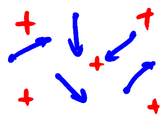
Models for solids

Drude —better→ **Sommerfeld** —best→ **Band structure**

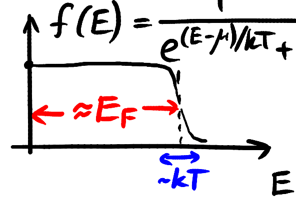
Drude



free electron gas
(MB statistics)
collide with ions
don't feel each other

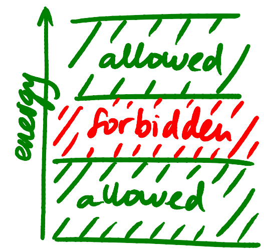
Sommerfeld

$$f(E) = \frac{1}{e^{(E-\mu)/kT}+1}$$



degenerate Fermi gas of free electrons

Band structure



electrons in a solid not "free"

	σ ($\times 10^7 \frac{1}{\Omega\cdot m}$)	$\varkappa$ ($\frac{W}{m\cdot K}$)	C (kJ/kg·K) ← specific heat
Ag	6.2	410	0.23
Cu	5.9	390	0.39
Au	4.6	310	0.13
Al	3.7	210	0.91
Fe	1.0	80	0.45
Pb	0.48	35	0.13
Hg	0.10	8	0.14
glass	$10^{-22}-10^{-18}$	0.0025	0.20

① Electrical conductivity

* classical picture (= Drude model)

e^-'s bounce around, mean free time τ, mean free path ℓ } $\ell = v_{rms}\tau$
↑ thermal (?)

After collision : $\vec{v}$ is random

In $\mathcal{E}$-field : $\frac{d}{dt}m\vec{v} = e\vec{\mathcal{E}}$, =>

drift velocity $\vec{v}_d \sim \frac{e\vec{\mathcal{E}}\tau}{m}$ $\quad v_d \ll v_{rms}$ (small but not random)

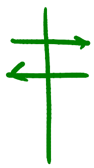
$\vec{j} = ne\vec{v}_d$, $\vec{j} \equiv \sigma\vec{\mathcal{E}}$ – Ohm's law

$$\Rightarrow \boxed{\sigma = \frac{ne^2\tau}{m}} \quad \text{or} \quad \sigma = \frac{ne^2\ell}{m v_{rms}} \quad \underbrace{\left(v_{rms} = \sqrt{3k_BT/m}\right)}_{\text{thermal ??}}$$

② Thermal conductivity

similar to Ohm's law : $\frac{1}{A}\frac{dQ}{dt} \equiv j_Q = -\varkappa \frac{dT}{dx}$

equal net part. fluxes



$T_2 > T_1$

but particles transfer heat (KE) : $\frac{3}{2}k_B(T_2 - T_1) = \frac{3}{2}k_B \frac{dT}{dx}\ell$

$\Rightarrow j_Q = \frac{3}{2} n v_{rms} k_B \frac{dT}{dx}\ell$, $\varkappa = \frac{3}{2} n v_{rms} k_B \ell$ or

$\varkappa = \frac{3}{2} n v_{rms}^2 k_B \tau \quad (\ell = v_{rms}\tau)$

$v_{rms}^2 = \frac{3k_BT}{m}$

Wiedemann-Franz :

$$\frac{\varkappa}{\sigma} = \frac{3}{2}\frac{k_B^2}{e^2}T$$

Ratio : $\frac{\varkappa}{\sigma T} \equiv L$ Lorentz number

$$= \frac{3k_B^2}{2e^2} = 1.1 \times 10^{-8} \frac{W\Omega}{K^2}$$

same carriers for heat and charge $\Rightarrow$ transport coefficients must be related

Lorentz number : differs by a factor of 2-3 from measured values for most metals, though $\varkappa/\sigma T$ is indeed a const, indep. of T

③ Problems with the Drude model

Several, but the main one is

too big heat capacity (from free electrons)

