Chapter 8: Some elements of transport theory

So far:
- Bloch electrons → solutions to a static Hamiltonian H_e
- Phonons → also solutions to an exact (harmonic) Hamiltonian

→ describes thermodynamic equilibrium
- stability through E_{gs}
- heat capacities
- ...

→ but not anything that needs interaction between particles:

- electrical current
- heat transport
- photons in wave guide
- ...

But eigenstates of an exact Hamiltonian do not interact
→ how to transport anything at all?

Recall: Simple picture of

transport in metals (Drude model)

$n = \frac{N}{V}$ electrons in box with ions to scatter at

Current: $j = -n e \cdot \underline{v}$ ← average velocity of electrons

if electrons scatter on average after time $\bar{\tau}$:

$$\underline{v} = \underline{v}_0 - \frac{e \underline{E} \bar{\tau}}{m}$$

- $\underline{v}_0$: velocity after last collision (random)
- $\frac{e \underline{E} \bar{\tau}}{m}$: acceleration in field since last collision

average velocity: $-\frac{e \underline{E} \bar{\tau}}{m}$

$$\underline{j} = \left(\frac{n e^2 \bar{\tau}}{m} \right) \underline{E} = \sigma \underline{E}$$ Ohm's law

Remarkably simple, (from our point of view) but totally incorrect model

Electrons are Bloch electrons —

- they do not scatter with the ion-s lattice

  define H^{el}

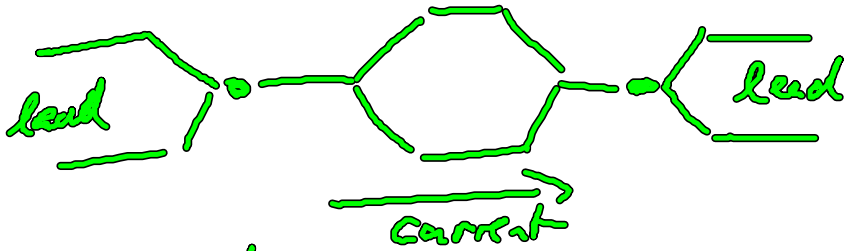
- there are no free electrons (strictly)

How does all this fit together?

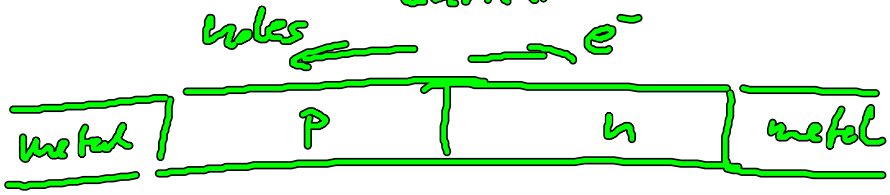
Transport theory – rigorous description

Problem classes:

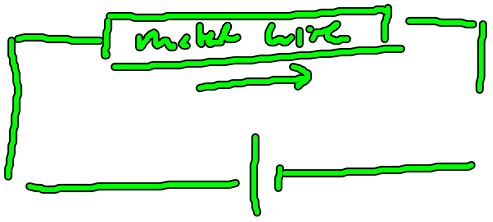
"nano"



"meso"



macroscopic



Approach: quantum statistical mechanics

$$H_{tot} = H^{el} + H^{ph} + H^{int} + \dots$$

Could use : • Green's function based methods

• Master equation formalism (Density matrix)

idea : unperturbed states (H_0 i-teraction) $|m\rangle$ with probability $P_m(t)$ at t.

Require: Time development of $P_m(t)$

e.g. $|m\rangle \to |l\rangle$: probability $P_m(t) \cdot dt \cdot a^*_{lm}$

$|l\rangle \to |m\rangle$: $P_l(t) \cdot dt \cdot a^*_{ml}$

$$\frac{dP_l}{dt} = \sum_m \left(a^*_{lm} P_m(t) - a^*_{ml} P_l(t) \right)$$

Master Equation

→ need to know a^*_{lm} !

given by interaction H^{int} between states

more practically:

