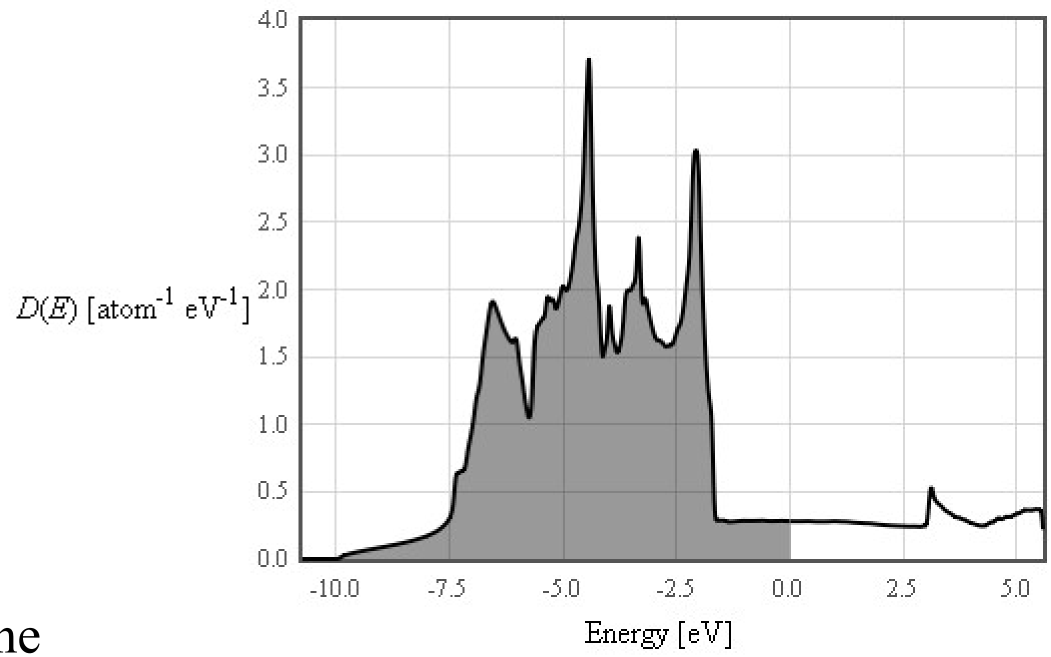
Electrical and thermal transport in metals

Thermodynamic properties of metals

From the band structure measurements, we obtain the electron density of states.

Electron density of states for fcc gold



E [eV]	$D(E)$ [atom^{-1} eV^{-1}]
-10.74913	0
-10.73552	0
-10.72192	0

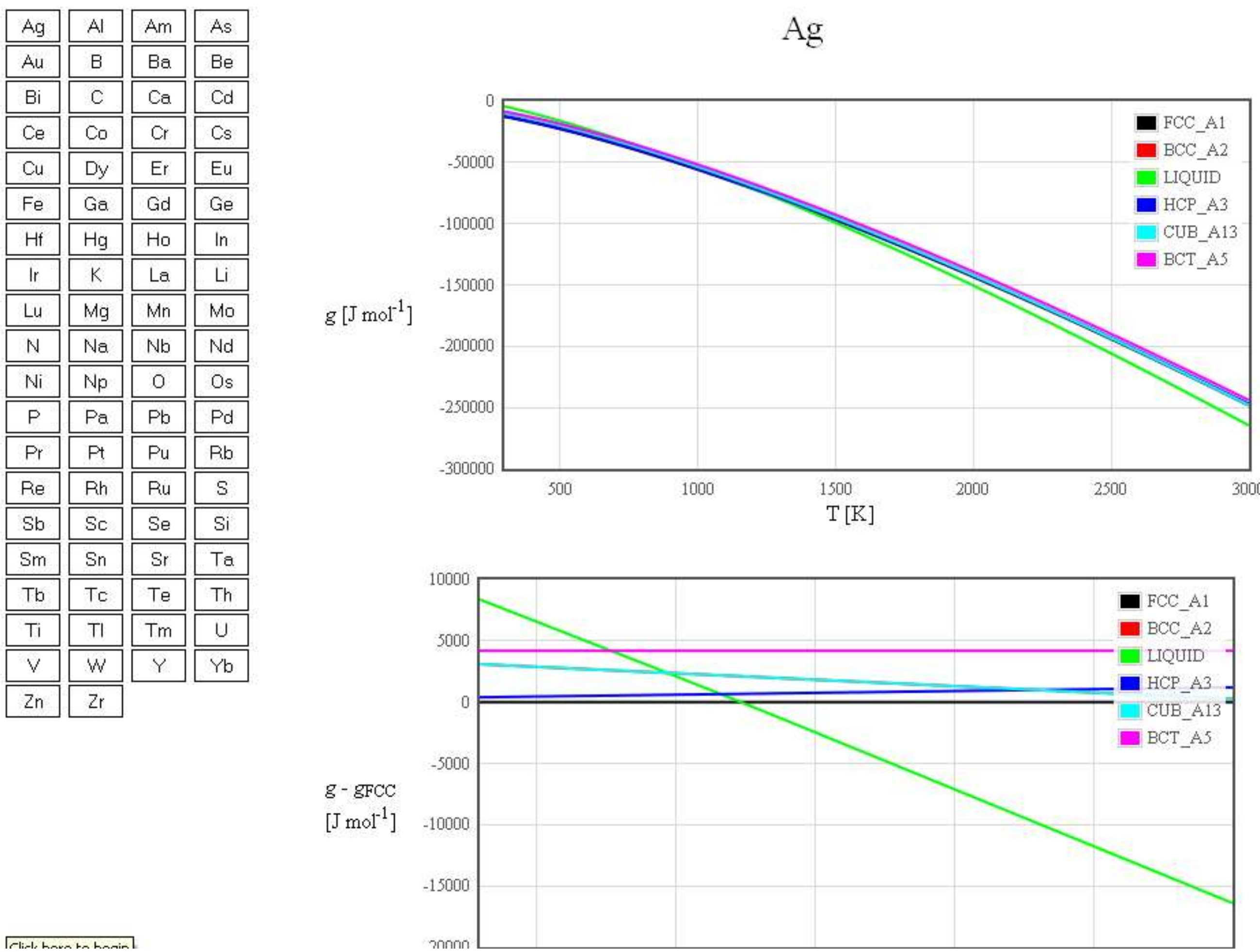
Thermodynamic properties can be calculated from the tabulated data for the density of states

