C. The Boltzmann Transport Equation

- A semi-classical, but general otherwise, approach to Transport Properties
- Works for $\vec{\mathcal{E}}$, $\vec{\mathcal{B}}$, $\vec{\nabla} T$, $\vec{\nabla} n(\vec{r})$ and all kinds of collisions
- Under a "driving force", $f_{\text{non-equilibrium}} \neq f^{\circ}(\varepsilon)$

$f^{\circ}(\varepsilon)$ here is formally $f^{\circ} = \dfrac{1}{e^{(\varepsilon - E_F)/kT} + 1} = \dfrac{1}{e^{(\varepsilon(\vec{k}) - E_F)/kT} + 1} = f^{\circ}(\varepsilon) = f^{\circ}(\vec{k})$

If picking up the tail, then

$$f^{\circ} = e^{-(\varepsilon - E_F)/kT} = e^{-(\varepsilon(\vec{k}) - E_F)/kT} = e^{-(\frac{1}{2} m^* v^2 - E_F)/kT}$$

$$= f^{\circ}(\varepsilon) = f^{\circ}(\vec{k}) = f^{\circ}(\vec{v})$$

In Equilibrium, $$f^{\circ}(\vec{k}) = f^{\circ}(\varepsilon(\vec{k})) = \frac{1}{e^{(\varepsilon(\vec{k}) - E_F)/kT} + 1} \tag{17}$$

When system is out of equilibrium, introduce $f(\vec{r}, \vec{k}, t)$

Aside: Recall phase space (x, p) or (x, k). We are generalizing $f^0(\vec{k})$ (no $\vec{r}$-dependence because temp. T is the same everywhere at equilibrium) to phase space. More generally, a band index "n" $f_n(\vec{r}, \vec{k}, t)$ should be included. But we consider only one band (e.g. CB for electrons).

In thermal equilibrium (1 band):

$$\underset{\substack{\#\text{ electrons} \\ \text{in CB} \\ \text{(for example)}}}{N} = \overset{\text{spin}}{2} \cdot \frac{V}{(2\pi)^3} \int d^3k \, f^0(\vec{k})$$

$$= \underbrace{\iint d^3r}_{\text{gives } V} \, d^3k \left(2 \cdot \frac{V}{(2\pi)^3} f^0(\vec{k}) \right)$$

$\left[\frac{N}{V} = n = \text{electron \# density} \right]$

[recall: $d^3k \to 4\pi k^2 dk$, with $\mathcal{E} = \frac{\hbar^2 k^2}{2m^*}$, then

$$\int \frac{2V}{(2\pi)^3} (\cdots) \, d^3k$$
$$\downarrow$$
$$\int \underbrace{g(\mathcal{E})}_{\text{DOS}} (\cdots) \, d\mathcal{E} \;]$$

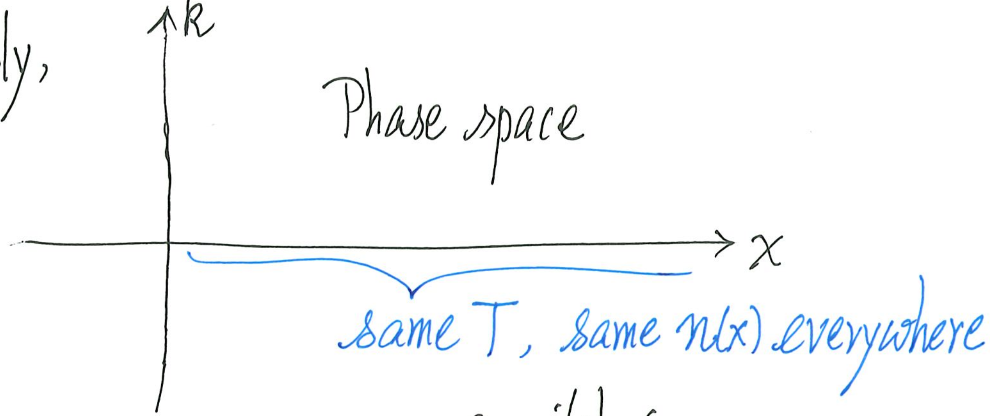
Driving Forces $\rightarrow$ $\underbrace{f(\vec{r}, \vec{k}, t)}$

