TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

# Solid State Theory (SS2020)

## Lecture 16: Boltzmann equation

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# § 4.3 Boltzmann equation

- Semiclassical wave-packet picture:

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

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

# § 4.3 Boltzmann equation

- Distribution function:

Thermal equilibrium (without external perturbation)

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

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

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

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

# § 4.3 Boltzmann equation

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

$$\underset{\text{spin}}{\underset{\uparrow}{2}}\, f(\vec{r},\vec{k},t)\, d\vec{r}\, \frac{d\vec{k}}{(2\pi)^3}$$

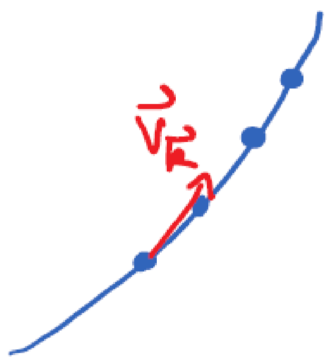
$$N_e = \int 2 f(\vec{r},\vec{k},t)\, d\vec{r}\, \frac{d\vec{k}}{(2\pi)^3}$$

# § 4.3 Boltzmann equation

- Establishing semiclassical equation of motion:

Wave packets move in phase space:

(semiclassical picture)


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

$$\Rightarrow \frac{1}{\hbar}\frac{\partial \varepsilon_{\vec{k}}}{\partial \vec{k}} = \frac{\hbar \vec{k}}{m^*} = \vec{v}_{\vec{k}}$$

(velocity of single-particle states)

# § 4.3 Boltzmann equation

- Establishing semiclassical equation of motion:

Wave packets move in phase space:

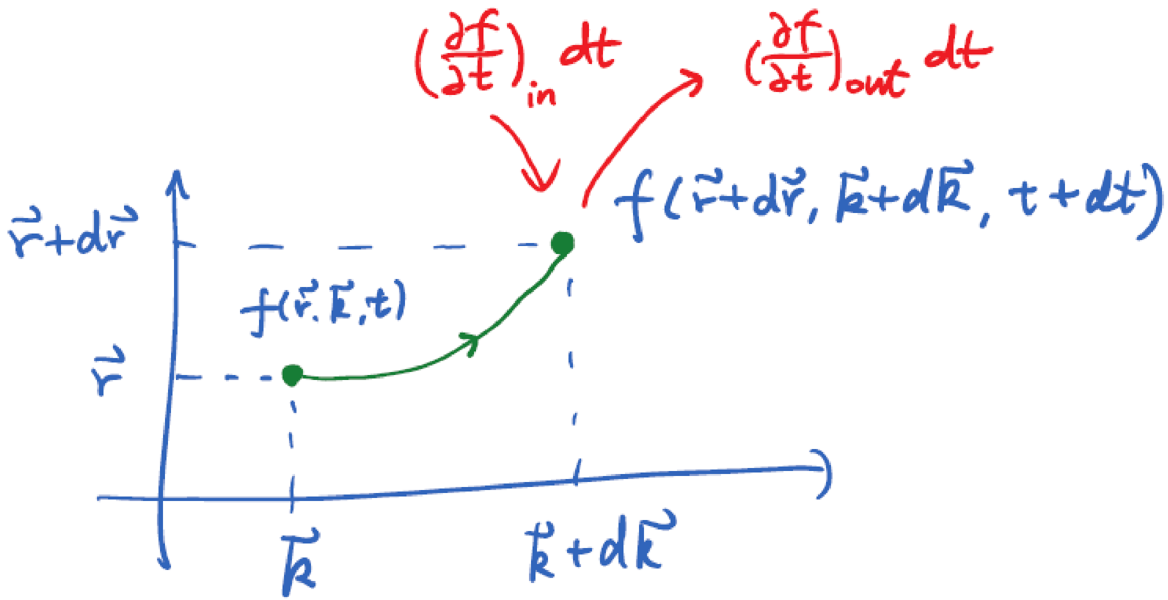
(semiclassical picture)