SGTE data for pure elements

SGTE thermodynamic data

The Scientific Group Thermodata Europe SGTE maintains thermodynamic databanks for inorganic and metallurgical systems. Data from their 'pure element database' is plotted below.

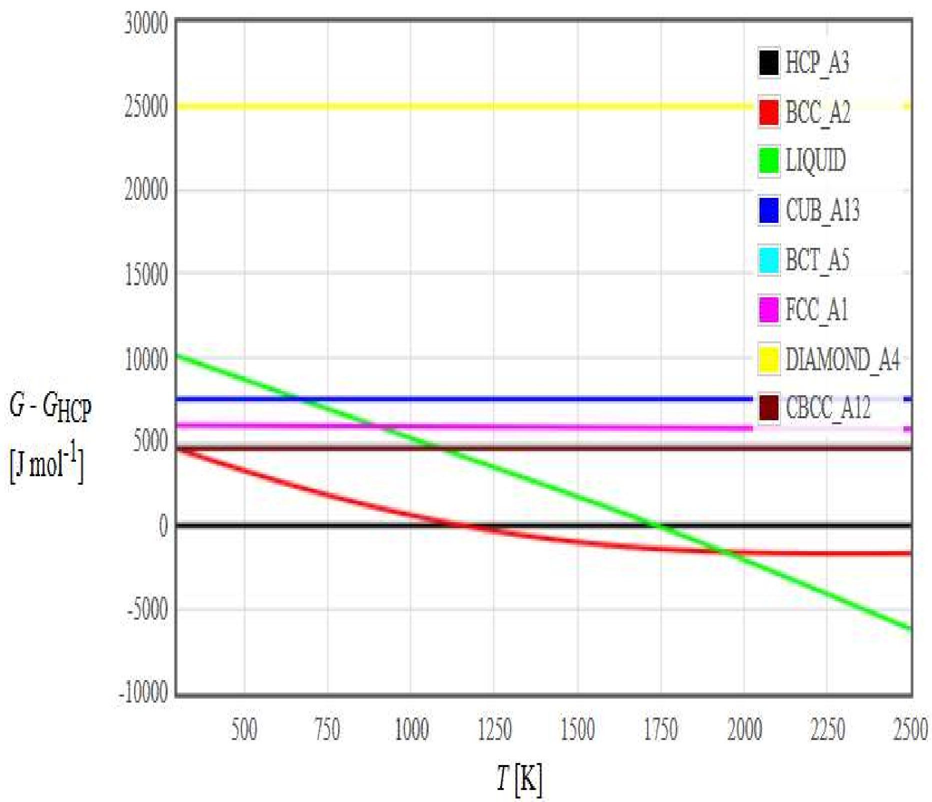
Typically, experiments are performed at constant pressure p, temperature T, and number N. Under these conditions, the system will go to the minimum of the Gibbs energy $G = U + pV - TS$. Here U is the internal energy, V is the volume, and S is the entropy. The top plot is the Gibbs energy per mole $g = u + pv - Ts$, where u is the internal energy per mole, v is the volume per mole, and s is the entropy per mole.



