17. Phonons, Electrons

May 24, 2018

Waves and particles

The eigen function solutions of the wave equation are plane waves. The scattering time is one over the rate for scattering from a given plane wave solution to any other.

Phonons are particles. The scattering time is the time before the phonons scatter and randomly change energy and momentum.

$$\vec{p} = \hbar\vec{k}$$

The average time between scattering events is $\tau_{sc} = 1/\Gamma$

Phonon scattering

Scattering randomizes the momentum of the phonons.

$$H = H_{HO} + H_1$$

Transition rates determined by Fermi's golden rule

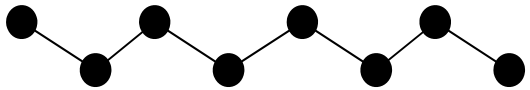
$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}\left|\left\langle \psi_f \left| H_1 \right| \psi_i \right\rangle\right|^2 \delta\left(E_f - E_i\right)$$

Any process (3 phonon, 4 phonon, 5 phonon. ...) that conserves energy and momentum is allowed.

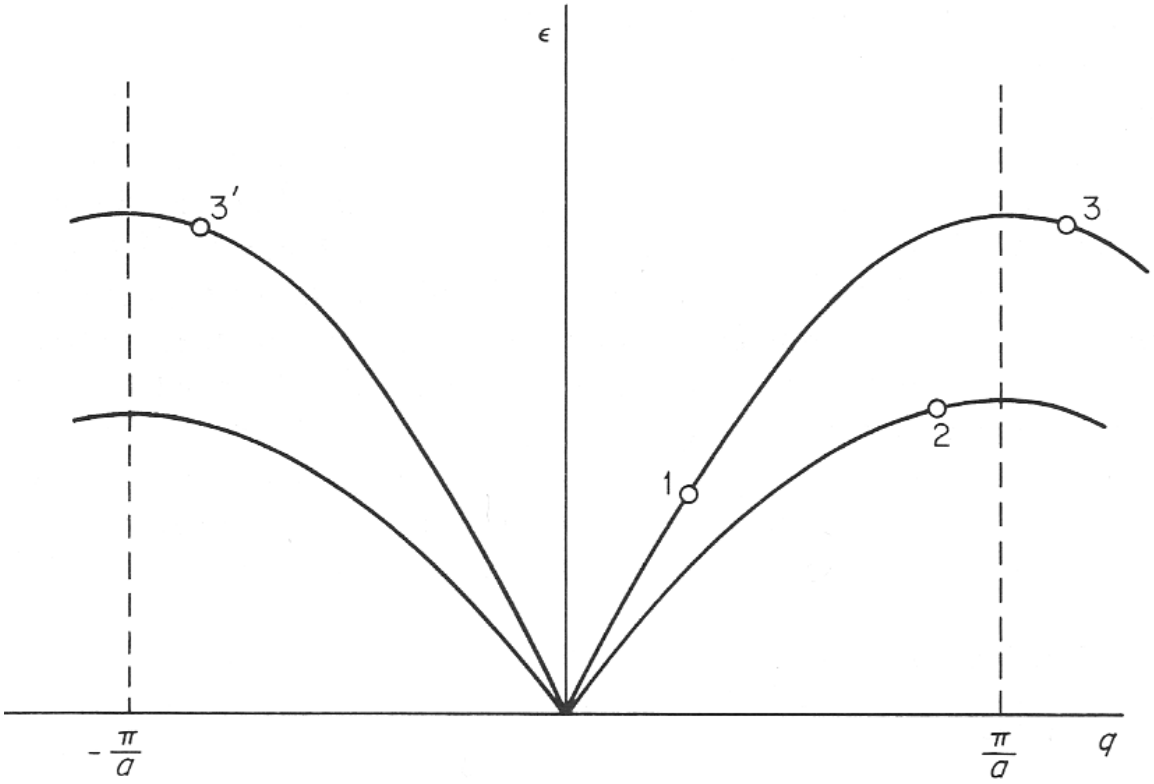
Results in attenuation of acoustic waves

