AM 16,17

Boltzmann transport equation

Before

semiclassical dynamics of "single particle" (single wave packet). Force: $F = -e(\hat{E} + \bar{v} \times \bar{B})$

$$\frac{d\vec{p}}{dt} = \vec{F} - \frac{\vec{p}}{\tau}$$

"collission" time τ

when $F=0 \Rightarrow p = p_0 e^{-t/\tau}$

τ = timescale of loss of momentum

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

band structure $m \rightarrow m^*_{ij} = \left[\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}\right]^{-1}$ ⓐ

$\downarrow$

Bloch states $\psi_k(\vec{r}) = u_k(\vec{r})\, e^{i k \cdot \vec{r}}$, $u_k(\vec{r})$ lattice periodic

- Hamilton operator (single band).

$$H = \sum_{k\sigma} E(k)\, |k\rangle\langle k|$$

- velocity $v(k) = \frac{1}{\hbar}\frac{\partial E}{\partial k}$
- mass → see above ⓐ
- occupation: $f^0(k) = \frac{1}{e^{\beta(E(k)-\mu)} + 1}$

$\beta = \frac{1}{k_B T}$; μ: chemical potential (for $T=0$ $\equiv E_F$)

- disadvantages:

  ad hoc introduction of τ

  more typically one has scattering from $k \to k'$

  so better would be $\psi_k \to \psi_k e^{-t/\tau}$ i.e. finite lifetime in state k.

~~and~~ better starting point:

consider small region in phase space $d\bar{r}\,d\vec{k}$ and see how # occupied states evolve with time.

① introduce distribution function $f(\bar{r}, \bar{k}, t)$, which describes occupation in $\frac{d\bar{r}\,d\bar{k}}{(2\pi)^3}$ at time t

② in ~~the~~ equilibrium $f(\bar{r}, \bar{k}, t) = f^0(k)$
i.e. FD distribution
- time independent
- homogeneous.

③ Forces change occupation,
i.e. forces drive $f(\bar{r}, \bar{k}, t)$ <u>away</u> from f_0.

④ Collissions drive $f(\bar{r}, k, t)$ <u>towards</u> f_0.
i.e. they restore ~~the~~ equilibrium

objective now is to study the distribution as a function of time ~~and space~~ since when $f(\bar{r}, \bar{k}, t)$ is known we can calculate properties: e.g. current

$$j(r,t) = \frac{1}{(2\pi)^3} \int d^3\bar{k} \cdot (-e\bar{v}) \cdot (f(\bar{r}, \bar{k}, \bar{t}) - f^0(\bar{k}))$$

since current is response of force F
one expects that $[f(r,k,t) - f^0(k)] \sim F$

When ~~no external forces~~ steady state situation $\Rightarrow \frac{df}{dt} = 0.$

effectively no scattering (i.e. $\frac{\partial f}{\partial t}\Big|_{\text{in scattering}} = \frac{\partial f}{\partial t}\Big|_{\text{out scattering}}$)

example $f(x, k_x, t)$.

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial f}{\partial k_x}\frac{\partial k_x}{\partial t} = 0.$$

$$= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\cdot v_x + \frac{\partial f}{\partial k_x}\cdot\frac{1}{\hbar}F_x = 0.$$

more general:

$$\frac{\partial f}{\partial t} + \bar{v}\cdot\bar{\nabla}_r f + \frac{1}{\hbar}\vec{F}\cdot\bar{\nabla}_k f = 0.$$

Relaxation time approximation

scattering "in" and "out" of element $\frac{d^3\bar{r}\,d^3k}{(4\pi)^3}$
leads to "restoring" equilibrium

if deviation from equil. is $\delta f = f - f^0$

then for homogeneous case with no fields.

$$\frac{\partial f}{\partial t} = -\frac{\delta f}{\tau_k}$$

($\bar{v}\cdot\bar{\nabla}_r f$ & $\frac{1}{\hbar}\bar{F}\cdot\bar{\nabla}_k f$ are zero)