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

$$\vec{v}_{\vec{k}} = \frac{1}{\hbar} \frac{\partial \varepsilon_{\vec{k}}}{\partial \vec{k}} \qquad \frac{d(\hbar \vec{k})}{dt} = \vec{F} \ \text{(external force)}$$

band information encoded

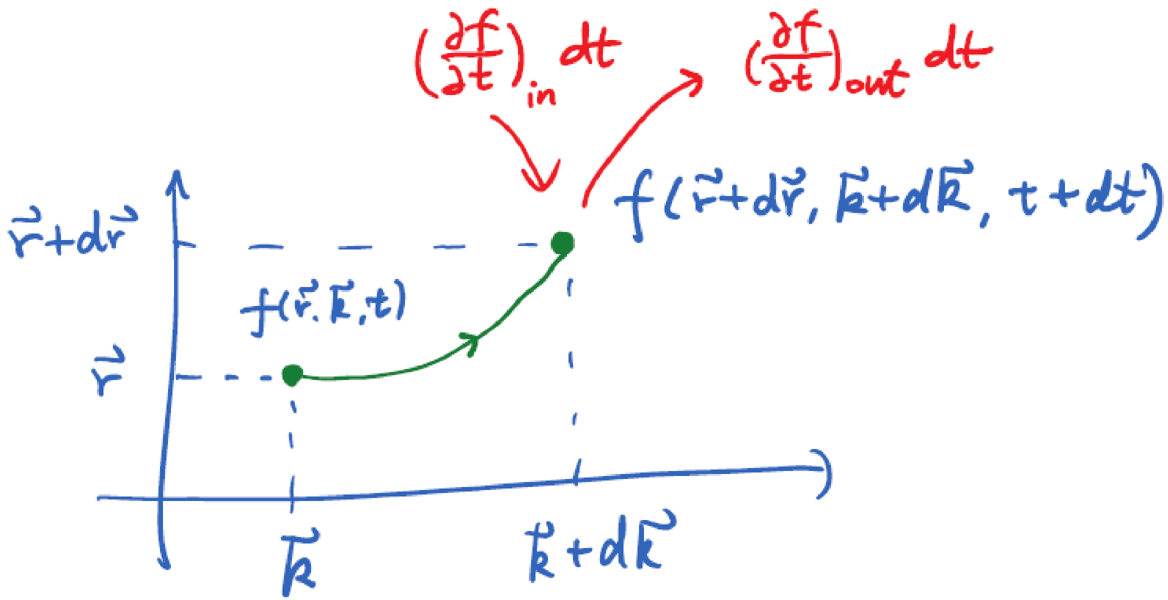
# § 4.3 Boltzmann equation




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

due to collisions

# § 4.3 Boltzmann equation




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

detailed balance

# § 4.3 Boltzmann equation

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

detailed balance

$$LHS \simeq f(\vec{r},\vec{k},t) + \frac{\partial f}{\partial \vec{r}}\cdot \underbrace{d\vec{r}}_{v_{\vec{k}}\,dt} + \frac{\partial f}{\partial \vec{k}}\cdot \underbrace{d\vec{k}}_{\frac{1}{\hbar}\vec{F}\,dt} + \frac{\partial f}{\partial t}dt$$

$$= RHS$$

# § 4.3 Boltzmann equation

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

detailed balance

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

How to model it ?

# § 4.3 Boltzmann equation

Relaxation time assumption:

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\frac{f-f_0}{\tau}$$

relaxation time, $\tau = \tau(\vec{r}, \vec{k})$

Boltzmann equation:

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

# § 4.3 Boltzmann equation

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

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

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

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

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

$\tau$ justified as "relaxation time"

# § 4.3 Boltzmann equation

- Example: Calculation of DC conductivity

Charge current density :

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

average velocity

# § 4.3 Boltzmann equation

- Example: Calculation of DC conductivity

Charge current density :

$$\vec{J} = 2\int \frac{d\vec{k}}{(2\pi)^3}\,(-e)\,\vec{v}_{\vec{k}}\, f(\vec{k}) \qquad \Big(\text{c.f. } \vec{J} = -en\underset{\text{average velocity}}{\vec{v}}\Big)$$

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

# § 4.3 Boltzmann equation

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

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

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

$e|\vec{E}| \ll \hbar k_F$

(electric field weak)

# § 4.3 Boltzmann equation

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

Change of distribution induced by the external electric field

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

$$\frac{1}{\hbar}\frac{\partial \varepsilon_{\vec{k}}}{\partial \vec{k}} = \vec{v}_{\vec{k}}$$

