Improving on Drude's Theory of Metals

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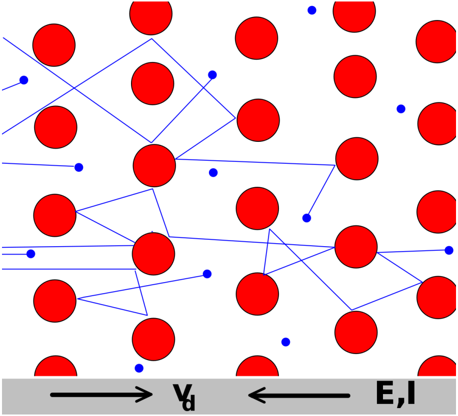
Drude's Model



from hyperphysics.phy-astr.gsu.edu

Electrons are treated independently and classically. In between collisions with ions, they obey the Lorentz force law. Immediately after colliding, they follow some isotropic velocity distribution.

Parameters of Drude's Model

- τ: mean free time between collisions.
- n: number density of conduction electrons.
- Carrier charge $-e$ and mass m.
- Velocity distribution after bouncing off an ion.

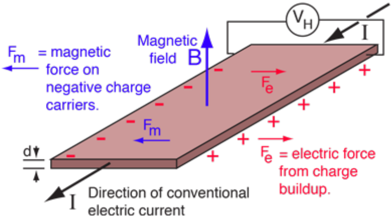
Conduction in Drude's Model

In a uniform electric field $\vec{E}$:

- Drift Velocity: $\vec{v_d} = \frac{e\tau}{m}\vec{E}$.
- Conductivity: $\vec{J} = ne\vec{v_d} = \frac{ne^2\tau}{m}\vec{E} \implies \boxed{\sigma = \frac{ne^2\tau}{m}}$.

With a perpendicular magnetic field B:

- Hall coefficient:
  $evB = eE_y \implies E_y = vB \implies R_H = \frac{E_y}{J_x B} = \frac{1}{ne}$.



Thermal Conduction in Drude's Model

Thermal Conductivity

In the absence of external forces,

$$\kappa = \frac{1}{3} v_{rms}^2 c_V \tau.$$

Wiedemann-Franz law

If we assume a Maxwell-Boltmann distribution...

$$\left.\begin{aligned} v_{rms}^2 &= \frac{3k_B T}{m} \\ c_V &= \frac{3}{2} n k_B \end{aligned}\right\} \implies \boxed{\kappa = \frac{3}{2}\frac{n\tau}{m} k_B^2 T}.$$

$$\frac{\kappa}{\sigma T} = \frac{3}{2}\left(\frac{k_B}{e}\right)^2.$$

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(Drude's fortuitous mistake.)

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$$\left.\begin{aligned} v_{rms}^2 &= \frac{3k_B T}{m} \\ \text{Much too large!} \left\{ c_V \right. &= \tfrac{3}{2} n k_B \end{aligned}\right\} \implies \boxed{\kappa = \frac{3}{2}\frac{n\tau}{m}k_B^2 T}.$$

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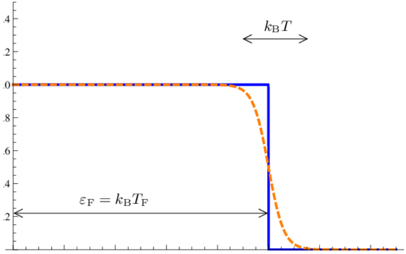
Drude-Sommerfeld Model

Maxwell-Boltzmann $\rightarrow$ Fermi-dirac distribution for free electrons:



Boettcher et al.

Wiedemann-Franz law again...

$$\left.\begin{aligned} v_{rms}^2 &= \frac{3k_B T}{m} \\ c_V &= \frac{3}{2} n k_B \end{aligned}\right\} \implies \kappa = 3\frac{n\tau}{m} k_B^2 T \implies \boxed{\frac{\kappa}{\sigma T} = 3\left(\frac{k_B}{e}\right)^2}.$$

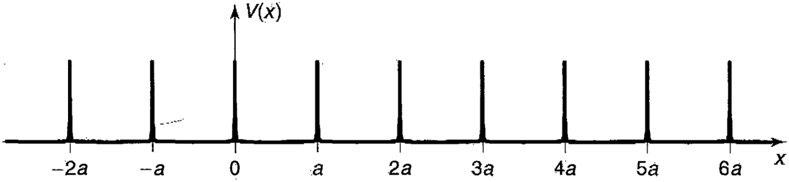
Maxwell-Boltzmann got the product $v_{rms}^2 c_V$ roughly correct.

Fundamental Failures of the Drude Model

- How do we determine n?
  - The sign of the Hall coefficient $\frac{1}{ne}$ can even reverse!
- What determines whether an element is a metal?
- How do we explain semiconductors and insulators?

- Are collisions with ions the true source of scattering? What determines τ?