Umklapp Processes

Three phonon scattering



$$\hbar\vec{k}_1 + \hbar\vec{k}_2 = \hbar\vec{k}_3 + \hbar\vec{G}$$

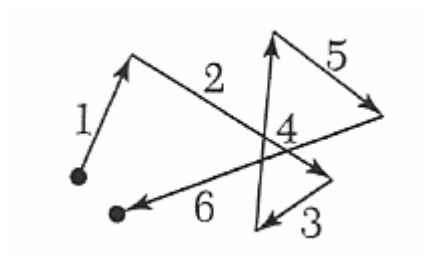


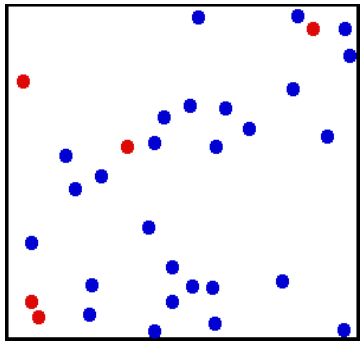
from: Hall, Solid State Physics

Heat transport (Kinetic theory)

Treat phonons as an ideal gas of particles that are confined to the volume of the solid.

Phonons move at the speed of sound. They scatter due to imperfections in the lattice and anharmonic terms in the Hamiltonian.





The average time between scattering events is τ_{sc}

The average distance traveled between scattering events is the mean free path: $\boldsymbol{l} = v\tau_{sc} \sim 10$ nm