$\Rightarrow$ BTE in relaxation time approximation: !!

$$\boxed{\frac{\partial f}{\partial t} + \bar{v}\cdot\bar{\nabla}_r f + \frac{1}{\hbar}\bar{F}\cdot\bar{\nabla}_k f = -\frac{f - f_0}{\cancel{2}\tau_k}}$$

Example

electrical conductivity

$$\bar{F} = -e\bar{E}$$ (homogeneous DC field)

look for homogeneous (current is same everywhere). steady state solution of BTE:

$$\frac{\bar{F}}{\hbar}\cdot\frac{\partial f}{\partial \bar{k}} = -\frac{f-f^0}{\tau_k} \Rightarrow f = f^0 - \frac{\tau_k \vec{F}}{\hbar}\frac{\partial f}{\partial k}.$$

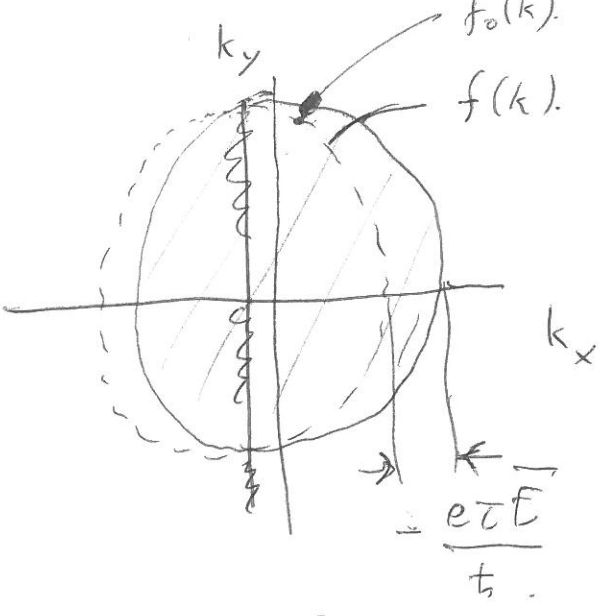
If not far from equil. (i.e. $f^0 \approx f$.). then.

$$f = f(k)^0 - \frac{\tau_k \vec{F}}{\hbar}\frac{\partial f^0(k)}{\partial k} = f^0(k) + \frac{e\tau_k \bar{E}}{\hbar}\frac{\partial f^0(k)}{\partial k}$$

$$\simeq f^0\left(\bar{k} + \frac{e\tau_k \bar{E}}{\hbar}\right).$$

prove yourself

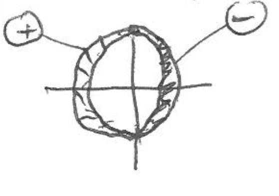
distribution is "shifted" by $\frac{e\tau_k \bar{E}}{\hbar}$



Field $\vec{E} = E_x \vec{e}_x$

shift of fermi surface.

for transport only consider changed parts.



homogeneous -

=0 steady state.

· now current:

$$\vec{j} = \frac{1}{(2\pi)^3}\int d^3k \cdot (-e\vec{v}) \cdot \left(f(k,\cancel{r},\cancel{t}) - f(k)\right)$$

$$= \frac{1}{(2\pi)^3}\int d^3\vec{k}\,(-e\vec{v})\,\frac{e\tau_k\vec{E}}{\hbar}\,\frac{\partial f^0}{\partial k}.$$

Tensor!

$$\vec{j} = \bar{\sigma}\vec{E} \Rightarrow \bar{\sigma} = -\frac{1}{(2\pi)^3}\frac{e^2}{\hbar}\int d^3\vec{k}\;\tau_k\,\vec{v}\,\frac{\partial f^0}{\partial k}.$$

when $\tau_k=\tau$ and spherical fermi surface then.

$$\sigma = \frac{ne^2\tau}{m}\,\mathbb{1} \qquad \text{(show yourself).}$$

$\vec{j}$ is like drude result

but physical assumptions are different!!

more general BTE:

$$\frac{\partial f}{\partial t} + \vec{v}\cdot\vec{\nabla}_r f + \frac{1}{\hbar}\vec{F}\cdot\vec{\nabla}_k f = G(\vec{r},\vec{k},t) - R(\vec{r},\vec{k},t)$$

e.g. absorption
~~at t=0~~ ~~$k_1 \to k_2$~~.
$\delta(t)\cdot\delta(r)\cdot\delta(k)$.
abs. at t=0
at r=0.
into state k=0.