* classically : $\frac{3}{2}k_BT$ per e^-

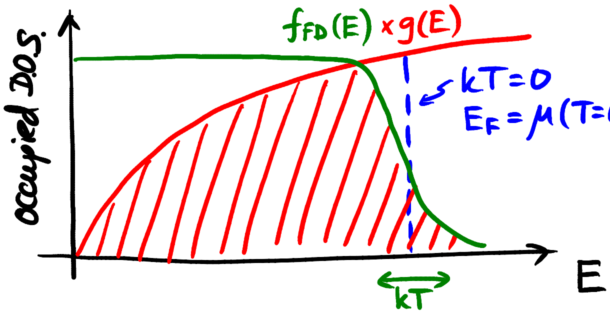
$$\Rightarrow \frac{dU}{dT} = C = \frac{3}{2}k_B N$$

(e.g. we expect good conductors to have larger C than for insulators. But in reality $C_{insulator} \sim C_{conductor}$)

$$g(E) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$$

$$U = \int_0^\infty g(E)\cdot f_{FD}(E)\cdot E\cdot dE$$

total income (U) — # of rooms (g(E)) — visitors' willingness ($f_{FD}(E)$) — $$$ they pay (E)



$$\frac{dU}{dT} = C = \frac{3}{2} k_B N_{eff}$$

N_{eff}: # of electr. participating in energy change

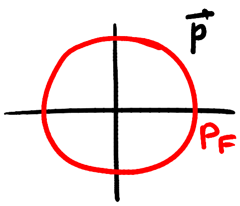
$$N_{eff} = N \cdot \frac{}{} = N \frac{k_B T}{E_F}$$

$$\Rightarrow \quad C = \frac{3}{2} N k_B \frac{T}{T_F}$$

good agreement with exp. observations : electrons don't contribute to heat capacity

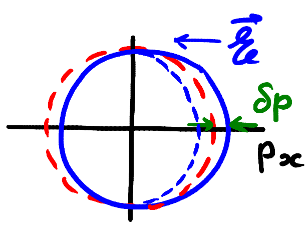
④ Conductivity revisited (Sommerfeld)

metal at $T=0$, $\Rightarrow$ Fermi sphere (in p-space)



electric field $\frac{d}{dt}\vec{p} = e\vec{\mathcal{E}}$

$\Rightarrow$ entire Fermi sphere moves



$\delta\vec{p} = e\vec{\mathcal{E}}\tau$ relaxation sets in after time τ

$\delta p \ll p_F$, displaced electrons have $v \approx v_F$!

Energy span corresponding to displaced electrons :

$$\delta E_{kin} = \frac{1}{2m}\left[(\vec{p}_F + \delta\vec{p})^2 - (\vec{p}_F - \delta\vec{p})^2\right] \simeq \frac{2\,\delta\vec{p}\cdot\vec{p}_F}{m} = 2\underbrace{\frac{p_{F,x}}{m}}_{v_{F,x}} e\mathcal{E}\tau$$

contibution to current density $(\vec{\mathcal{E}} = \mathcal{E}\hat{x})$: $j_x = e n v_x$

(v) $$dj_x = e\, g(E_F)\, \delta E\, v_{F,x} \frac{d\hat{p}}{4\pi}$$

unit vector, to be integrated ...

(V) $j_x = e\, g(E_F) \int_{\text{half space}} \frac{d\varphi}{2\pi}\, e \mathcal{E} \tau\, v_{F,x}^2$ integrated over half space

$$= e^2 v_F^2\, g(E_F)\, \mathcal{E} \tau \underbrace{\int_0^{\pi} \frac{d\varphi}{2\pi}}_{1/2} \underbrace{\int_0^{\pi} d\theta \sin\theta \cos^2\theta}_{2/3}$$