all currents should be due to the out-of-equilibrium $f(\vec{r}, \vec{k}, t)$

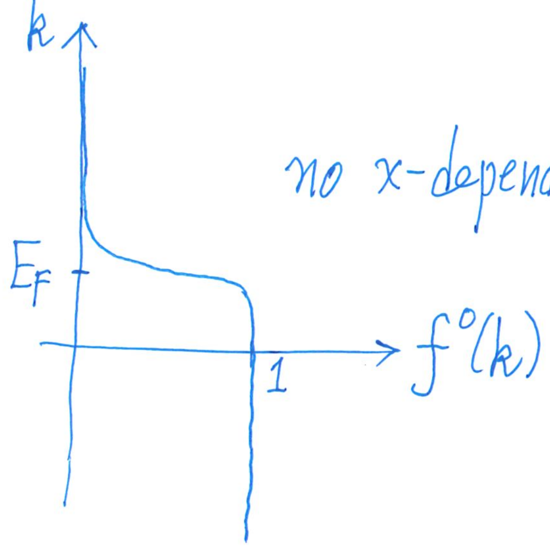
Meaning

$$\boxed{2 \cdot \frac{1}{(2\pi)^3} f(\vec{r}, \vec{k}, t)\, d^3r\, d^3k = dn(\vec{r}, \vec{k}, t) = \text{\# electrons in volume element } d^3r \text{ at } \vec{r} \text{ AND in the reciprocal space volume element } d^3k \text{ at } \vec{k} \text{ at time } t} \qquad (18)$$

Previously,

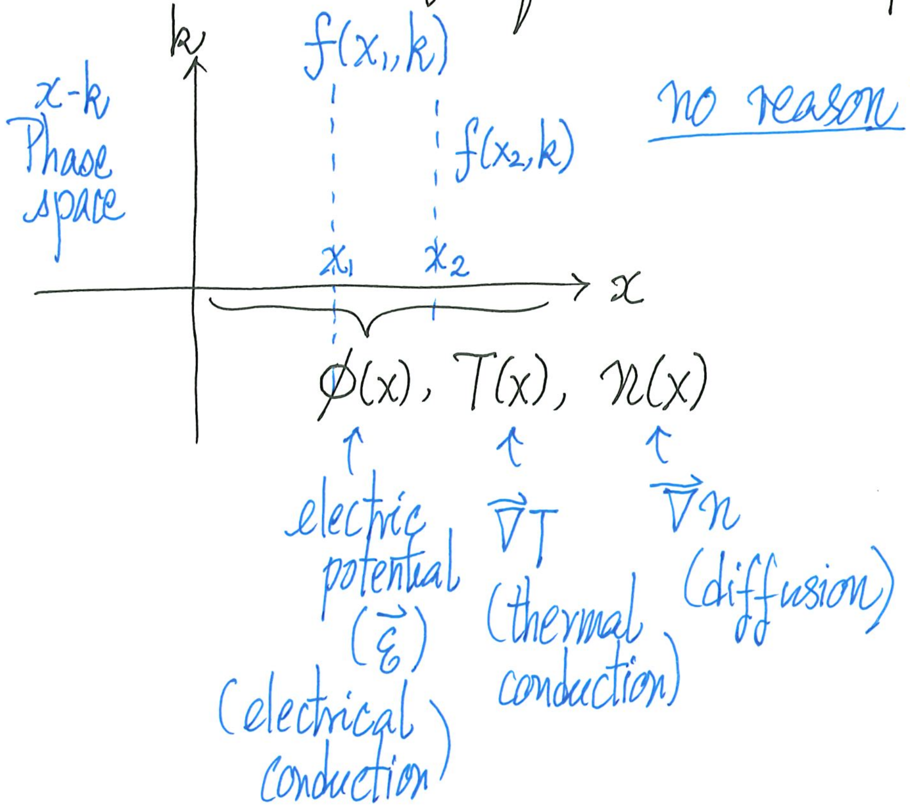


equilibrium



no x-dependence

But driven out of equilibrium in presence of driving forces...