Periodic Potential

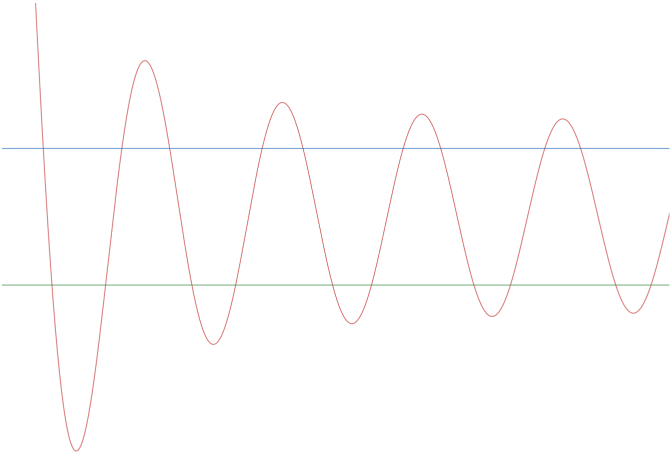


Dirac Comb, from Griffiths

Bloch's theorem: for a periodic potential with period a, solution to Schrodinger's Equation takes the form $\psi(x) = e^{-ika}u(x)$, where $u(x) = u(x + a)$.

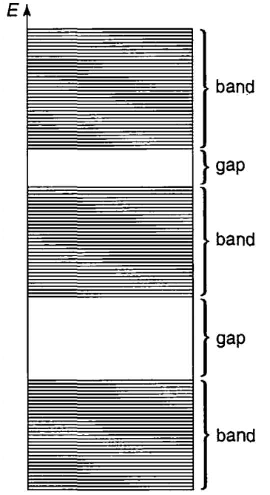
Bands for the Dirac Comb

We can solve the Dirac comb potential by letting $u(x)$ be a wave function with definite momentum over $[0, a)$.



A qualitative plot of $cos(ka)$ against E.

Bands more generally



From Ashcroft and Mermin.

$\psi_n(\boldsymbol{k})$ is the state in band n with *crystal momentum* $\boldsymbol{k}$. By Bloch's theorem, we can write

$$\psi_n(\boldsymbol{k}) = e^{-\boldsymbol{k}\cdot\boldsymbol{r}} u_n(k), \qquad (1)$$

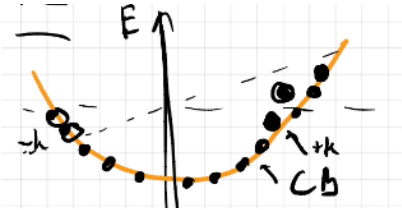
where $u_n(k)$ is periodic over the lattice's cells. Let $\epsilon_n(\boldsymbol{k})$ be the energy of $\psi_n(\boldsymbol{k})$.

Semiclassical Equations of Motion

$$\boldsymbol{v} = \frac{1}{\hbar} \nabla_{\boldsymbol{k}} \epsilon_n(\boldsymbol{k}),$$
$$\hbar \dot{\boldsymbol{k}} = -e(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}).$$

We assume: Electric and magnetic fields are suffiicently weak and slowly varying. Gap in energy between bands is large enough to prevent jumping between bands.

Formation of current



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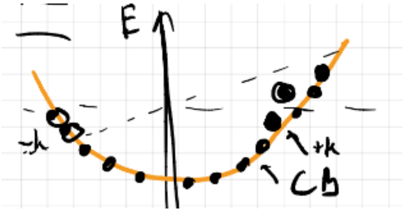

Bloch oscillations?

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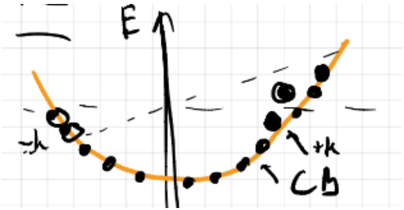

Bloch oscillations? Relaxation time still exists :(

Consequences of the model

Electrons in partially filled bands are Drude's conduction electrons.

- Metal: ϵ_F lies in the middle of a band $\implies$ partially filled.
- Insulator: ϵ_F lies between bands.
- Semiconductor: doping / creation of holes leads to a small number of electrons in partially filled bands.

Band Mass

When the occupied crystal momentums $\boldsymbol{k}$ of a partially filled band are centered around some local extremum, we can approximately write (in one dimension),

$$\epsilon_n(k) = \epsilon_n(k_0) - A(k - k_0)^2, \tag{2}$$

for some A. So,

$$\boldsymbol{v}(\boldsymbol{k}) = \frac{1}{\hbar}\frac{d\epsilon_n(\boldsymbol{k})}{dk} = +\frac{\hbar(k - k_0)}{m_{eff}}, \tag{3}$$

where $m_{eff} = \frac{\hbar^2}{2A}$.

Implications for the Drude Model

Although the new theory is a lot more general, we can see what it implies for the Drude model. When m_{eff} and τ are roughly constant, applying the relaxation time approximation in a uniform electric field gives $\sigma = \frac{n_h e^2 \tau}{m_{eff}}$, where n_h is the density of occupied states in the partially filled band.

Holes

When $m_{eff} < 0$. we can think of the carriers as having positive charge e and positive mass $-m^*$. This explains why the sign of the Hall coefficient can flip.

Sources of Scattering?

- ~~Collisions with ions~~
- Phonons (vibrations of the ions).
- Electron-electron interaction.
- Impurities.