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

# § 4.3 Boltzmann equation

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

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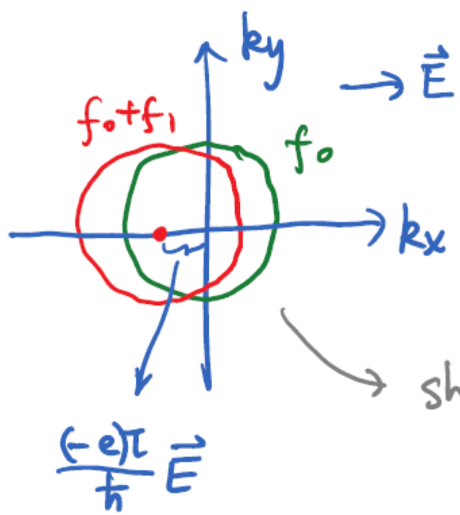
$$= e\tau\frac{\partial f_0}{\partial \varepsilon}\vec{v}_{\vec{k}}\cdot\vec{E}$$




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

$$\simeq f_0\left(\vec{k} + \frac{e\tau}{\hbar}\vec{E}\right)$$

shift of the Fermi sphere

# § 4.3 Boltzmann equation

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

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

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

# § 4.3 Boltzmann equation

$$\vec{J} = 2\int \frac{d\vec{k}}{(2\pi)^3}(-e)\,\vec{v}_{\vec{k}}\,\underbrace{f(\vec{k})}_{f_0(\vec{k})+f_1(\vec{k})}$$

$f_0(\vec{k})$ ⟶ no contribution since there is no DC current without $\vec{E}$

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

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

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

# § 4.3 Boltzmann equation

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

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

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

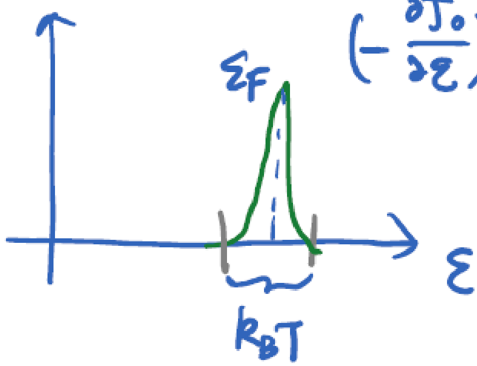
$$\Rightarrow \quad \sigma_0 = \frac{J}{|\vec{E}|} = \frac{e^2}{4\pi^3} \int d\vec{k}\; \tau_{\vec{k}} \left(-\frac{\partial f_0}{\partial \varepsilon}\right) \left(\hat{e} \cdot \vec{v}_{\vec{k}}\right)^2$$

# § 4.3 Boltzmann equation

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

$$\left(-\frac{\partial f_0}{\partial \varepsilon}\right) \simeq \delta(\varepsilon_{\vec{k}} - \varepsilon_F)$$

(at low T)




Contribution mainly from electrons close to $\varepsilon_F$ !

# § 4.3 Boltzmann equation

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

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

$(\vec{e} \cdot \vec{v}_{\vec{k}})^2 \simeq \frac{1}{3} v_{\vec{k}}^2$ (isotropic)

# § 4.3 Boltzmann equation

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

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

$(\vec{e} \cdot \vec{V}_{\vec{k}})^2 \simeq \frac{1}{3} V_{\vec{k}}^2$ (isotropic)

$$\delta(\varepsilon_F - \varepsilon_{\vec{k}}) = \delta\left(\varepsilon_F - \frac{\hbar^2 |\vec{k}|^2}{2m^*}\right)$$

$$= \frac{2m^*}{\hbar^2} \delta(k_F^2 - k^2)$$

$$= \frac{2m^*}{\hbar^2} \frac{1}{2k_F} \left[\delta(k - k_F) + \delta(k + k_F)\right]$$

# § 4.3 Boltzmann equation

$$\Rightarrow \sigma_0 = \frac{e^2}{4\pi^3}\int \underbrace{d\vec{k}}_{4\pi k^2 dk}\, \tau_{\vec{k}}\, \frac{1}{3} v_{\vec{k}}^2\, \underbrace{\delta(\varepsilon_F - \varepsilon_{\vec{k}})}_{\frac{2m^*}{\hbar^2}\frac{1}{2k_F}\delta(k-k_F)}$$

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

$$v_F = \frac{\hbar k_F}{m^*}$$

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

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

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

# § 4.3 Boltzmann equation

$$\Rightarrow \sigma_0 = \frac{e^2}{4\pi^3}\int \underbrace{d\vec{k}}_{4\pi k^2 dk}\, \tau_{\vec{k}}\, \frac{1}{3} v_{\vec{k}}^2\, \underbrace{\delta(\varepsilon_F - \varepsilon_{\vec{k}})}_{\frac{2m^*}{\hbar^2}\frac{1}{2k_F}\delta(k-k_F)}$$

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

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

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

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