<u>no reason</u> to expect $f(x_1, k) = f(x_2, k)$

$\therefore$ Need $\underbrace{\text{an equation}}_{\boxed{\text{Boltzmann Equation}}}$ for $f(\vec{r}, \vec{k}, t)$ to <u>include the effects</u> of

(i) external forces (driving forces)

and (ii) scatterings

How to use $f(\vec{r},\vec{k},t)$, if we have solved it?

- Physical quantities (responses) can be expressed in terms of $f(\vec{r},\vec{k},t)$

e.g. $\vec{J}_e(\vec{r},t)$ = electrical current density (the $\vec{J}(\vec{r},t)$ in EM Theory)

$$\boxed{\vec{J}_e(\vec{r},t) = (-e)\int_{1^{st}\text{ B.Z.}} d^3k\, \frac{2}{(2\pi)^3} f(\vec{r},\vec{k},t)\cdot \underbrace{\vec{V}(\vec{k})}_{\text{velocity of electron at } \vec{k}\ \left(\frac{1}{\hbar}\vec{\nabla}_{\vec{k}} \underbrace{E(\vec{k})}_{\text{band structure}}\right)}} \quad (19)$$

Note: If $f = f^0(\vec{k})$, $\vec{J}_e = 0$ (due to symmetry of $\overbrace{E(\vec{k})}^{\text{band structure}}$)

e.g. energy current density

$$\vec{J}_U(\vec{r},t) = \int_{1^{st}\text{ B.Z.}} d^3k\, \frac{2}{(2\pi)^3} f(\vec{r},\vec{k},t)\cdot \overbrace{E(\vec{k})\,\vec{V}(\vec{k})}^{\text{energy moves}} \quad (20)$$

(useful in study thermal conduction)

Setting up the Boltzmann Equation

Ideas: Both external forces and scattering cause electrons to change in $\vec{r}$ and in $\vec{k}$ $\Rightarrow$ $f(\vec{r},\vec{k},t)$ changes with time in general

Steady state: when external forces and scattering work together to maintain an out-of-equilibrium $f(\vec{r},\vec{k})$ (no time, $\because$ steady state)

Key idea

$$\boxed{\underbrace{\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}}_{\text{How does } f \text{ change?}} = \underbrace{\left(\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right)_{\text{field}}}_{\text{due to fields } (\vec{\mathcal{E}},\, \vec{B},\, -\vec{\nabla}T,\, -\vec{\nabla}n)} + \underbrace{\left(\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right)_{\text{scattering}}}_{\text{due to scatterings (phonons, impurities, defects, ...)}}} \quad (21)$$

This is the Boltzmann Equation (primitive form)

$\left(\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right)_{field}$ term: $\left(\frac{\partial f}{\partial t}\right)_{field} = \lim_{\Delta t \to 0}\left(\frac{f(\vec{r},\vec{k},t+\Delta t) - f(\vec{r},\vec{k},t)}{\Delta t}\right)_{field}$

<u>Key idea</u>: If an electron has $\vec{r}$ and $\vec{k}$ at time $t+\Delta t$, then <u>at an earlier time t</u>, its position was $(\vec{r} - \underbrace{\vec{v}(\vec{k})\Delta t}_{\text{moved this much in } \Delta t \text{ to reach } \vec{r}})$ and its wavevector was $(\vec{k} - \underbrace{\dot{\vec{k}}\Delta t}_{\text{moved this much in } \Delta t \text{ to reach } \vec{k}})$

$$\therefore f(\vec{r},\vec{k},t+\Delta t) = f(\vec{r} - \vec{v}(\vec{k})\Delta t,\ \vec{k} - \dot{\vec{k}}\Delta t,\ t)$$

