

Transport theory

Basis for Quantum Stat Mech:

Master Equation

$$\frac{dP_e}{dt} = \sum_m (a_{em} P_m(t) - a_{me} P_e(t))$$

$|e\rangle$ states of some unperturbed Hamiltonian interactions through (c.g.)

$$H_{tot} = H^{el} + H^{e-e} + H^{e-ph} + H^{impurities} + \dots$$

$$\frac{df}{dt} = \left(\frac{\partial}{\partial t} + \underline{v} \cdot \underline{\nabla}_{\underline{r}} + \frac{1}{\hbar m} \underline{F} \cdot \underline{\nabla}_{\underline{k}} \right) f = \left(\frac{\partial f}{\partial t} \right)_{coll.}$$

$$f = f(t, \underline{r}, \underline{k}) \equiv P_e(t)$$

nonequilibrium distribution function

Next: how about transport in a metal with "impurities"

$$\begin{aligned} \left(\frac{\partial f}{\partial t} \right)_{\text{coll}}^{\text{coll}} &= \bar{I}(f) \\ &= \frac{2\pi}{\hbar} \frac{N_i}{V} \int d^3k' |V_{\underline{k}, \underline{k}'}| \cdot \delta(\epsilon(\underline{k}') - \epsilon(\underline{k})) \\ &\quad \cdot (f(\underline{k}') - f(\underline{k})) \quad (*) \end{aligned}$$

but how to get (or not?) Ohm's law from here?

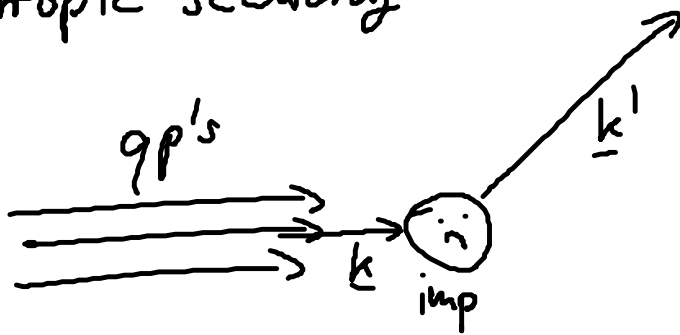
• small electrical fields, small temperature gradients; stationary state

$$f(t, \underline{r}, \underline{k}) = \underbrace{f_0(\epsilon(\underline{k}))}_{\text{equilibrium distribution function}} + f_1(\underline{k})$$

$$|f_1| \ll f_0$$

then: replace $(f(\underline{k}) - f(\underline{k}'))$
by $(f_1(\underline{k}) - f_1(\underline{k}'))$ in *

• isotropic scattering



spherical impurity;

$$V_{\underline{k}, \underline{k}'} = V(\Theta)$$

f_1 is weakly perturbing addition to f_0

- scalar
- should be linear in \underline{E}
- should also retain some dependence on ϵ

$$\rightarrow f_1(\underline{k}) = \eta(\epsilon) \cdot (\underline{k} \cdot \underline{E})$$

$$\Rightarrow I(f) = \frac{2\pi}{\hbar} \int d^3k' |v(\theta)|^2 \cdot \delta(\epsilon(k) - \epsilon(k'))$$

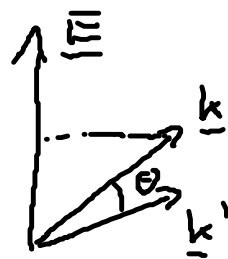
$$\cdot \underline{k} \cdot \underline{E} \cdot \eta(\epsilon) \left(\underbrace{\cos(k', E) - \cos(k, E)}_{\text{from } \underline{k}' \cdot \underline{E} - \underline{k} \cdot \underline{E}} \right)$$

replace: $\int d^3k'$

by $\int_{\text{cons. } \epsilon \text{ surface}} d\epsilon \cdot \underbrace{\int \frac{d\Omega}{4\pi}}_{\text{angle of } k'}$

$$\Rightarrow I(f) = \frac{2\pi}{h} \cdot k \cdot E \cdot \eta(\epsilon) \cdot g(\epsilon) \cdot$$

$$\cdot \int \frac{d\Omega}{4\pi} |v(\theta)|^2 \cdot (\cos(\underline{k}' \cdot \underline{E}) - \cos(\underline{k} \cdot \underline{E}))$$



$$\downarrow$$

$$\cos(\underline{k} \cdot \underline{E})$$

$$\cdot \cos(\underline{k}, \underline{k}')$$

+ terms that depend on $\sin \theta$

\rightarrow

$$I(f) = p \cdot E \cdot \cos(\underline{k}, \underline{E})$$

$$\cdot \eta(\epsilon) \cdot \int \frac{d\Omega}{4\pi} W(\theta) \underline{\underline{(\cos \theta - 1)}}$$

$$= \underbrace{p \cdot E \cdot \eta(\epsilon)}_{f_1} \cdot \int \frac{d\Omega}{4\pi} \dots$$

$$\therefore -\frac{f_1}{\tau} = -\frac{f - f_0}{\tau}$$

τ : "relaxation time"

$$\tau = - \left(\int \frac{d\Omega}{4\pi} W(\theta) \cdot (\cos \theta - 1) \right)^{-1}$$

can we take this to Drude?