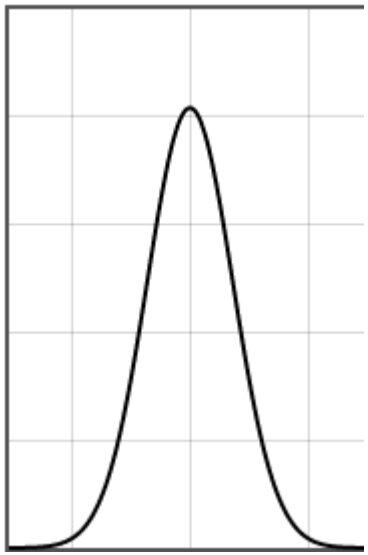
Diffusion equation/ heat equation

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

Diffusion constant

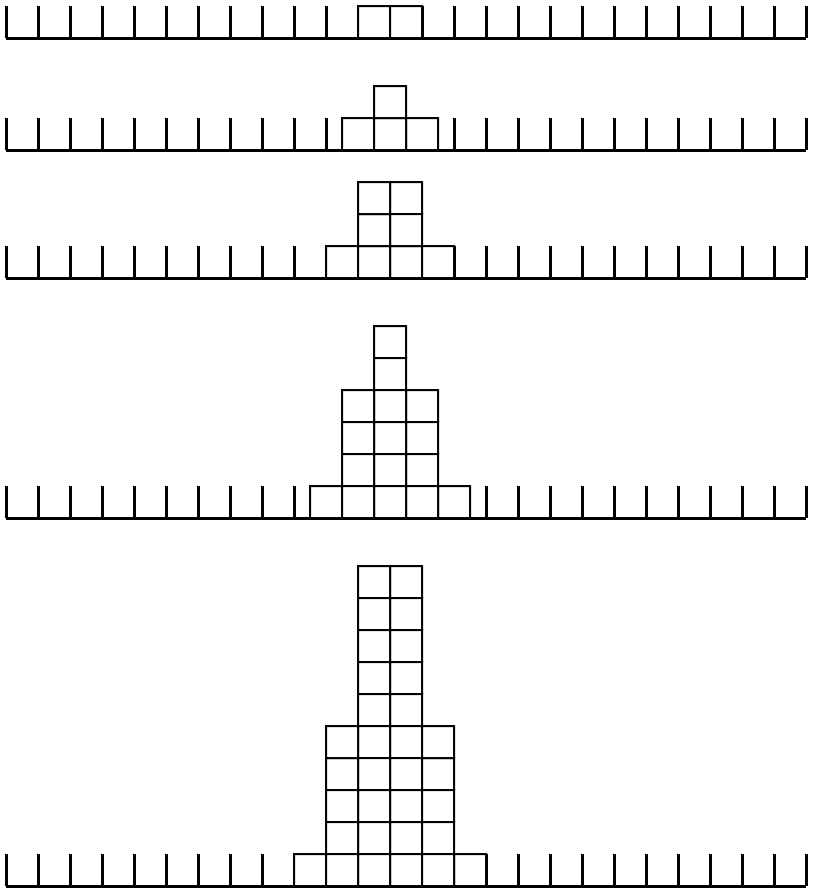
Fick's law $\vec{j} = -D\nabla n$

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

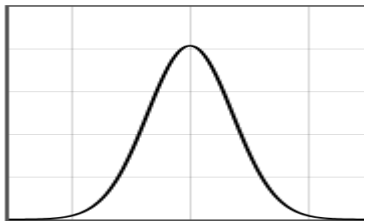


$$n = \frac{1}{\sqrt{4\pi Dt}} \exp\left(\frac{-r^2}{4Dt}\right)$$

Random walk



$$\frac{\Delta n_s}{\Delta t} = n_{s+1} - 2n_s + n_{s-1}$$



$$\exp\left(-x^2\right)$$

Central limit theorem: A function convolved with itself many times forms a Gaussian

Thermal conductivity

$$\vec{j}_U = \bar{E}\vec{j}$$

Average particle energy

$$u = \bar{E}n$$

internal energy density

$$\vec{j}_U = -\bar{E}D\nabla n = -D\nabla u$$

$$\vec{j}_U = -D\frac{du}{dT}\nabla T = -Dc_v\nabla T$$

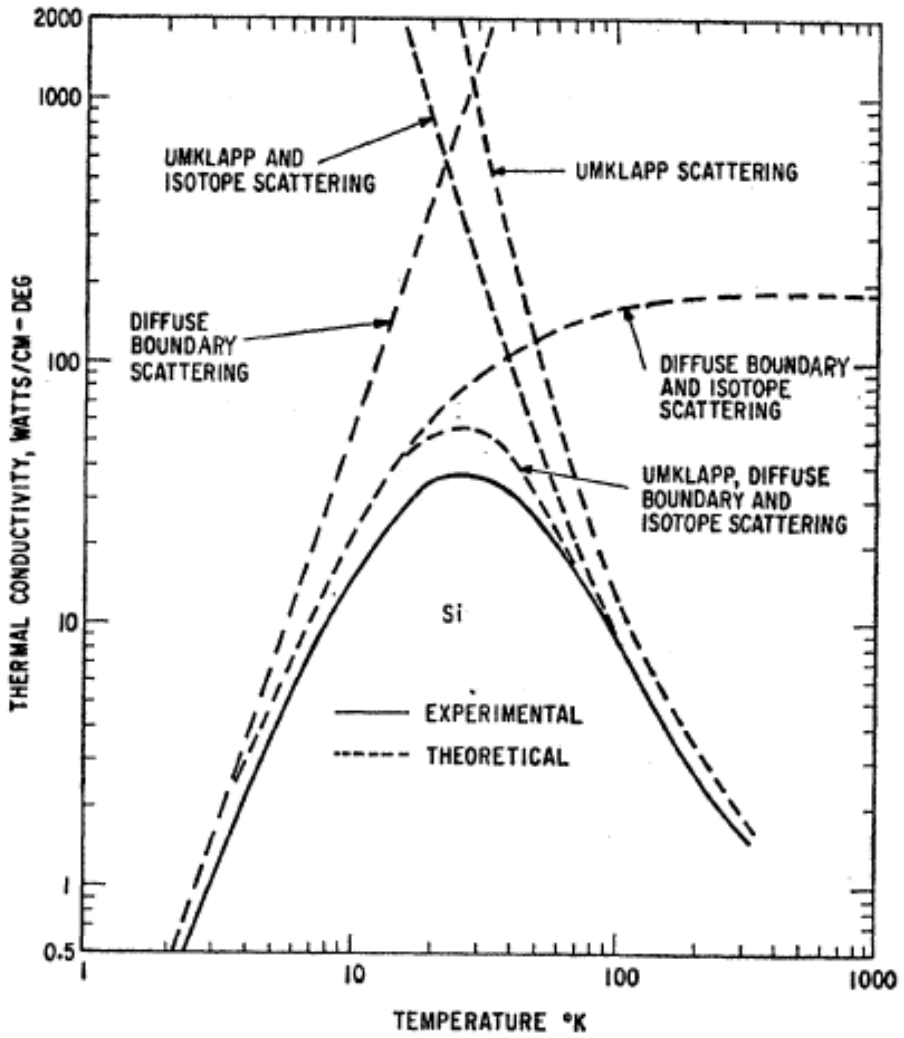
$$\vec{j}_U = -K\nabla T$$

Thermal conductivity

$$K = Dc_v$$

$$K \to 0 \quad \text{as} \quad T \to 0$$

Thermal conductivity $\vec{j}_U = -K\nabla T$



Imperfections in the crystal or grain boundaries decrease the mean free path and the thermal conductivity.

