial \vec{E}}\right) \vec{v}_{\vec{k}} (\vec{v}_{\vec{k}} \cdot \vec{E})$$

(relaxation time generally depends on \vec{k})

DC conductivity:

$$J^\alpha = \sum_{\beta} \sigma_{\alpha\beta} E_{\beta} \quad , \quad \alpha, \beta = x, y, z$$

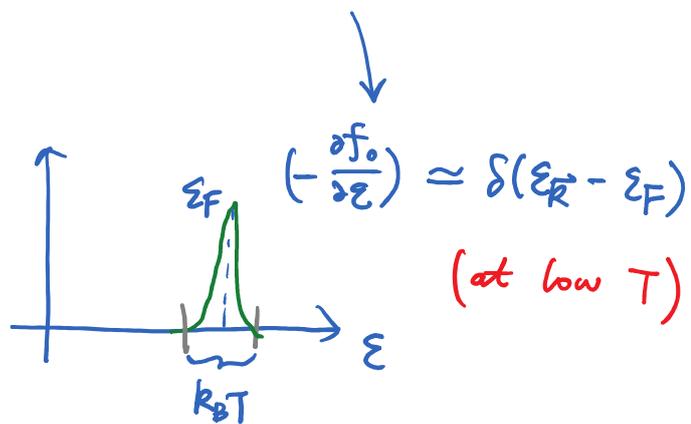
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⑦

electric field direction: $\hat{e} = \frac{\vec{E}}{|\vec{E}|}$

$$\begin{aligned} J &= \vec{J} \cdot \hat{e} \\ &= \frac{e^2 |\vec{E}|}{4\pi^3} \int d\vec{k} \tau_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon} \right) (\hat{e} \cdot \vec{v}_{\vec{k}})^2 \end{aligned}$$

$$\Rightarrow \sigma_0 = \frac{J}{|\vec{E}|} = \frac{e^2}{4\pi^3} \int d\vec{k} \tau_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon} \right) (\hat{e} \cdot \vec{v}_{\vec{k}})^2$$



Contribution mainly from electrons close to ε_F !

Estimations: $-\frac{\partial f}{\partial \varepsilon} \approx \delta(\varepsilon_F - \varepsilon_{\vec{k}})$ (low T)

$$(\hat{e} \cdot \vec{v}_{\vec{k}})^2 \approx \frac{1}{3} v_{\vec{k}}^2 \quad (\text{isotropic})$$

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$$\varepsilon_{\vec{k}} = \frac{\hbar^2 |\vec{k}|^2}{2m^*}$$

$$\begin{aligned} \delta(\varepsilon_F - \varepsilon_{\vec{k}}) &= \delta\left(\varepsilon_F - \frac{\hbar^2 |\vec{k}|^2}{2m^*}\right) \\ &= \frac{2m^*}{\hbar^2} \delta(k_F^2 - k^2) \\ &= \frac{2m^*}{\hbar^2} \frac{1}{2k_F} [\delta(k - k_F) + \delta(k + k_F)] \end{aligned}$$

$$\Rightarrow \sigma_0 = \frac{e^2}{4\pi^3} \int d\vec{k} \tau_{\vec{k}} \frac{1}{3} v_{\vec{k}}^2 \delta(\varepsilon_F - \varepsilon_{\vec{k}})$$

\downarrow
 $4\pi k^2 dk$

$$= \frac{e^2}{4\pi^3} \cdot 4\pi k_F^2 \tau_F \frac{1}{3} v_F^2 \frac{2m^*}{\hbar^2} \frac{1}{2k_F}$$

$$= \frac{e^2 m^*}{3\pi^2 \hbar^2} k_F \left(\frac{\hbar k_F}{m^*}\right)^2 \tau_F \quad v_F = \frac{\hbar k_F}{m^*}$$

$$= \frac{e^2 k_F^3}{3\pi^2 m^*} \tau_F \quad k_F^3 = 3\pi^2 n$$

$$= \frac{ne^2}{m^*} \tau_F$$

$$\sigma_0 = \frac{ne^2 \tau}{m} \quad (\text{Drude's theory})$$