Dynamics of electrons in Solids (= Crystals)

Friday, 28. October 2022 10:08

* Drude model / free electrons
* Add Quantum mechanics (Sommerfeld Model)
* Add Lattice (Bloch)

① Why is the transport / dynamics of electrons interesting.

Electrons are charged so they are put in motion by EM field and/or by thermal gradient.
This results in a "current" of electricity or heat that is related to the applied field but also to the intrinsic properties of materials

$$U = R \cdot I$$

voltage (U) ; "transport coefficient" (R) ; flow of electrons (I)

	B = 0, M = 0	
	$\hat{\boldsymbol{E}} = -\boldsymbol{\nabla}\phi_{el}$	$-\boldsymbol{\nabla}T$
J_q	Electrical Conductivity ($\overleftrightarrow{\sigma}$) or resistivity ($\overleftrightarrow{\rho}$)	Seebeck-Effect (S)
J_H	Peltier-Effect (P)	Heat Conductivity ($\overleftrightarrow{\kappa}$)
	$\mathbf{B} \neq 0$	
	$-\boldsymbol{\nabla}\phi_{el}\times\hat{\mathbf{B}}$	$-\boldsymbol{\nabla}T\times\hat{\mathbf{B}}$
J_q	Magnetoresistance σ_{xx}(B) Hall Effect (R_H)	Nernst Effect (N)
J_H	Ettinghausen-Effect	Thermal Hall Effect

② A brief Recollection on Drude Model 1897

Key Idea: Classical gas of electrons which follow Maxwell-Boltzmann statistics.

Probability of having an electron with a velocity $\vec{v}$ between $\vec{v}$ and $\vec{v}+d\vec{v}$ is given by:

$$f(\vec{v}) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} 4\pi v^2 \exp\left(-\frac{m v^2}{2 k_B T}\right)$$

or equivalently since $E = \frac{1}{2} m v^2$

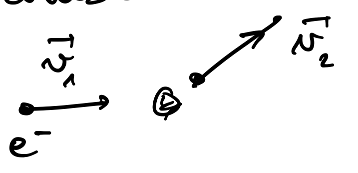
$$f(E) = 2\left(\frac{E}{\pi (k_B T)^3}\right)^{1/2} e^{-E/k_B T}$$

Average electronic energy $\langle E\rangle = \int_0^\infty f(E) \cdot E \cdot dE$

$$= \frac{3}{2} k_B T = U$$

Assumption: thermal equilibrium is achieved through collisions

① No interactions between the collisions
② Instantaneous change of the velocity after the collision



③ Probability of collision is given by τ, $1/\tau$ = scattering rate [given in s^{-1}]
⇒ electronic mean free path = average distance between two collisions
$$\ell = \langle v\rangle \cdot \tau$$

Main Result: estimate of the electrical conductivity

$$\vec{J}_q = \overleftrightarrow{\sigma} \cdot \vec{E}$$

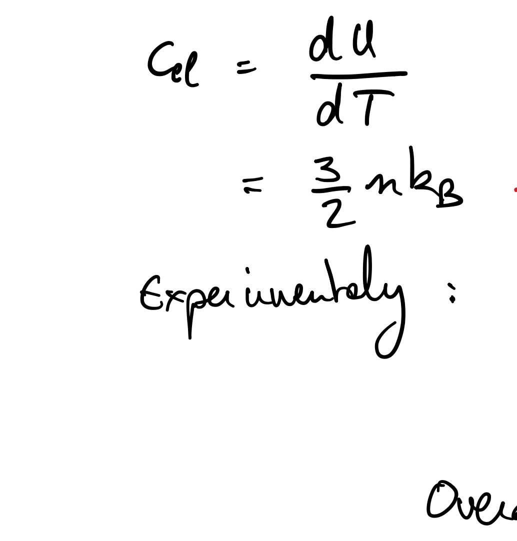
↳ conductivity tensor

. DC - conductivity $\boxed{\sigma_0 = \frac{n e^2 \tau}{m}}$
  . n = charge density
  . m = mass of the charge carriers
  . e = charge.

. AC / optical conductivity = conductivity at finite frequency ω

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau} = \underbrace{\frac{\sigma_0}{1+\omega^2\tau^2}}_{\text{re part}} + i\,\underbrace{\frac{\omega\tau\sigma_0}{1+\omega^2\tau^2}}_{\text{imaginary part}}$$

al



(Source: Wikipedia)

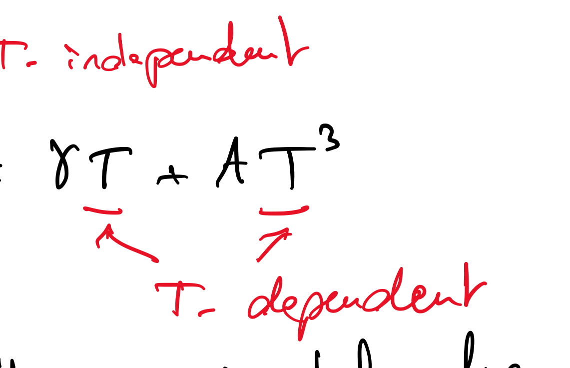


Figure 2 | Conductivity spectrum of UPd_2Al_3 at temperature 2.75 K; both real and imaginary parts (σ_1 and σ_2, respectively) are shown. The fit ($\sigma_1 + i\sigma_2 = \sigma_0(1 - i\omega\tau)^{-1}$, $\sigma_0 = 0.105\,\mu\Omega^{-1}\,cm^{-1}$, $\tau = 4.8\times10^{-11}$ s) documents the excellent agreement of experimental data and the Drude prediction. The characteristic relaxation rate $1/\tau$ is marked by the decrease in σ_1 and the maximum in σ_2 around 3 GHz.

Source: Scheffler et al. Nature 438, 1135 (2005)

Main failures: * electronic heat capacity: energy to provide to the system to increase its temperature by 1K

$$C_{el} = \frac{dU}{dT} \qquad U = \text{internal energy}$$
$$= \frac{3}{2} n k_B \rightarrow T\text{-independent}$$

Experimentally: $C = \gamma T + A T^3$ ← T-dependent

Overall the experimental value is 2 orders of magnitude smaller than $\frac{3}{2} n k_B$

* thermal conductivity κ

$$\vec{J}_H = -\overleftrightarrow{\kappa} \cdot \vec{\nabla} T$$
$$\kappa = \frac{1}{3} v^2 \tau C_{el}$$ = also off by two orders of magnitude

* Wiedemann - Franz law: $\frac{\kappa}{\sigma T} = \mathcal{L}$ = constant
  OK (by chance)

* Hall Effect: $R_H = -\frac{1}{ne}$ = T-independent
  ↳ contradiction with experiment

③ Drude - Sommerfeld Model

Replace Boltzmann distribution with the Fermi Dirac one

$$f_D(E) = \frac{1}{\exp\left(\frac{E-\mu}{k_B T}\right) + 1}$$

$$\mu = \text{chemical potential} = E_F\left(1 - \frac{\pi^2}{12}\left(\frac{T}{T_F}\right)^2\right)$$
$$\approx E_F$$