"Make sense"!

$$= f(\vec{r},\vec{k},t) - \vec{v}(\vec{k}) \cdot \underbrace{\vec{\nabla}_{\vec{r}} f}_{\text{gradient in } \vec{r}}\,\Delta t - \dot{\vec{k}} \cdot \underbrace{\vec{\nabla}_{\vec{k}} f}_{\text{gradient in } \vec{k}}\,\Delta t$$

(Taylor expansion)
(order Δt)

$$= f(\vec{r},\vec{k},t) - \vec{v}(\vec{k}) \cdot \vec{\nabla}_{r} f\,\Delta t - \frac{\vec{F}_{ext}}{\hbar} \cdot \vec{\nabla}_{\vec{k}} f\,\Delta t$$

$\left(\because \hbar \frac{d\vec{k}}{dt} = \vec{F}_{ext}\right)$

$$\Rightarrow \boxed{\left(\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right)_{field} = -\vec{v}(\vec{k}) \cdot \vec{\nabla}_{r} f - \frac{\vec{F}_{ext}}{\hbar} \cdot \vec{\nabla}_{\vec{k}} f} \qquad (22)$$

Up to now, Boltzmann Equation becomes

$$\frac{\partial f(\vec{r},\vec{k},t)}{\partial t} = -\vec{v}(\vec{k})\cdot\vec{\nabla}_{\vec{r}} f - \frac{\vec{F}_{ext}}{\hbar}\cdot\vec{\nabla}_{\vec{k}} f + \left(\frac{\partial f}{\partial t}\right)_{scattering} \qquad (23)$$

- If nothing is there to cause spatially non-uniform distribution, then $f(\vec{k},t)$ only and $\vec{\nabla}_{\vec{r}} f$ term vanishes $\underbrace{\text{(e.g. no } -\vec{\nabla} n(\vec{r})\text{, or } \underbrace{-\vec{\nabla}\mu(\vec{r})}_{\text{gradient of chemical potential}})}_{\text{no } \vec{\nabla}_r f \text{ term}}$

Next, we handle $\left(\frac{\partial f}{\partial t}\right)_{scattering}$

$\left(\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right)_{scattering}$ term under the Relaxation Time Approximation

- Recall: $f(\vec{r},\vec{k},t)$ relaxes back to $f^0(\vec{k})$ by scattering processes

$$\boxed{\left(\frac{\partial f}{\partial t}\right)_{scattering} \cong -\frac{\left(f(\vec{r},\vec{k},t) - f^0(\vec{k})\right)}{\tau(\vec{k})}} \quad (24)$$

This is the Relaxation Time Approximation

- $\tau(\vec{k})$ (or $\tau(\vec{v})$, $\tau(\varepsilon)$, $\tau(\vec{p})$) is relaxation time for an electron in Bloch state $\vec{k}$
- In principle, $\tau(\vec{k})$ (or $1/\tau(\vec{k})$) can be calculated quantum mechanically (time-dependent perturbation theory) for given scattering process
- $\tau(\vec{k})$ depends on $\vec{k}$ (or energy ε, or velocity $\vec{v}$) in general
- $\underbrace{\tau(\vec{k}) \approx \tau}_{\text{simplest approximation}}$ for simplicity and $\tau(\vec{k})$ can be treated empirically

Boltzmann Equation within relaxation time approximation

$$\boxed{\left(\frac{\partial f}{\partial t}\right) = -\vec{v}(\vec{k})\cdot\vec{\nabla}_{\vec{r}} f - \frac{\vec{F}_{ext}}{\hbar}\cdot\vec{\nabla}_{\vec{k}} f - \frac{(f - f^{0}(\vec{k}))}{\tau(\vec{k})}} \qquad (25)$$