$$j_x = \frac{1}{3} e^2 v_F^2 \frac{g(E_F)}{V} \mathcal{E} \tau = \frac{1}{3} e^2 \underbrace{\frac{2E_F}{m}}_{v_F^2} \frac{g(E_F)}{V} \mathcal{E} \tau$$

$$\int_0^{E_F} g(E)\,dE = N \quad ; \quad g(E) = \text{Const}\, E^{1/2}$$

$$\frac{2}{3} \text{const}\, E^{3/2} \Big|_0^{E_F} = \frac{2}{3} \underbrace{\text{const}\, E_F^{1/2}}_{g(E_F)} E_F = N$$

$$\frac{g(E_F)}{V} = \frac{N/V}{E_F} \frac{3}{2} = \frac{3}{2} \frac{n}{E_F}$$

$$\Rightarrow \boxed{j_x = \frac{n \mathcal{E} \tau e^2}{m}}$$ same as Drude!

* can do the same for thermal conductivity
one finds

$$\boxed{\frac{\kappa}{\sigma T} = \frac{\pi^2 k_B^2}{3 e^2}} = 2.45 \times 10^{-8} \frac{W\Omega}{K^2}$$

good agreement with expt. (ranges b/w 2.3 to $3 \times 10^{-8} \frac{W\Omega}{K^2}$)

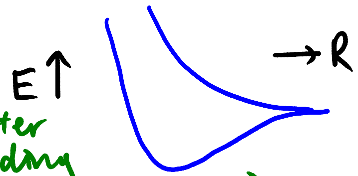
⑤ Problems with Sommerfeld model

good: describes heat capacity
electric conductivity
thermal conductivity
Hall effect
plasma frequency (e.g. shiny metal)
. . . .
metals

bad: cannot explain difference between
metals, semiconductors, and insulators

⑥ Energy band structure of solids

* recall level splitting in HW6, prob 2

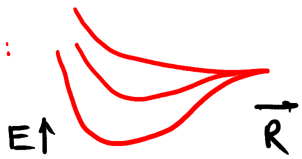


(after adding nuclear repulsion)

level splitting

Q: what if 3 atoms are brought together?

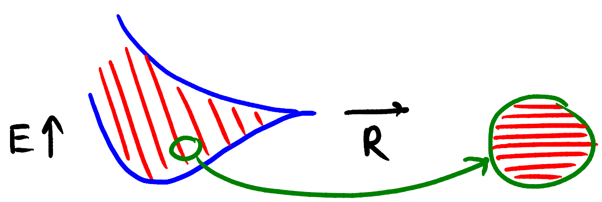
A:



3-splitting of energy levels

Q: N atoms?

A: each atom level is split into N levels

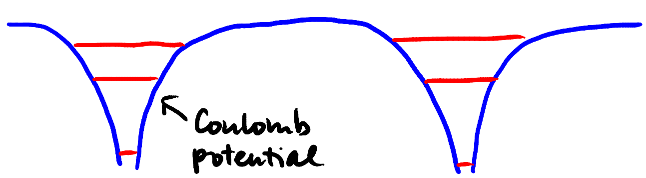


indiv. levels are very close (e.g. 1 mole ~ 6×10^{23}, $\Rightarrow 10^{-23}$ eV spacing)

"energy bands"

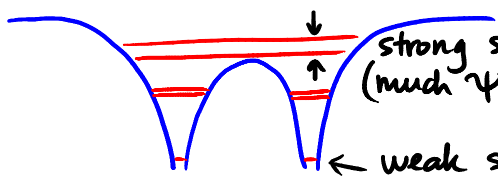
⑦ Splitting of valence vs. inner shells

two atoms far apart



Coulomb potential

two atoms close by



strong splitting (much Ψ overlap)

weak splitting (no Ψ overlap)

inner shells: no appreciable splitting at typical inter-atom sep.
fully occupied

valence shells: continuous energy bands
may be partially filled

Energy band structure and occupancy:
determine whether a metal, a semiconductor, or an insulator