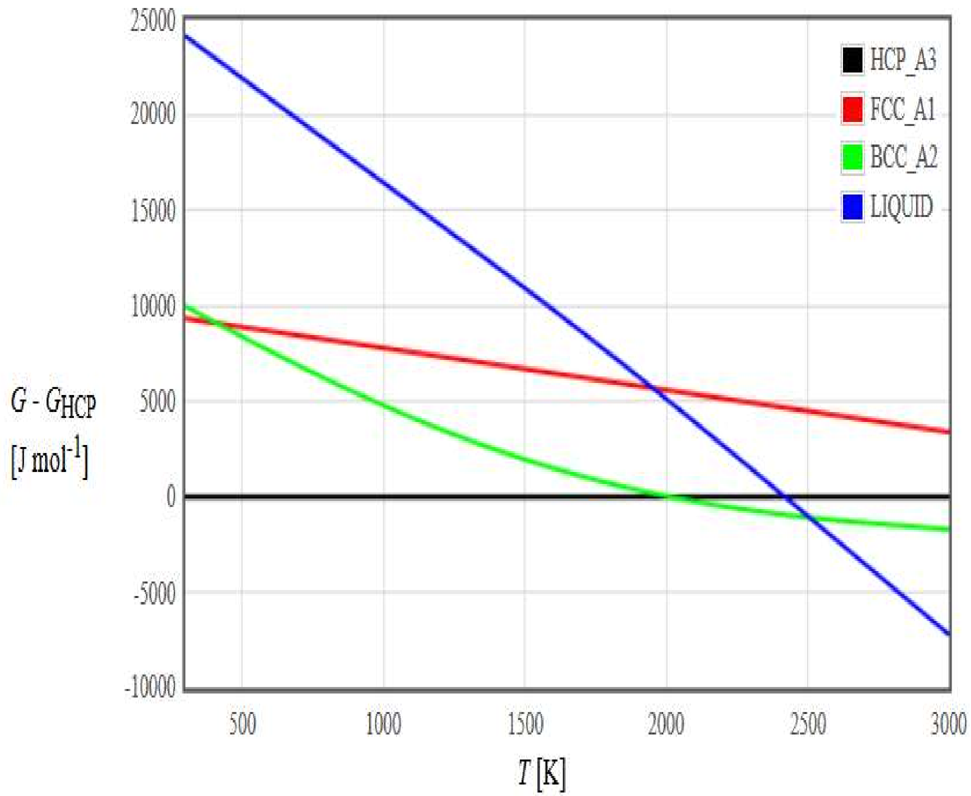
http://www.sciencedirect.com/science/article/pii/036459169190030N

Close packed → bcc

Ti



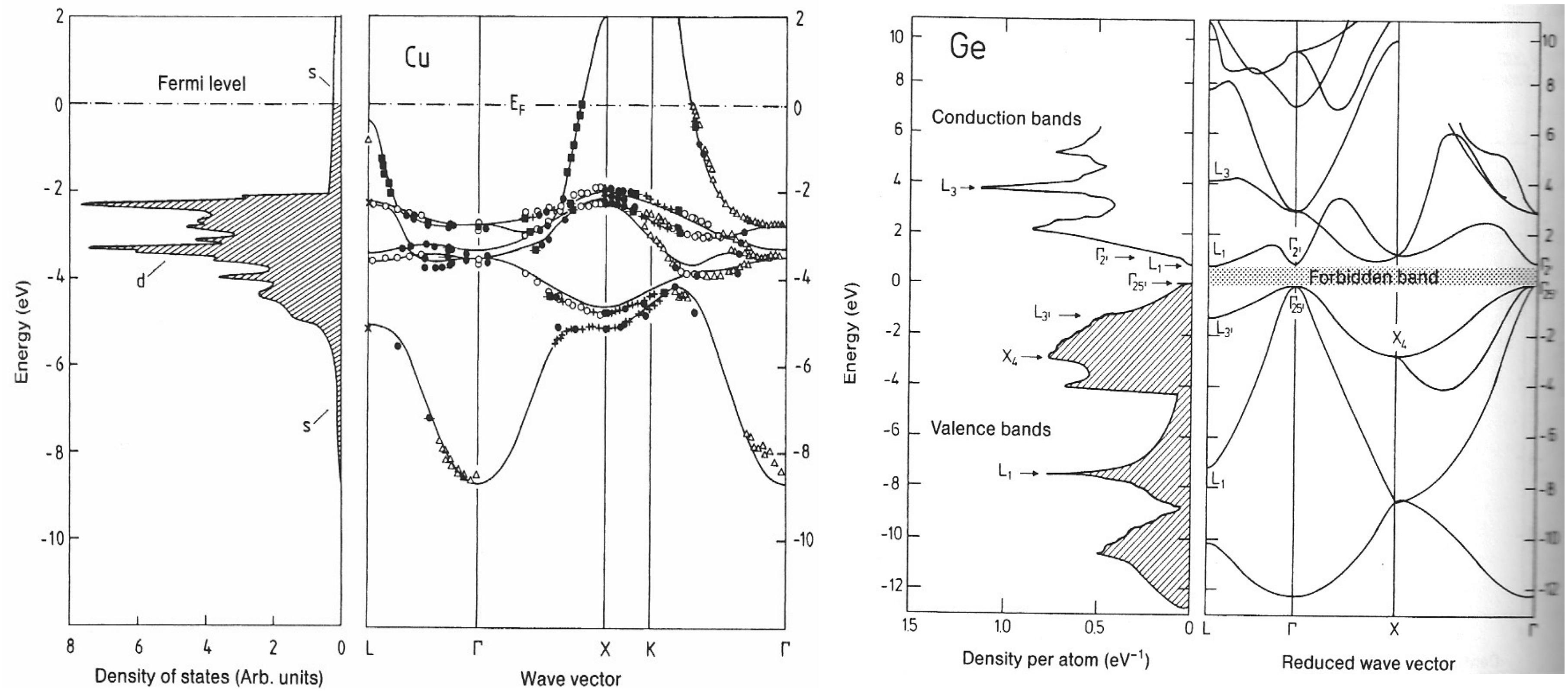
Hf



Close packed → bcc: Am, Be, Ca, Gd, Nd, Pr, Hf, Sc, Sm, Sr, Ti, Tb, Th, Tl, Y, Yb, Zr