- Still very general
- Starting point for studying transport properties
- Good for $\vec{\mathcal{E}}$, $\vec{B}$, $-\vec{\nabla}T$, $-\vec{\nabla}\mu(\vec{r})$, $\cdots$; and various scattering processes
- Can solve for $f(\vec{r},\vec{k},t)$, thus transient response (time before steady state)
- For studying <u>Steady State</u> properties, set $\left(\frac{\partial f}{\partial t}\right) = 0$, solve for $f(\vec{r},\vec{k})$
- $\underbrace{\vec{\mathcal{E}}, \vec{B} \text{ go into } \vec{F}_{ext} ; \vec{\nabla}T, \vec{\nabla}\mu(\vec{r}) \text{ go into } \vec{\nabla}_{\vec{r}} f}$

  can solve $f(\vec{r},\vec{k})$ to any order of forces (linear and nonlinear response)
- Readily generalized to study out-of-equilibrium <u>phonon</u> distributions

  ($f(\vec{r},\vec{k},t)$ here is electron distribution)

Linear Response : a humble strategy with a big idea

Idea: $\vec{F}_{ext} = -e\vec{\mathcal{E}}$, solve steady state $f \cong \underset{\vec{J}_e = 0}{f^0} + \underbrace{\delta f}_{\text{gives } \vec{J}_e \neq 0}$

and aim at $\underbrace{\delta f \text{ to } \mathcal{E}^1}_{1^{st} \text{ order in } \mathcal{E}}$ (not-so-strong $\mathcal{E}$) and ignore $\sim \mathcal{E}^2, \sim \mathcal{E}^3$ terms

$$\vec{J}_e \sim \delta f \sim \vec{\mathcal{E}}, \text{ so } \vec{J}_e = \sigma \vec{\mathcal{E}}$$

- σ does not depend on $\vec{\mathcal{E}}$ ($\because \vec{\mathcal{E}}^1$ explicitly taken out)
- σ can be expressed in terms of quantities evaluated at equilibrium!

$\therefore$ In linear response, we aim at finding $f(\vec{r}, \vec{k})$ to 1st order in the driving (external) forces.

The response can then be evaluated in terms of quantities referred to equilibrium.

Stimulations		Response Functions
$\vec{\mathcal{E}}$	electric field	conductivity
plus $\vec{B}$	magnetic field	Magnetoresistance, Hall coefficient
$-\vec{\nabla}T$	temperature gradient	thermal conductivity
$-\vec{\nabla}\mu$	gradient of chemical potential	thermal power, Peltier coefficient
⋮		⋮

Scattering Processes for achieving Steady State

- electron-phonon, impurities (ionized, un-ionized (low-temp)), defects, sample boundary

All can be treated under one roof! (The Boltzmann Equation)

Remarks

(i) $(\vec{r}, \vec{p})$ phase space (instead of $(\vec{r}, \vec{k})$) useful in Solid States, then $f(\vec{r}, \vec{p}, t)$

$$\frac{\partial f}{\partial t} = -\vec{v} \cdot \vec{\nabla}_{\vec{r}} f - \vec{F} \cdot \vec{\nabla}_{\vec{p}} f - \frac{(f - f^0)}{\tau} \tag{26}$$

(ii) There is a quantum version of Boltzmann's approach based on Wigner Functions

(iii) Statistical Dynamics: How systems approach equilibrium (beyond equilibrium statistical mechanics)

e.g. See Balescu, "Statistical Dynamics: Matter out of Equilibrium"

D. Electrical Conductivity σ

Q: What is that "τ" in $\frac{ne^2}{m^*}\tau$?