$$\frac{\partial f}{\partial t} + \underline{v} \cdot \frac{\partial f}{\partial \underline{r}} + \frac{e \underline{E}}{\hbar} \cdot \frac{\partial f}{\partial \underline{k}} = - \frac{f - f_0}{\tau}$$

Stationary state: $\frac{\partial f}{\partial t} = 0$ $\frac{\partial f}{\partial \underline{r}} = 0$

$$e \cdot \underline{E} \cdot \frac{1}{\hbar} \frac{\partial f}{\partial \underline{k}} = - \frac{f - f_0}{\tau}$$

$$f = f_0 + f_1, \quad |f_1| \ll f_0$$

$$\Rightarrow \frac{\partial f}{\partial \underline{k}} \approx \frac{\partial f_0}{\partial \underline{k}} = \frac{\partial f_0}{\partial E} \underbrace{\frac{\partial E}{\partial \underline{k}}}_{\hbar \underline{v}}$$

and $f_1 = -e \cdot \underline{E} \cdot \underline{v} \cdot \tau \cdot \frac{\partial f_0}{\partial E}$

$$\underline{j} \sim e \int d^3 k \underline{v} \underbrace{f(\underline{k})}_{f(\underline{k}) = f_0 + f_1}$$

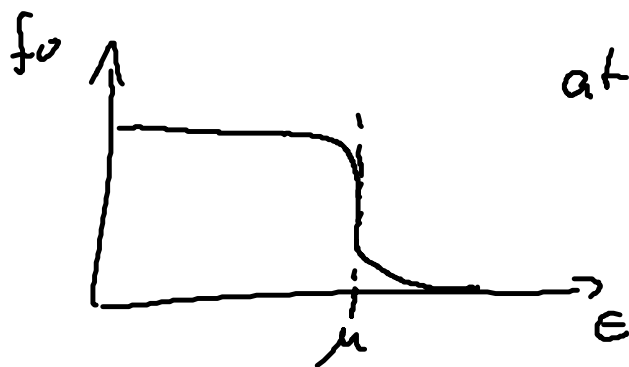
and in equilibrium (f_0):

$$\underline{j} = 0$$

$$= e \cdot \int d^3 k \cdot \underline{v} \cdot f_1$$

but $\int d^3k \rightarrow \int d\epsilon \cdot g(\epsilon) = \int \frac{d\Omega}{4\pi}$
 constant energy surface (at Fermi surface)

and Electron energies:



at reasonable kT :

$$f_0 \sim \Theta(\mu - \epsilon)$$

$$\rightarrow \frac{\partial f_0}{\partial \epsilon} = \delta(\mu - \epsilon)$$

$$\rightarrow j \sim e^2 \cdot \tau(\mu) \cdot g(\mu) \cdot \int \frac{d\Omega}{4\pi} \underline{v} \cdot (\underline{v} \cdot \underline{E})$$

'almost there'?

but: $\int \frac{d\Omega}{4\pi} \underline{v} \cdot (\underline{v} \cdot \underline{E})$

projects out only \underline{v} components along \underline{E}

if $\int \frac{d\Omega}{4\pi} (\dots) \parallel \underline{E}$

(isotropic metal)

$$j \sim e^2 \cdot \underline{E} \cdot [v^2 \cdot \tau \cdot g(\epsilon)]_{\epsilon=\mu}$$

$$= \sigma \cdot \underline{E} \quad \text{Ohm's law.}$$

$$\text{if } \underline{E} \neq \int \frac{d\Omega}{4\pi} \dots$$

$\rightarrow \sigma$ becomes σ_{ij} (tensor)
with $i, j = 1, \dots, 3$
(anisotropic metals)

Assumptions :

- elastic scattering
 - isotropic scattering
 - small fields, small T gradients
 - stationary state.
- } τ approximation

Summary: Transport theory

- qm level: predictive theory for conductivities, ...
active area at nanoscale

- Mesoscopic systems: Boltzmann's Equ + quasiparticles
quantitatively useful when combined with experiments

- Macroscopic conductivities (e.g. Ohm's law) linked to microscopic world

Many other applications (textbooks)

- thermal conductivities

(electrons: carry QP $f = e^{-\mu}$)
can show that $k \propto \sigma \cdot T$
↑
thermal cond.