http://lampx.tugraz.at/~hadley/ss1/materials/sgte/SGTE.html

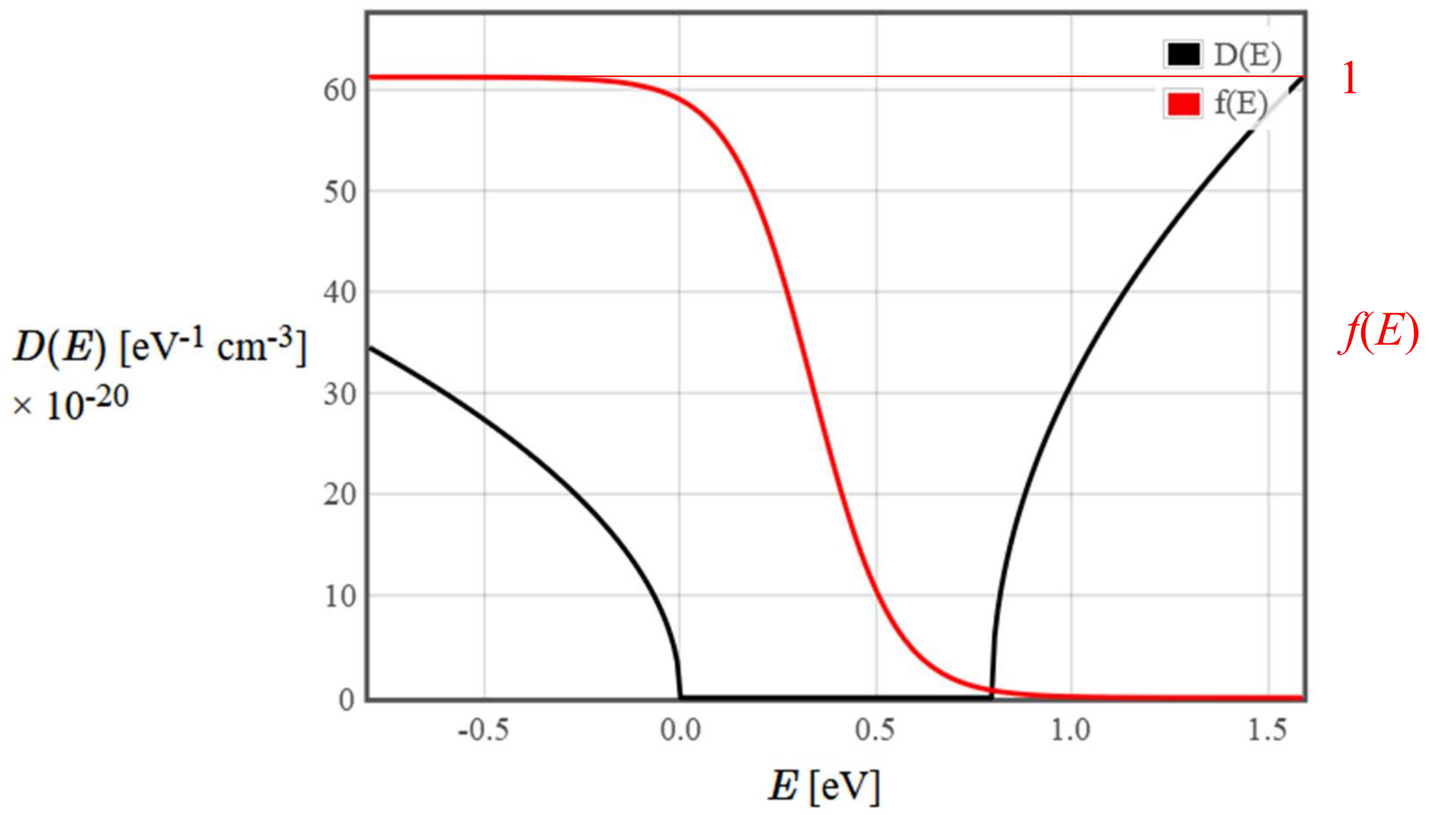
Metals, semiconductors, and insulators



Insulators: band gap > 3 eV

From Ibach & Lueth

Chemical potential of semiconductors and insulators



μ is in the middle of the band gap

Ballistic transport

$$\vec{F} = m\vec{a} = -e\vec{E} = m\frac{d\vec{v}}{dt}$$

$$\vec{v} = \frac{-e\vec{E}t}{m} + \vec{v}_0$$

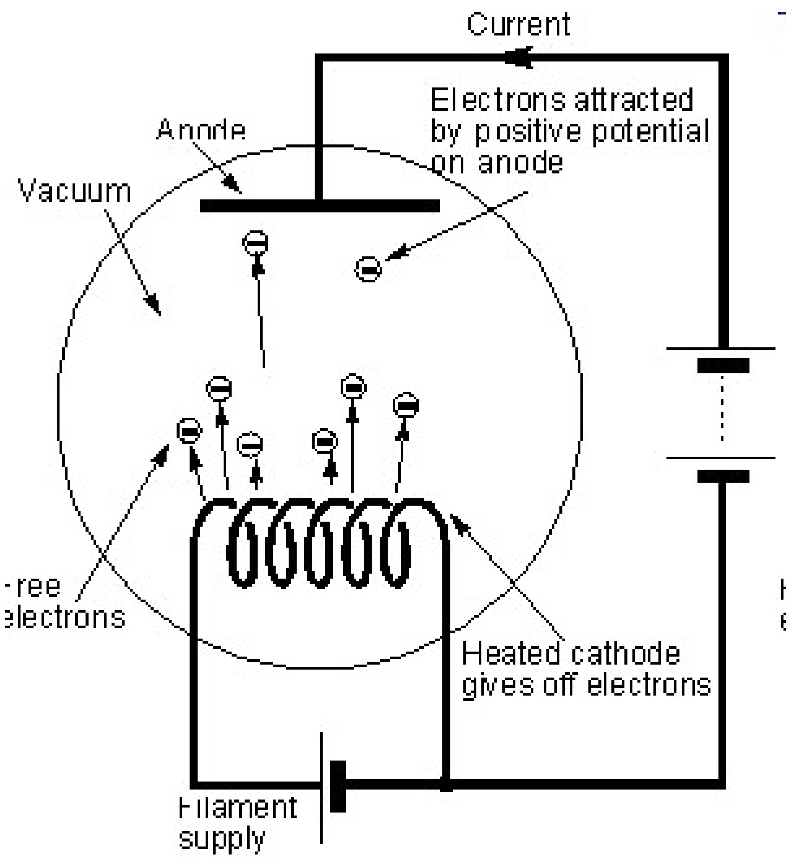
$$\vec{x} = \frac{-e\vec{E}t^2}{2m} + \vec{v}_0 t + \vec{x}_0$$