$\begin{cases} \text{an averaged } \tau\text{, what is the average? [in semiconductors]} \\ \text{a characteristic } \tau\text{, what is it? [in metals]} \end{cases}$

- Static, Uniform (no $\vec{r}$-dependence) electric field only $\vec{\mathcal{E}}$ ($\therefore \vec{F}_{ext} = -e\vec{\mathcal{E}}$)
- $f(\vec{r},\vec{k})$ in steady state is $f(\vec{k})$ only $\Rightarrow$ $\vec{\nabla}_{\vec{r}} f$ term vanishes

$\therefore$ Steady state Boltzmann Equation becomes (see Eq. (25))

Steady state $\rightsquigarrow$ $$0 = \frac{e\vec{\mathcal{E}}}{\hbar}\cdot\vec{\nabla}_{\vec{k}} f - \frac{\delta f(\vec{k})}{\tau(\vec{k})}$$

$\delta f \equiv f - f^0$

$\Rightarrow f = f^0 + \underbrace{\delta f}_{\text{wants this to 1st order in } \vec{\mathcal{E}}}$

one factor of $\vec{\mathcal{E}}$ out here

$$\Rightarrow \frac{\delta f(\vec{k})}{\tau} = \frac{e\vec{\mathcal{E}}}{\hbar}\cdot\vec{\nabla}_{\vec{k}} \underbrace{f(\vec{k})}_{f^0(\vec{k}) + \delta f(\vec{k})} \qquad (27)$$

at least 1st order

$\therefore$ Linear Response $\Rightarrow$ $$\boxed{\delta f(\vec{k}) = \frac{e}{\hbar}\tau(\vec{k})\,\vec{\nabla}_{\vec{k}}\underbrace{f^{0}(\vec{k})}_{\text{equilibrium!}}\cdot\vec{\mathcal{E}}} \qquad (28)$$

linear in $\vec{\mathcal{E}}$

This is the general linear response result, good for systems (bands) in which carriers are electrons ($-e$ charged), i.e. semiconductors/metals

Further development

$$f^{0}(\vec{k}) = \frac{1}{e^{(\mathcal{E}(\vec{k})-E_F)/kT}+1}$$

(including metals and $\underbrace{\text{semiconductors}}_{\text{pick up the tails as } E_F \text{ in gap}}$)

$$\frac{1}{\hbar}\underbrace{\vec{\nabla}_{\vec{k}}f^{0}(\vec{k})}_{\text{a vector}} = \frac{\partial f^{0}}{\partial \mathcal{E}}\cdot\frac{1}{\hbar}\vec{\nabla}_{\vec{k}}\mathcal{E}(\vec{k})$$

energy

(chain rule)

$$= \left(\frac{\partial f^{0}}{\partial \mathcal{E}}\right)\underbrace{\vec{v}(\vec{k})}_{\text{a vector}}$$

$\left(\because\ \vec{v}(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}\underbrace{\mathcal{E}(\vec{k})}_{\text{band}}\right)$

Inspect
$$\frac{\partial f^\circ}{\partial \varepsilon} = \frac{\partial}{\partial \varepsilon}\left[\frac{1}{e^{(\varepsilon - E_F)/kT}+1}\right] = \frac{-1}{\left(e^{(\varepsilon-E_F)/kT}+1\right)^2}\cdot e^{(\varepsilon-E_F)/kT}\cdot\frac{1}{kT}$$
$$= -\frac{1}{kT}\cdot\left(\frac{1}{e^{(\varepsilon-E_F)/kT}+1}\right)\cdot\frac{e^{(\varepsilon-E_F)/kT}}{e^{(\varepsilon-E_F)/kT}+1}$$
$$= -\frac{1}{kT}\cdot f^\circ\cdot\left(1-f^\circ\right) \qquad (29)$$

(general)+

[or later see $f^\circ(1-f^\circ) \rightarrow -kT\left(\frac{\partial f^\circ}{\partial \varepsilon}\right)$]

+ $$\underbrace{\frac{\partial f^\circ}{\partial \varepsilon}}_{\text{a negative quantity}} = - \underbrace{\frac{1}{kT}}_{>0}\cdot\underbrace{f^\circ}_{>0}\,\underbrace{(1-f^\circ)}_{>0}$$

and it is!

