Transport theory

Basis for Quantum Stat Mech;

Master Equation

$$\frac{dP_\ell}{dt} = \sum_m \left(a_{\ell m} P_m(t) - a_{m\ell} P_\ell(t) \right)$$

$|\ell\rangle$ states of some unperturbed Hamiltonian

interactions through (e.g.)

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

$$\frac{df}{dt} = \left(\frac{\partial}{\partial t} + \underline{v}\,\underline{\nabla}_{\underline{r}} + \frac{1}{\hbar m}\underline{F}\,\underline{\nabla}_{\underline{k}} \right) f = \text{``}\left(\frac{\partial f}{\partial t}\right)_{coll.}\text{''}$$

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

nonequilibrium distribution function

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

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

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

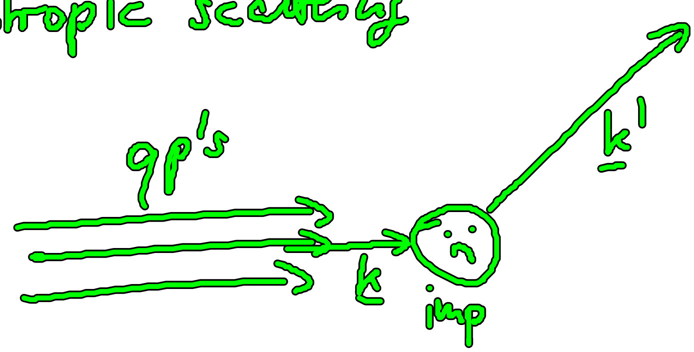
- small electrical fields, small temperature gradients; stationary state

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

$$|f_1| \ll f_0$$

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

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

$$\Rightarrow I(f) = \frac{2\pi}{\hbar} \int d^3k' \, |V(\theta)|^2 \cdot \delta(\epsilon(k) - \epsilon(k')) \cdot k \cdot E \cdot \eta(\epsilon) \underbrace{\left(\cos(k', E) - \cos(k, E)\right)}_{\text{from } \underline{k}' E - \underline{k} \underline{E}}$$

replace: $\int d^3k'$

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

$$\Rightarrow I(f) = \frac{2\pi}{\hbar} \cdot k \cdot E \cdot \eta(\epsilon) \cdot g(\epsilon) \cdot \int \frac{d\Omega}{4\pi} |v(\theta)|^2 \cdot \left(\cos(\underline{k}',\underline{E}) - \cos(\underline{k},\underline{E})\right)$$

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

+ terms that depend on $\sin\theta$

$\rightarrow$

$$I(f) = p \cdot E \cdot \cos(\underline{k},\underline{E}) \cdot \eta(\epsilon) \cdot \int \frac{d\Omega}{4\pi} W(\theta) \underline{\underline{(\cos\theta - 1)}}$$

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

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

τ: "relaxation time"

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

can we link this to Drude?

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

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

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

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

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

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

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

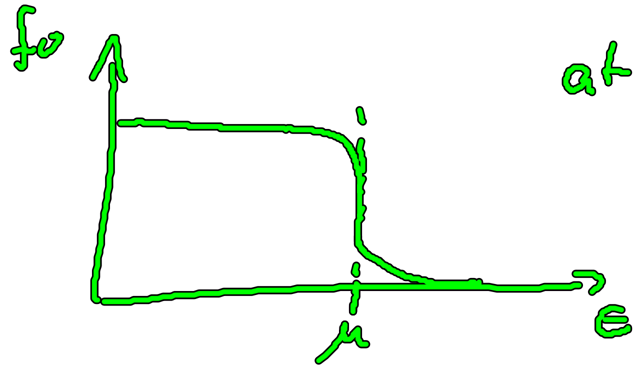
and in equilibrium (f_0):

$$j = 0$$

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

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

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 $\int \frac{d\Omega}{4\pi} (\ldots) \parallel \underline{E}$ (isotropic metal)

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

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

if $\underline{E} \nparallel \int \frac{d\Omega}{4\pi} \ldots$

$\rightarrow \sigma$ becomes σ_{ij} (tensor)

with $i,j = 1, \ldots 3$

(anisotropic metals)

Assumptions:

- elastic scattering
- isotropic scattering

$\Big\}$ τ approximation

- small fields, small T gradients
- stationary state.

Summary: Transport theory

- qm level: predictive theory for conductivities, ...

active area at nanoscale

- Mesoscopic systems: Boltzmann' Eqn
  + 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 $\xi = \epsilon - \mu$)
  can show that $\kappa \sim \sigma \cdot T$
  $\uparrow$ 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?