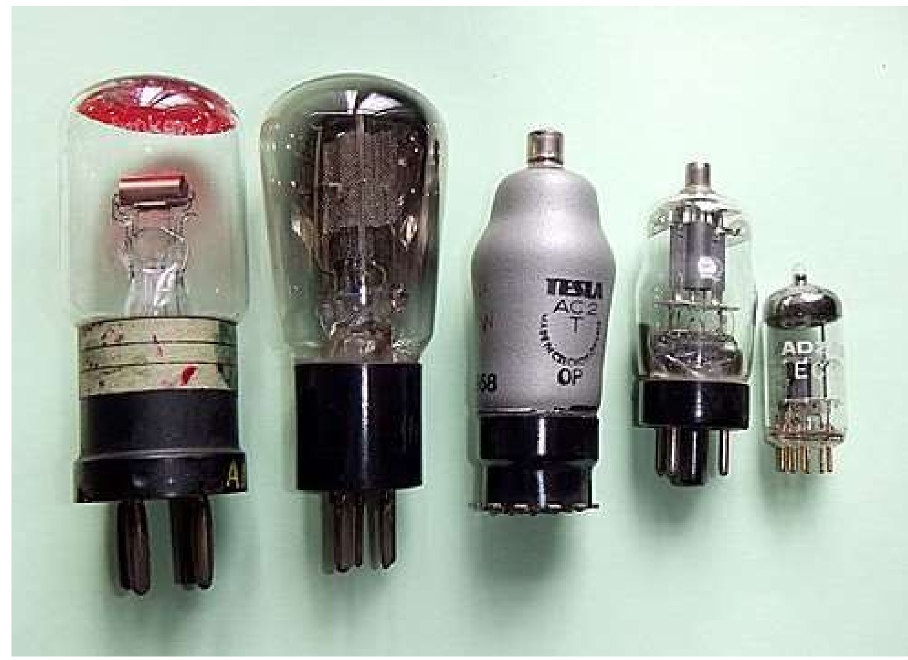
electrons in an electric field follow a parabola.

electrons in a magnetic field move in a spiral

electrons crossed electric and magnetic fields spiral along the direction perpendicular to the electric and magnetic fields

Ballistic motion

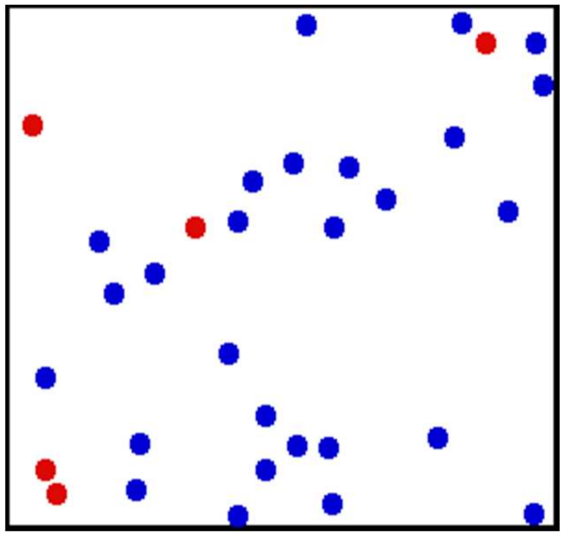




diode

kinetic theory

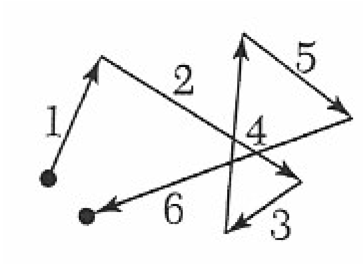
describe electrons as a gas of particles



$v_F = 10^8$ cm/s.