true for semiconductors and metals

$$\therefore\ \delta f(\vec{k}) = e\tau(\vec{k})\left(\frac{\partial f^0}{\partial \mathcal{E}}\right)\vec{v}(\vec{k})\cdot\underbrace{\vec{\mathcal{E}}}_{\text{order } \vec{\mathcal{E}}^1} = -\frac{1}{kT}e\tau(\vec{k})f^0(1-f^0)\,\vec{v}(\vec{k})\cdot\vec{\mathcal{E}}$$

$$\Rightarrow \boxed{\begin{aligned} f(\vec{k}) &= f^0(\vec{k}) + e\tau(\vec{k})\left(\frac{\partial f^0}{\partial \mathcal{E}}\right)\vec{v}(\vec{k})\cdot\vec{\mathcal{E}} \\ &= f^0(\vec{k}) - \frac{e}{kT}\tau(\vec{k})f^0(1-f^0)\,\vec{v}(\vec{k})\cdot\vec{\mathcal{E}} \end{aligned}} \quad (30)$$

both forms are general

Remark: $f^0(1-f^0)$ will behave differently for $\begin{cases}\text{metals (degenerate gas)} \\ \text{semiconductors (non-degenerate gas)}\end{cases}$

(i) metals: E_F inside band, $f^0(1-f^0) = kT\,\delta(\mathcal{E}-E_F)$

or $\dfrac{\partial f}{\partial \mathcal{E}} \to -\delta(\mathcal{E}-E_F)$

(ii) Semiconductors: E_F in gap, $f^0 \sim e^{-(\mathcal{E}-E_F)/kT}$ tail in CB ($\ll 1$)

$1-f^0 \sim 1$

$$f^0(1-f^0) \sim e^{-(\mathcal{E}-E_F)/kT} = e^{E_F/kT}\cdot e^{-\mathcal{E}/kT} \quad \text{and} \quad \frac{\partial f}{\partial \mathcal{E}} = -\frac{1}{kT}\cdot f^0$$

Appreciating the physics in $f(\vec{k})$:

$$\underbrace{f(\vec{k})}_{\text{(3) giving rise to steady state}} = \underbrace{f^{0}(\vec{k})}_{\text{not giving } \vec{J}_e \text{ [equilibrium term]}} + e\,\underbrace{\tau(\vec{k})}_{\text{(2) counteracted by scattering}}\left(\frac{\partial f^{0}}{\partial \varepsilon}\right)\underbrace{\vec{v}(\vec{k})\cdot\vec{\varepsilon}}_{v_z(\vec{k})\,\varepsilon \text{ if } \vec{\varepsilon}\,/\!/\,\hat{z}} \tag{30}$$

(1) effect of ε to shift equilibrium f^{0} is...

Read (1), (2), (3) in order

- $f(\vec{k})$ replaces $f^{0}(\vec{k})$ in presence of $\vec{\varepsilon}$
- Need to consider states at different $\vec{k}$'s (DOS) to obtain responses

Formal Expression of Electrical Conductivity Tensor

$$\vec{J}_e = (-e)\int_{1^{st}\,B.Z.} d^3k \, \frac{2}{(2\pi)^3} \cdot \Big[\underbrace{f^0(\vec{k})}_{\text{gives "0" for } \vec{J}_e} + e\,\tau(\vec{k}) \left(\frac{\partial f^0}{\partial \varepsilon}\right) \underbrace{\vec{v}(\vec{k})\cdot\vec{\varepsilon}}_{\sum_j v_j(\vec{k})\,\varepsilon_j} \Big] \, \vec{v}(\vec{k}) \qquad \text{(see Eq. (19))}$$

$$\vec{\varepsilon} = \varepsilon_i \hat{i} + \varepsilon_j \hat{j} + \varepsilon_k \hat{k}$$