Can rewrite using density matrix :

$$\Sigma = \sum_{n,m} f_{nm} |n\rangle\langle m|$$

e.g. $$\Sigma = \sum_{\ell} P_\ell |\ell\rangle\langle\ell|$$

Expectation values of observables A

$$\langle A \rangle = \mathrm{Tr}(\Sigma A)$$

$$= \sum_n \langle n | \Sigma A | n \rangle$$

$$= \sum_n \sum_\ell P_\ell \langle n|\ell\rangle\langle\ell|A|n\rangle$$

$$= \sum_\ell P_\ell \langle \ell | A | \ell \rangle$$

$\{|n\rangle\}$ is any complete orthonormal basis

Textbook: Can write down time evolution of Σ:

$$\frac{\partial}{\partial t}\Sigma = -\frac{i}{\hbar}[H_{tot}, \Sigma]$$

Recipe:
- Define appropriate H_{tot} & $\hat{V}$ (incl: interactions, thermodyn. bath, ...)
- obtain e^-, ph stationary states from QM
- calculate currents etc $j = Tr(\Sigma \cdot \hat{j})$

Summary:
- QSM exists and is an active research area for the nanoscale.
- Serious open questions still to be resolved. (e.g.: which electronic eigenenergies $\epsilon_n(k)$ should we use?)

"Mesoscale": full quantum description is overkill!

A step back:

Boltzmann Equation and Quasiparticles

Classical gas: Boltzmann Equation

Equilibrium defined by distribution function f_0

Particles are distributed according to

$$f_0(k) = \frac{1}{1 + e^{\frac{\omega(k) - \mu}{k_B T}}} \qquad \text{Fermions}$$

$$f_0(k) = \frac{1}{e^{\frac{\omega(k) - \mu}{k_B T}} - 1} \qquad \text{Bosons}$$

What about inhomogeneities?

$$f = f(t, \underline{r}, \underline{k}) = f(t + dt, \underline{r} + \underline{v}\,dt, \underline{v} + \frac{\underline{F}}{m} dt)$$

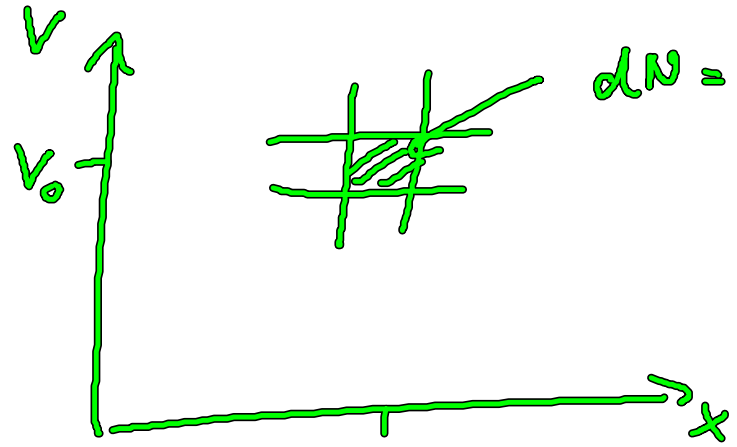
stationary state
no collisions

By simple Taylor expansion:

$$\frac{d}{dt} f(t, \underline{r}, \underline{v}) = \left(\frac{\partial}{\partial t} + \underline{v} \cdot \underline{\nabla}_{\underline{r}} + \frac{\underline{F}}{m} \underline{\nabla}_{\underline{v}} \right) f(t, \underline{r}, \underline{v})$$

$$= 0 \quad \text{in equilibrium.}$$

Microscopic meaning: Phase space



$$dN = f(x, v_x)\, dx\, dv_x$$

x_v

if no force acts: change of dN

$dN(t+dt) - dN(t)$

$= dN_{in} - dN_{out}$

if we follow $dN_{in}, dN_{out} \Rightarrow$

get $\left(\frac{\partial}{\partial t} + \underline{v} \cdot \frac{\partial}{\partial \underline{r}} + \frac{\underline{F}}{m} \frac{\partial}{\partial \underline{v}}\right) f = 0$

as above.

But: dN will change

if there are collisions:

we lose or gain an extra amount

of particles in our phase space element

$$\left(\frac{\partial}{\partial t} + \underline{v} \cdot \underline{\nabla}_r + \frac{\underline{F}}{m} \underline{\nabla}_{\underline{v}}\right) f(\underline{r}, \underline{v}, t)$$

$$=: \left(\frac{\partial f}{\partial t}\right)_{coll}$$

$$= I(f)$$

"collision integral"

Boltzmann's transport equation.