The average time between scattering events τ_{sc} can be calculated by Fermi's golden rule

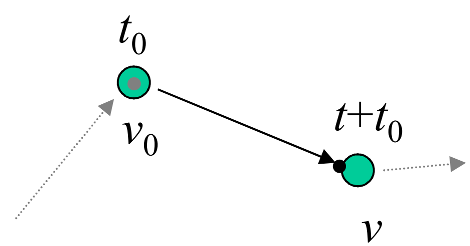
mean free path: $\boldsymbol{l} = v_F\tau_{sc}$ ~ 1 nm - 1 cm



Diffusive transport

$$\vec{F} = -e\vec{E} = m^{*}\vec{a} = m^{*}\frac{d\vec{v}}{dt}$$

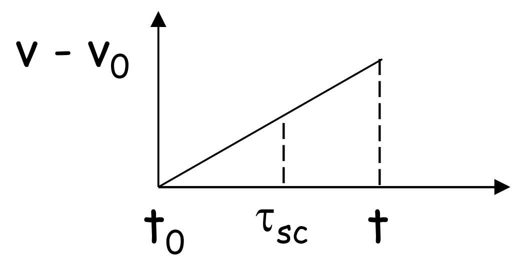
time between two collisions



$$\vec{v} = \vec{v}_0 - \frac{e\vec{E}}{m^{*}}(t - t_0)$$

$\langle v_0 \rangle = 0$

$\langle t - t_0 \rangle = \tau_{sc}$ < average time between scattering events



$$\vec{v}_d = \frac{-e\vec{E}\tau_{sc}}{m^{*}} = \frac{-e\vec{E}\ell}{m^{*}v_F}$$

drift velocity: $\vec{v}_d = -\mu\vec{E}$

Ohm's law: $\vec{j} = -ne\vec{v}_d = ne\mu\vec{E} = \sigma\vec{E}$

Matthiessen's rule

$$\frac{1}{\tau_{sc}} = \frac{1}{\tau_{sc,lattice}} + \frac{1}{\tau_{sc,impurity}}$$

mostly temperature independent

phonons, temperature dependent

$$\frac{1}{\mu} = \frac{1}{\mu_{lattice}} + \frac{1}{\mu_{impurity}}$$

Waves or Particles

Scattering between Bloch states can be calculated by Fermi's golden rule.

The particle picture is not rigorously correct.

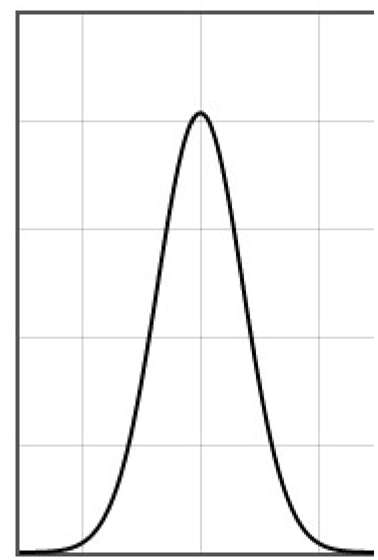
Diffusion equation/ heat equation

$$\frac{dn}{dt} = -D\nabla^2 n$$

Diffusion constant (→ D)