$$= e^2 \int_{1^{st}\,B.Z.} d^3k \, \frac{2}{(2\pi)^3} \left(-\frac{\partial f^0}{\partial \varepsilon}\right) \sum_j v_j(\vec{k})\,\varepsilon_j \;\; \tau(\vec{k}) \; \vec{v}(\vec{k}) \qquad (31)$$

$$\underbrace{(J_e)_i}_{i^{th}\text{ component}} = \sum_j \underbrace{\left[\frac{2}{(2\pi)^3} e^2 \int d^3k \, \underbrace{\left(-\frac{\partial f^0}{\partial \varepsilon}\right)}_{\text{positive}} v_i(\vec{k}) \, v_j(\vec{k}) \, \tau(\vec{k}) \right]}_{\equiv\, \sigma_{ij}} \varepsilon_j \equiv \sum_j \sigma_{ij}\,\varepsilon_j \qquad (32)$$

band structure information (m^* comes in)

The "τ" in $\frac{ne^2}{m^*}\tau$ is an average (non-trivial) as a consequence of Boltzmann Transport Theory

For $\varepsilon(\vec{k}) \sim \frac{\hbar^2 k^2}{2m^*}$ (isotropic),

$\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma, \quad \sigma_{ij} = 0 \; (i \neq j)$

In a discrete summation form:

$$\underbrace{\vec{J}_e}_{\substack{3\times 1\\ \text{(vector)}}} = \frac{(-e)}{V} \underbrace{\sum_{\vec{k}\,(\text{in B.Z.})}}_{\int \frac{V}{(2\pi)^3} d^3k} \underbrace{\sum_{\text{spin}}}_{\text{"2"}} \underbrace{e\tau(\vec{k})\left(\frac{\partial f^0}{\partial \mathcal{E}}\right)\vec{v}(\vec{k})\cdot\vec{\mathcal{E}}}_{\delta f(\vec{k})}\ \vec{v}(\vec{k}) = \underbrace{\underbrace{\overleftrightarrow{\sigma}}_{3\times 3}\cdot\underbrace{\vec{\mathcal{E}}}_{3\times 1}}_{3\times 1}$$

$$\boxed{\sigma_{ij} = \frac{e^2}{V}\sum_{\vec{k}}\sum_{\text{spin}}\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right) v_i(\vec{k})\, v_j(\vec{k})\, \tau(\vec{k})} \qquad (32a)$$

Expression for Mobility

N_e = # electrons in band ; $\frac{N_e}{V} = n$ = electron number density

$$\langle \vec{v}\rangle_{av} = \frac{1}{N_e}\sum_{\vec{k}}\sum_{\text{spin}}\left[e\tau(\vec{k})\left(\frac{\partial f^0}{\partial \mathcal{E}}\right)\vec{v}(\vec{k})\cdot\vec{\mathcal{E}}\right]\vec{v}(\vec{k}) = (-e)\frac{V}{N_e}\vec{J}_e$$

average drift velocity

$$\therefore \boxed{\underbrace{\vec{J}_e}_{\overleftrightarrow{\sigma}\cdot\vec{\mathcal{E}}} = (-e)\, n \underbrace{\langle \vec{v}\rangle_{av}}_{-\overleftrightarrow{\mu}\cdot\vec{\mathcal{E}}}}$$

mobility tensor (positive)

$$\therefore \boxed{\sigma_{ij} = e\, n\, \mu_{ij}}$$

positive

Remarks

- Obtained general expression for the conductivity (within linear response)
- See Eq. (32) (32a):
  - involve $-\frac{\partial f^0}{\partial \varepsilon}$ ← equilibrium f^0's derivative
  - involve $e^2 v_i(\vec{k})\, v_j(\vec{k})$ ≈ correlation function
  - involve $\tau(\vec{k})$ inside $\sum_{\vec{k}}$ (etc.) $\Rightarrow \frac{ne^2 \text{"}\tau\text{"}}{m}$ ← non-trivial average
- Can derive general expressions for other responses