Obviously, we need:

- particles that we can somehow count
- good expression for $\left(\frac{\partial f}{\partial t}\right)_{coll}$

Quasiparticles and Wave Packets

non-interacting electrons, exact eigenstates:

∞ lifetimes, Fermi statistics

"Fermi gas"

Reality: $H_{tot} = H^{el} + H^{e-e} + H^{e-ph} + H^{e-impurity} + \dots$

H^{el}: leading term

$+ \dots$: relatively weak perturbations

$\rightarrow$ real interacting electrons: "Fermi liquid"

Landau hypothesis:

energy spectrum in such a liquid is very similar to electron gas, but electrons behave as "quasiparticles":

QP energy: $\varepsilon_p(k) = \frac{\hbar^2 k^2}{2m^*} - \frac{\hbar^2 k_0^2}{2m^*}$

where m^* is some effective mass and ϵ_0 a reference energy

and $|\psi_p\rangle \sim e^{-i\frac{\xi_p(k)t}{\hbar}} \cdot e^{-\frac{\gamma(k)t}{\hbar}}$

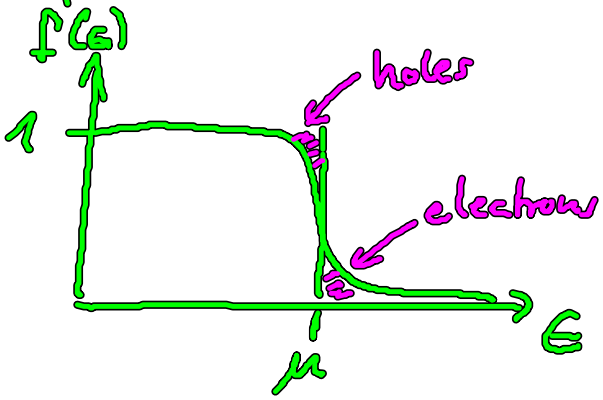
$e^{-i\frac{\xi_p(k)t}{\hbar}}$: non-interacting wave

$e^{-\frac{\gamma(k)t}{\hbar}}$: over time, exact qp solution decays

to be meaningful:

$\gamma \ll |\xi_p|$ QP wave fn should exist reasonably long.

In metals:



Landau: $\boxed{\xi = \epsilon_n(k) - \mu}$ for electrons and holes

If only e-e scattering at finite T:

Can show that $\gamma = \alpha \cdot \frac{\xi^2}{\mu}$

i.e. $\gamma \ll |\xi|$

Full justification for Fermi liquid theory:
Perturbation / Green's fn based.

Not every system is a Fermi liquid,
but metals usually are.

Wave packets

Individual Bloch states extend over
the full crystal, cannot transport anything!

Solution: form localized wave packets:

$$\sum_{k} a(k)\, e^{ik\cdot r} \cdot u_k(r)$$

such that $|\Delta r| \ll l$, average length
travelled by a qp
before it scatters
elastically

$$|\Delta k| \ll |k|$$

elastic mean free path $l \ll$ decay length given by γ (inelastic)

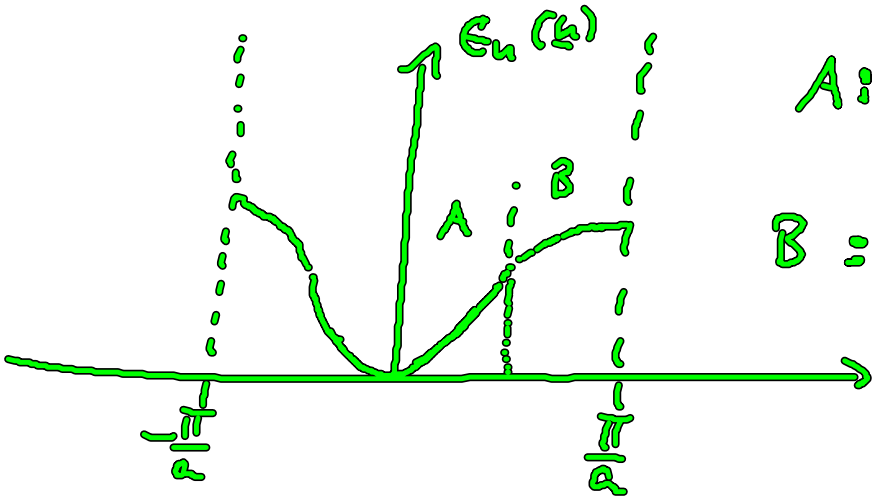
$$l \gg \lambda_{\text{de Broglie}} = \frac{1}{k} \sim a$$