• ...

Chapter 9: Magnetism

In principle: "everyday phenomenon"

historically: can understand through classical concepts (currents) → Maxwell!

But not clear:

→ how do Ferromagnets (permanent!) fit into this?

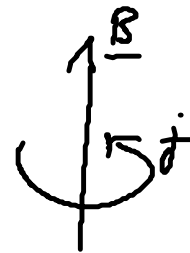
→ how can we understand the different response of different materials to mag. fields?

Illustrates: Significance of cl. correlations:

"magnetic interactions" that lead to e.g. Ferromagnetism are not magnetic in nature!

Prelude: Classical description of B field

Ring currents generate B



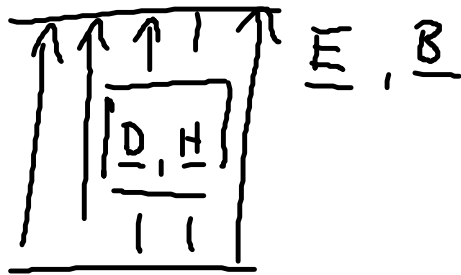
Vacuum: E, B fields

$$\begin{array}{ccc} \downarrow & & \downarrow \\ \frac{V}{m} & & \left(\frac{Vs}{m^2} = T\right) \end{array}$$

E electrical field

B "flux density"

Solids:



$$\underline{D} = \underline{D}(\underline{E}, \underline{B}) \quad \text{"electrical displacement"}$$

$$\underline{H} = \underline{H}(\underline{E}, \underline{B}) \quad \text{"magnetic field"}$$

in general:

$$\underline{E} = \underline{E}(\underline{r}, t) \quad \underline{D}(\underline{r}, t)$$
$$\underline{B} = \underline{B}(\underline{r}, t) \quad \underline{H}(\underline{r}, t)$$

(Maxwell's Eqs)

Here: Homogeneous fields (ω \underline{r}, t dep)

"linear response":

$$\underline{D} = \epsilon_0 \underline{E} + \underline{P} \quad \underline{P}: \text{electrical polarisation}$$

$$\underline{H} = \frac{1}{\mu_0} \underline{B} - \underline{M} \quad \underline{M}: \text{magnetization}$$

with:

$$\underline{P} = \epsilon_0 \underline{\chi}^{el} \underline{E}$$

$$\underline{M} = \underline{\chi}^{mag} \cdot \underline{H}$$

χ^{el} , χ^{mag} "susceptibility tensors"

here (and for most relevant solids):

- scalars χ^{el} , χ^{mag}

- no non-linear terms in H (B)

Thus: $\underline{M} = \chi^{mag} \underline{H}$

$$\underline{P} = \epsilon_0 \chi^{el} \underline{E}$$

or more familiar:

$$\underline{D} = \epsilon_0 \epsilon \underline{E}$$

$$\underline{H} = \frac{1}{\mu_0 \mu} \underline{B}$$

$$\epsilon = 1 + \chi^{el}$$

$$\mu = 1 + \chi^{mag} \quad \text{"permeability"}$$

$$\mu > 1 : \quad |\underline{H}| > \left| \frac{1}{\mu_0} \underline{B} \right| \quad \text{"paramagnetic case"}$$

$$\chi^{\text{mag}} > 0 :$$

$$\mu < 1 : |\underline{H}| < \left| \frac{1}{\mu_0} \underline{B} \right| \quad \text{"diamagnetic case"}$$

$$\chi^{\text{mag}} < 0$$

In practice: Susceptibilities:

$$\text{vacuum} : \chi = 0$$

$$\text{H}_2\text{O} : -8 \cdot 10^{-6} \quad \text{diamagnetic}$$

$$\text{Bi} : -166 \cdot 10^{-6} \quad \text{(strongest case)}$$

$$\text{Cu} : \sim -10^{-5} \quad \text{diamagnetic}$$

$$\text{Al} : 2 \cdot 10^{-5} \quad \text{paramagnetic}$$

$$\text{Steel} : \sim 700$$

Magnetic Energy

$$\text{Can define: } M(H) = -\frac{1}{\mu_0 V} \left. \frac{\partial E(H)}{\partial H} \right|_{S, V}$$

$$\chi^{\text{mag}} = \frac{\partial M(H)}{\partial H} = -\frac{1}{\mu_0 V} \left. \frac{\partial^2 E}{\partial H^2} \right|_{S, V}$$

Plausibility:

Investigate work done to insert a solid into a magnetic field!