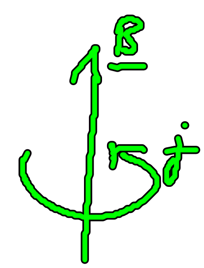
→ how can we understand the different response of different materials to mag. fields?

Illustrates: Significance of el. correlations:

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

Prelude: Classical description of $\underline{B}$ field

Ring currents generate $\underline{B}$



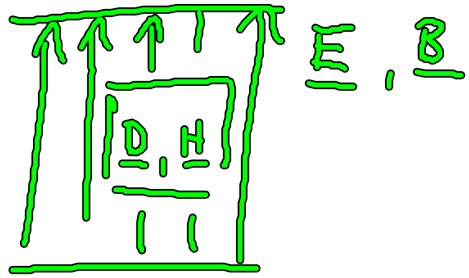
Vacuum: $\underline{E}$, $\underline{B}$ fields

$\frac{V}{m}$ $\left(\frac{Vs}{m^2} = T\right)$

$\underline{E}$ electrical field

$\underline{B}$ "flux density"

Solids:



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

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

in general:

$$\underline{E} = \underline{E}(\underline{r}, t) \qquad D(\underline{r}, t)$$

$$\underline{B} = \underline{B}(\underline{r}, t) \qquad H(\underline{r}, t)$$

(Maxwells Eqns)

Here: Homogeneous fields (no $\underline{r}, t$ dep)

"linear response":

$$\underline{D} = \epsilon_0 \underline{E} + \underline{P}$$

$\underline{P}$: electrical polarisation

$$\underline{H} = \frac{1}{\mu_0} \underline{B} - \underline{M}$$

$\underline{M}$: magnetization

with:

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

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

$\underline{\underline{\chi}}^{el}$, $\underline{\underline{\chi}}^{mag}$ "susceptibility tensors"

here (and for most relevant solids):

- scalars χ^{el}, χ^{mag}
- no non-linear terms in $\underline{H}$ ($\underline{B}$)

Thus:

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

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

or more familiar:

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

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

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

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

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

$\chi^{mag} > 0$:

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

$\chi^{mag} < 0$

In practice: Susceptibilities:

vacuum	:	$\chi = 0$	
H_2O	:	$-8 \cdot 10^{-6}$	diamagnetic
Bi	:	$-166 \cdot 10^{-6}$	(strongest case)
Cu	:	$\sim -10^{-5}$	diamagnetic
Al	:	$2 \cdot 10^{-5}$	paramagnetic
Steel	:	~ 700	

<u>Magnetic Energy</u>

Can define:

$$M(H) = -\frac{1}{\mu_0 V} \frac{\partial E(H)}{\partial H}\bigg|_{S,V}$$

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

Plausibility:

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

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

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

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

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

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

This can be used:

- Find gsm energy of solid as fn of $\underline{H}$
- $\rightarrow M, \chi, \ldots$

Limiting case: <u>Magnetism</u> of <u>atoms</u>

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

n, l, m_l, m_s

principal q.n — n

angular momentum — l

orbital magnetic qn — m_l

spin quantum number. — m_s

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

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

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

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

Total angular momentum of (many-electron) atom:

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

and total: $J = L + S$

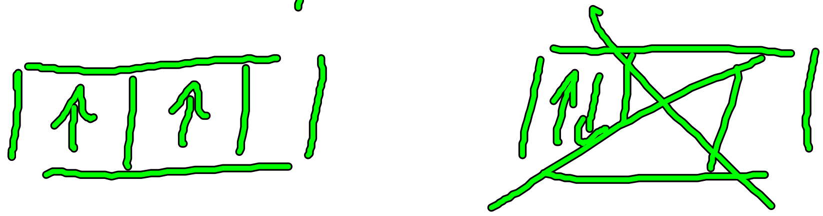
if L-S-coupling is weak: L, S are good quantum numbers

How to fill an atom with electrons?

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

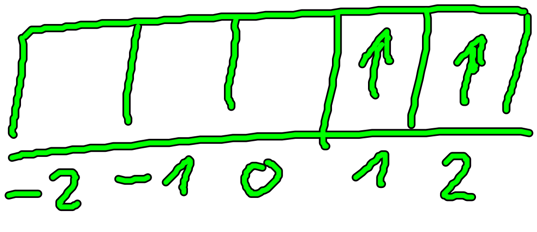
Hund's rules:

1. Within each subshell, we maximize S



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

e.g. d:



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

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

Notation: $^{(2S+1)}L_J$

e.g. Ti $4s^2 3d^2$ $\quad {}^3F_2$