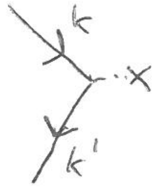
e.g.
relaxation
time
approx.

- in relaxation time approximation
- T-dep. is essentially $\tau(T)$.

collision term.

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = -\frac{f-f^0}{\tau_k(T)}.$$

~~[illegible]~~ impurity scattering as example.



transition rate for scattering $k \to k'$:

Fermi golden rule.

elastic scattering

$$W_{k\to k'} = \frac{2\pi}{\hbar}\left|\langle k'|V_I|k\rangle\right|^2 \cdot \delta(E(k')-E(k))$$

~~total rate for k to some k'~~

~~$\frac{1}{\tau_k^I} = \frac{1}{(2\pi)^3}\int d^3k'\, W_{k\to k'}$~~

scattering rate into and out of state k is then.

$$-\left.\frac{\partial f}{\partial t}\right|_{coll} = \frac{1}{(2\pi)^3}\int d^3k'\, -\underset{\nearrow \text{out}}{W_{k\to k'}}\cdot\left[f(k)\cdot(1-f(k'))\right] + \underset{\nearrow \text{in}}{W_{k'\to k}}\left[f(k')(1-f(k))\right]$$

if impurity pot. is ~~central~~ ~~isotropic (central force)~~ ~~not~~ t-reversal symmetric.

$$W_{k\to k'} = W_{k'\to k}.$$

then
$$\left.\frac{\partial f}{\partial t}\right|_{coll} = \frac{1}{(2\pi)^3}\int d_3\vec{k}' \cdot W_{k\to k'}\cdot\left(f(k)-f(k')\right).$$

now BTE,

$$\cancel{\frac{\partial f}{\partial t}}^{①} + \cancel{\bar{v}\cdot\nabla_r f}^{②} + \frac{1}{\hbar}\overline{F}^{③}\,\nabla_k f = -\frac{\partial f}{\partial t}\Big|_{coll.}$$

$\varepsilon = \frac{\hbar^2 k^2}{2m}$

$\frac{\partial \varepsilon}{\partial k} = \frac{\hbar^2 k}{m} = \hbar\frac{p}{m} = \hbar v$

① steady state, no explicit t-dep of f.

② homogeneous.

$$\left.\begin{aligned}&\nabla_k f = \frac{\partial f}{\partial k} = \frac{\partial \varepsilon}{\partial k}\frac{\partial f}{\partial \varepsilon} = \hbar v(k)\cdot\frac{\partial f_0}{\partial \varepsilon}\\ &F = -eE\end{aligned}\right\}\ ③ = -e\bar{E}\cdot\bar{v}(k)\,\frac{\partial f^0}{\partial \varepsilon}$$

collission term. (fill in $W_{k\to k'}$).

$= \langle k'|V_{imp}|k\rangle|^2$

$$⑤\quad -\frac{\partial f}{\partial t}\Big|_{coll} = n_{imp}\cdot\frac{2\pi}{\hbar}\cdot\int\frac{d^3\bar{k'}}{(2\pi)^3}\cdot|\hat{u}(k-k')|^2\cdot\delta\left(\frac{\hbar^2k^2}{2m}-\frac{\hbar^2k'^2}{2m}\right)\cdot(\delta f_{k'}-\delta f_k).$$

$\leftrightarrow f_{\cancel{k}} = f^0 + \delta f$.