Field energy $E^{\text{mag}} = V \cdot \frac{1}{2} B \cdot H$

$$dE^{\text{mag}} = \frac{1}{2} B dH + \frac{1}{2} H dB$$

$$= B dH = \underbrace{(\mu_0 H)}_{\text{vacuum expression}} + \underbrace{\mu_0 M(H)}_{\text{response of the solid}} dH$$

\uparrow
 $H \sim B$

$$\Rightarrow dE^{\text{mag}}_{\text{solid}} = -\mu_0 M(H) V \cdot dH$$

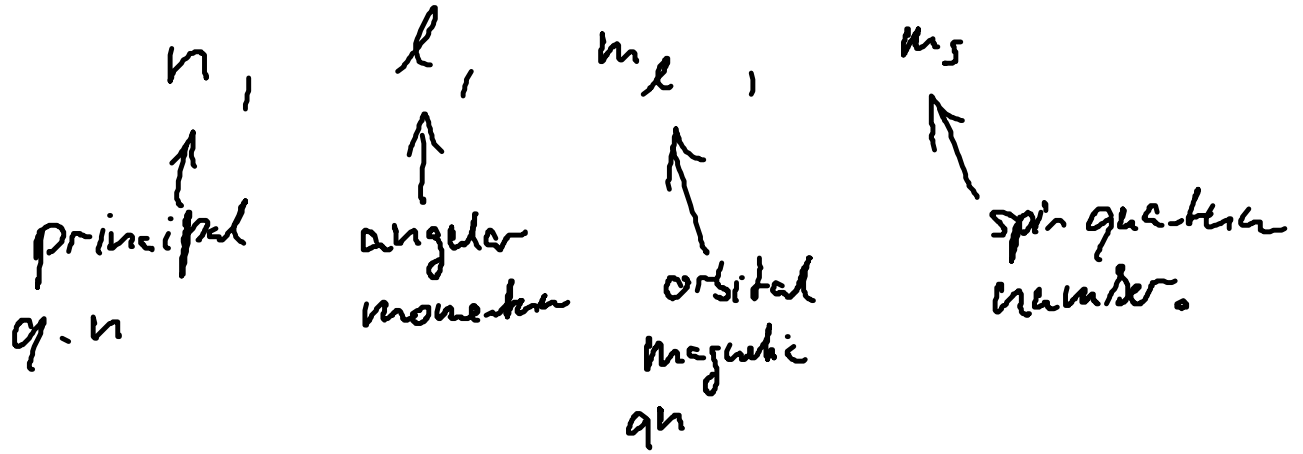
$$\rightarrow \frac{\partial E_{\text{solid}}}{\partial H} = -\mu_0 V M(H) \text{ as above.}$$

This can be used:

- Find ground energy of solid as f of H
- $\rightarrow M, \chi, \dots$

Limiting case: Magnetism of atoms

Individual electrons (orbitals) in atoms can be labelled by quantum numbers:



$$n = 1, 2, 3, \dots$$

$$l = 0, \dots, n-1 \equiv s, p, d, f, \dots$$

$$m_l = -l, \dots, +l$$

$$m_s = \pm \frac{1}{2}$$

Total angular momentum of (many-electron) atom:

$$L = \sum m_l \quad S = \sum m_s$$

and total: $J = L + S$

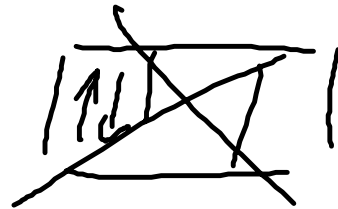
if L-S-coupling is weak: L, S are good quantum numbers

How to fill an atom with electrons?

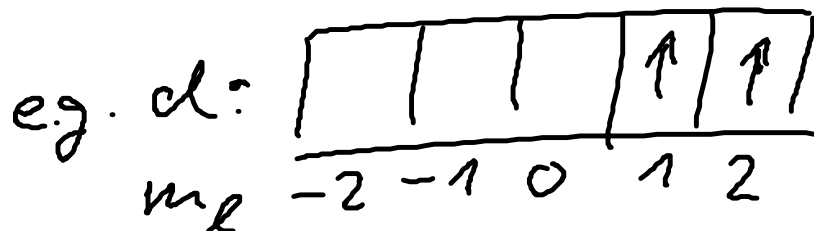
Filled subshells n, l : $L = S = 0$

Hund's rules:

1. Within each subshell, we maximize S



2. If S max., choose l as high as possible:



3. J follows from L and S by shell filling:

- less than half-filled: $J = L - S$
- exactly half-filled: $L = 0, J = S$
- more than half-filled: $J = L + S$

Notation: $(2S+1)L_J$