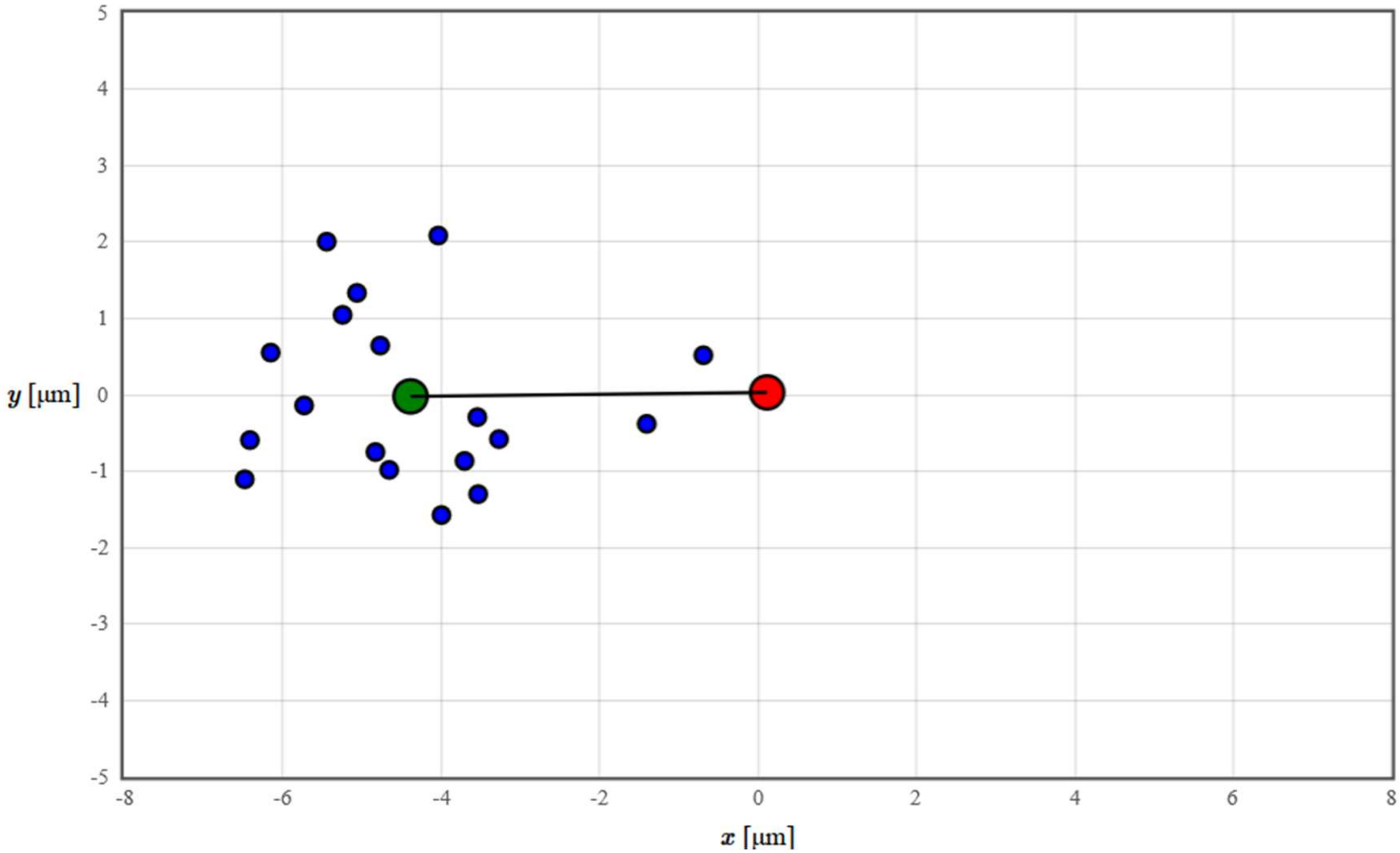
Fick's law $\vec{j} = -D\nabla n$

Continuity equation $\frac{dn}{dt} = \nabla \cdot \vec{j}$



$$n = \frac{1}{\sqrt{4\pi Dt}} \exp\left(\frac{-r^2}{4Dt}\right)$$

Drift and Diffusion

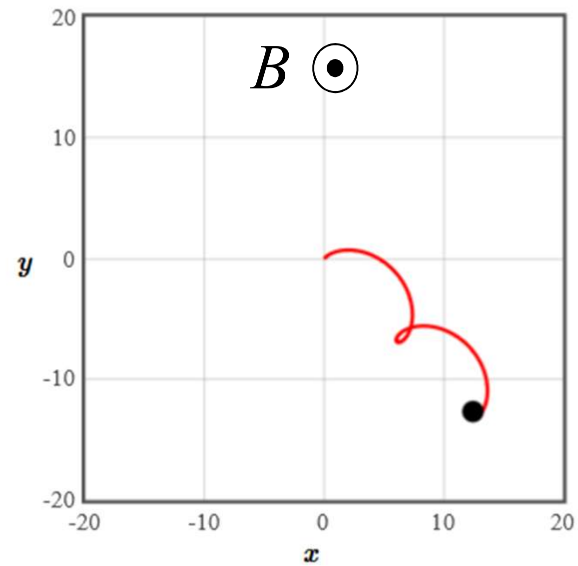


http://lampx.tugraz.at/~hadley/ss2/transport/drude.php

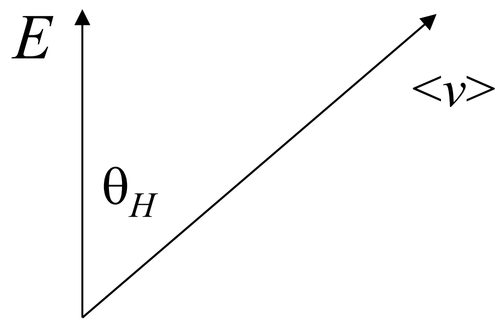
Crossed *E* and *B* fields

Ballistic transport

$$\vec{F} = m\vec{a} = -e\left(\vec{E} + \vec{v} \times \vec{B}\right)$$



Diffusive transport



Hall angle: $\theta_H = \tan^{-1}\left(-\frac{eB_z\tau_{sc}}{m}\right)$

Magnetic field (diffusive regime)

$$\vec{F} = m\vec{a} = -e\vec{E} = m\frac{\vec{v}_d}{\tau_{sc}} \qquad -\frac{e\tau_{sc}}{m}\vec{E} = \vec{v}_d$$

$$\vec{F} = m\vec{a} = -e\left(\vec{E} + \vec{v}\times\vec{B}\right) = m\frac{\vec{v}_d}{\tau_{sc}}$$

If B is in the z-direction, the three components of the force are

$$-e\left(E_x + v_{dy}B_z\right) = m\frac{v_{dx}}{\tau_{sc}}$$

$$-e\left(E_y - v_{dx}B_z\right) = m\frac{v_{dy}}{\tau_{sc}}$$

$$-e\left(E_z\right) = m\frac{v_{dz}}{\tau_{sc}}$$

Magnetic field (diffusive regime)