Ansatz:

$$④\quad \frac{\delta f_k}{\tau_k} \sim \frac{1}{\hbar}\bar{F}\cdot\nabla_k f\Big|_{|k|} \Rightarrow \delta f_k = \tau(\varepsilon(k))\cdot e\bar{E}\cdot\bar{v}(k)\cdot\frac{\partial f^0}{\partial \varepsilon}\Big|_{\varepsilon(k)}$$

only energy dep.

then from ③ and ④⑤

$$-e\bar{E}\cdot\bar{v}(k)\frac{\partial f^0}{\partial \varepsilon} = \frac{2\pi}{\hbar}n_{imp}\,e\bar{E}\cdot\int\frac{d^3\bar{k}}{(2\pi)^3}\cdot|\hat{u}(k-k')|^2\cdot\delta\left(\frac{\hbar^2k^2}{2m}-\frac{\hbar^2k'^2}{2m}\right)\cdot$$

$$\times\left(\tau(\varepsilon(k'))\,\bar{v}(k')\cdot\frac{\partial f^0}{\partial \varepsilon}\Big|_{\varepsilon(k')} - \tau(\varepsilon(k))\,\bar{v}(k)\cdot\frac{\partial f^0}{\partial \varepsilon}\Big|_{\varepsilon(k)}\right).$$

$v \to \frac{\hbar k}{m}$, divide by $\bar{E}\cdot\bar{v}(k)$, divide by $\frac{\partial f^0}{\partial \varepsilon}$ bring τ to left.

after some manipulation:

$\bar{k}\cdot\bar{k}'^2/k^2$

$$\tau = \tau(\varepsilon(k)).\qquad \frac{1}{\tau} = \frac{2\pi}{\hbar}n_{imp}\cdot\int\frac{d^3k}{(2\pi)^3}|u(\bar{k}-\bar{k}')|^2\cdot(1-\cos(\angle k,k'))$$

this means that forward scattering ($k \cdot k' = 0$, $\theta = 0$.)
does not contribute to τ.

makes sense $\Rightarrow$ transport does not change.

τ = transport lifetime
which is different from "lifetime".
↳ obtained by putting $\frac{k \cdot k'}{k^2} = \cos\theta$ to zero).

This gives scattering → finite conductivity
but not T-dep.

T-dep comes from ① e-e scattering ($\sim T^2$. only measurable in very pure samples)

② e-p scattering: $T > T_D \sim T$
$T < T_D \sim T^5$

all contribute to τ.
$\Rightarrow$ matthiesen's rule $\frac{1}{\tau} = \sum_i \frac{1}{\tau_i}$

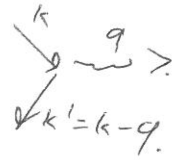
e-e scattering

- Coulomb interaction strong → strong scattering???
  no → pauli!
- Energy conservation + momentum conservation + pauli $\Rightarrow$ phase space restrictions
- relatively weak $\Rightarrow$ only seen at low T in very pure samples.
  (i.e. no impurity
  no phonon scattering)).

e-p scattering.

$T \gg T_D$.

- inelastic process (e loses p & E to phonon)
- 

or


- matrix element. phonon emission

$$W_{k \to k-q} \approx |M_q|^2 \, |\langle \bar{k}-\bar{q}, n_q+1 | a_q^+ | k, n_q \rangle|^2$$

$$\sim |\langle n_q+1 | \overbrace{a_q^+ | k, n_q \rangle}^{= \sqrt{n_q+1} \cdot |k-q \; n_q+1\rangle} |^2$$

$$\sim \langle n_q \rangle \sim k_b T$$

$$\frac{1}{\tau} \sim W_{k \to k-q} \sim k_b T$$

$T \ll T_D$.

- approximately elastic since only acoustic long wavelengt phonons involved (i.e. $q \approx 0$ $E \approx 0$).
- calculation of $\frac{1}{\tau}$ yields $\sim T^5$. (Bloch grüneisen law)

Experimentally → studies of metals in past century.
see - kittel
- Ibach - Luth
- Ashcroft mermin.