↑ lattice parameter

and group velocity of wave packet:

$$\underline{v} = \frac{1}{\hbar} \frac{\partial \epsilon_n(\underline{k})}{\partial \underline{k}}$$

metal:



A: $\underline{v}$ increases with $\underline{k}$

B: $\underline{v}$ decreases with $\underline{k}$

Now:

Boltzmann's Equation using quasiparticles

Recall:

$$\left(\frac{\partial}{\partial t} + \underline{v}\,\underline{\nabla}_{\underline{r}} + \frac{\underline{F}}{m}\,\underline{\nabla}_{\underline{v}}\right) f(t, \underline{r}, \underline{v}) = \left(\frac{df}{dt}\right)_{\text{coll}}$$

Can apply this to quasiparticles

If we had f_i could e.g. compute

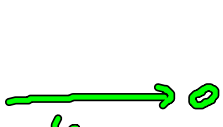
current $\quad j \sim e \int d^3k \; \underline{v} \cdot f(t, \underline{r}, \underline{k})$

Need $\left(\frac{\partial f}{\partial t}\right)_{coll} = I(f)$

e.g. metal with perturbation

$V = \sum_i V_i(\underline{r} - \underline{R}_i)$ at (some) lattice sites i

$$I(f) = \int d^3k' \left(P(\underline{k}', \underline{k}) - P(\underline{k}', \underline{k}) \right) \underbrace{\delta(\epsilon(\underline{k}) - \epsilon(\underline{k}'))}_{\text{elastic scattering}}$$



$P(\underline{k}', \underline{k})$ probability to scatter from $\underline{k}$ to $\underline{k}'$

$$P(\underline{k}', \underline{k}) = |V_{\underline{k}, \underline{k}'}|^2 \cdot f(\underline{k}) \cdot \underbrace{(1 - f(\underline{k}'))}_{\text{Pauli principle (need state at } \underline{k}' \text{ to scatter into!)}}$$

$|V_{\underline{k}, \underline{k}'}|^2$ ↑ matrix element = probability for scattering

$$I(f) = \int d^3k \; |V_{\underline{k}, \underline{k}'}| \, \delta(\epsilon(\underline{k}) - \epsilon(\underline{k}')) \cdot$$
$$\cdot \left[f(\underline{k}') (1 - f(\underline{k})) - f(\underline{k}) (1 - f(\underline{k}')) \right]$$

$$= \int d^3k \; |V_{k,k'}| \, \delta(\epsilon(k) - \epsilon(k')) \; (f(k') - f(k))$$

"Collision integral"

Boltzmann Eq: integro-differential equation for f

→ need to simplify to get (e.g.) Ohm's law.

$$V_{k,k'} = \frac{1}{V} \int d^3r \; e^{-i\underline{k}'\underline{r}} \, u^*_{k'}(r) \cdot \sum_i v_i(\underline{r} - \underline{R}_i) \cdot e^{i\underline{k}\underline{r}} \cdot u_k(r)$$

$$= \langle \psi_{k'} | V | \psi_k \rangle$$

$$= \frac{1}{V} \sum_i e^{i(\underline{k} - \underline{k}')\underline{R}_i} \cdot \int d^3r \; V(r) \cdot e^{-i(\underline{k} - \underline{k}')\underline{r}} \cdot \underbrace{u^*_{k'}(r) \cdot u_k(r)}$$

Scattering of indiv. perturb.

So $|V_{k,k'}|^2 = |v_{k,k'}|^2 \cdot \underbrace{\sum_{i,j} e^{i(\underline{k} - \underline{k}')\cdot(\underline{R}_i - \underline{R}_j)}}_{V_{k,k'}}$

only contributes for

$\underline{R}_i = \underline{R}_j$

$\Rightarrow = N_i$ number of impurities.

$$\Rightarrow \quad \bar{I}(f) = \frac{2\pi}{\hbar} \frac{N_i}{V} \int d^3k \underbrace{|V_{\underline{k},\underline{k}'}|^2}_{\text{local scattering}} \delta(\epsilon(k) - \epsilon(k'))$$

$$\cdot (f(\underline{k}') - f(\underline{k}))$$

We now need:

- some model for scattering process (now local)
- some expression for $f_1 := f - f_0$

  i.e. the deviation from equilibrium.