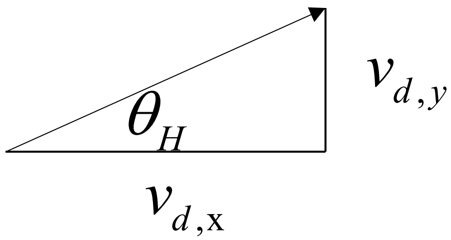
$$v_{d,x} = -\frac{eE_x \tau_{sc}}{m} - \frac{eB_z}{m}\tau_{sc} v_{d,y}$$

$$v_{d,y} = -\frac{eE_y \tau_{sc}}{m} + \frac{eB_z}{m}\tau_{sc} v_{d,x}$$

$$v_{d,z} = -\frac{eE_z \tau_{sc}}{m}$$

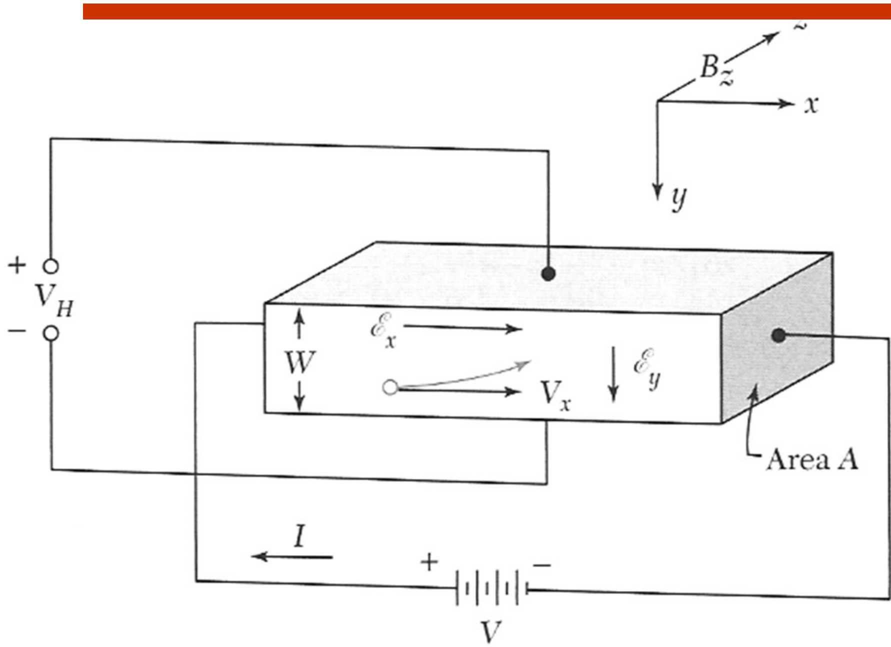
If $E_y = 0, E_z = 0$

$$v_{d,y} = -\frac{eB_z}{m}\tau_{sc} v_{d,x}$$



$$\tan\theta_H = -\frac{eB_z}{m}\tau_{sc}$$

The Hall Effect (diffusive regime)



$$v_{d,x} = -\frac{eE_x\tau_{sc}}{m} - \frac{eB_z}{m}\tau_{sc}v_{d,y}$$

$$v_{d,y} = -\frac{eE_y\tau_{sc}}{m} + \frac{eB_z}{m}\tau_{sc}v_{d,x}$$

$$v_{d,z} = -\frac{eE_z\tau_{sc}}{m}$$

If $v_{d,y} = 0$,

$E_y = v_{d,x}B_z = V_H/W = R_H j_x B_z$ V_H = Hall voltage, R_H = Hall Constant

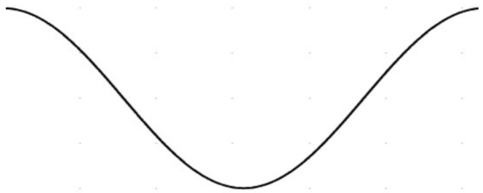
$j_x = - nev_{d,x}$

$$R_H = E_y/j_xB_z = -1/ne$$

Metal	Method	Experimental R_H, in 10^{-24} CGS units	Assumed carriers per atom	Calculated $-1/nec$, in 10^{-24} CGS units
Li	conv.	−1.89	1 electron	−1.48
Na	helicon	−2.619	1 electron	−2.603
	conv.	−2.3		
K	helicon	−4.946	1 electron	−4.944
	conv.	−4.7		
Rb	conv.	−5.6	1 electron	−6.04
Cu	conv.	−0.6	1 electron	−0.82
Ag	conv.	−1.0	1 electron	−1.19
Au	conv.	−0.8	1 electron	−1.18
Be	conv.	+2.7	—	—
Mg	conv.	−0.92	—	—
Al	helicon	+1.136	1 hole	+1.135
In	helicon	+1.774	1 hole	+1.780
As	conv.	+50.	—	—
Sb	conv.	−22.	—	—
Bi	conv.	−6000.	—	—

Kittel

Einstein relation



$$n(x) = A\exp\left(\frac{-U_{pot}(x)}{k_B T}\right)$$ Boltzmann factor

$$\vec{F} = -\nabla U_{pot} = -e\vec{E}$$

In equilibrium, drift = diffusion

$$en\mu\vec{E} + eD\nabla n = 0$$

$$\nabla n = -\frac{1}{k_B T} A\exp\left(\frac{-U_{pot}}{k_B T}\right)\nabla U_{pot} = -\frac{n}{k_B T}\nabla U_{pot} = \frac{-en\vec{E}}{k_B T}$$

$$en\mu\vec{E} - e^2 D\frac{n\vec{E}}{k_B T} = 0$$

$$\boxed{D = \frac{\mu k_B T}{e}}$$

Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen, A. Einstein (1905).