At high temperatures, the mean free path is limited by Umklapp processes. At low temperatures the Umklapp processes freeze out and the mean free path is limited by imperfections.

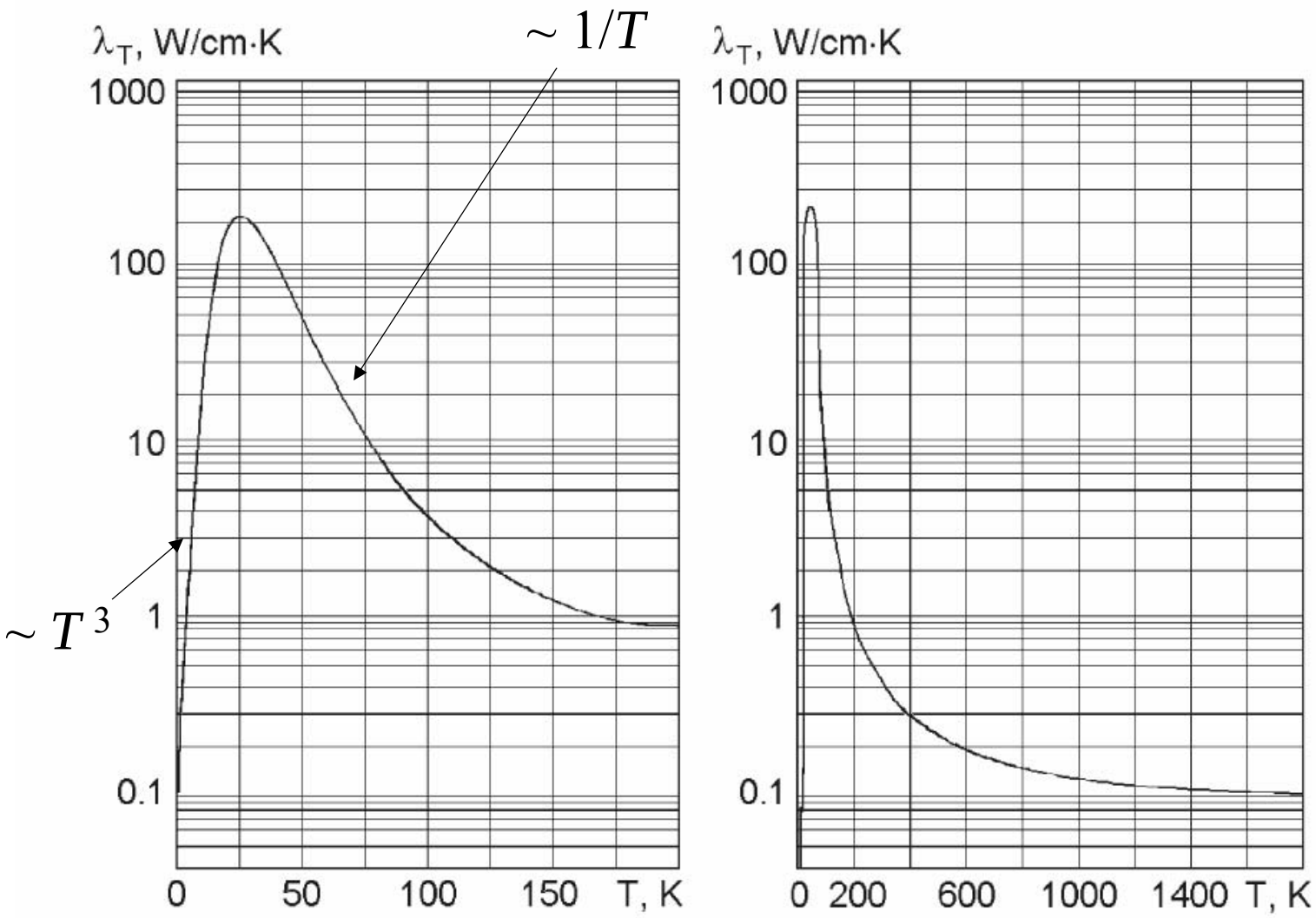
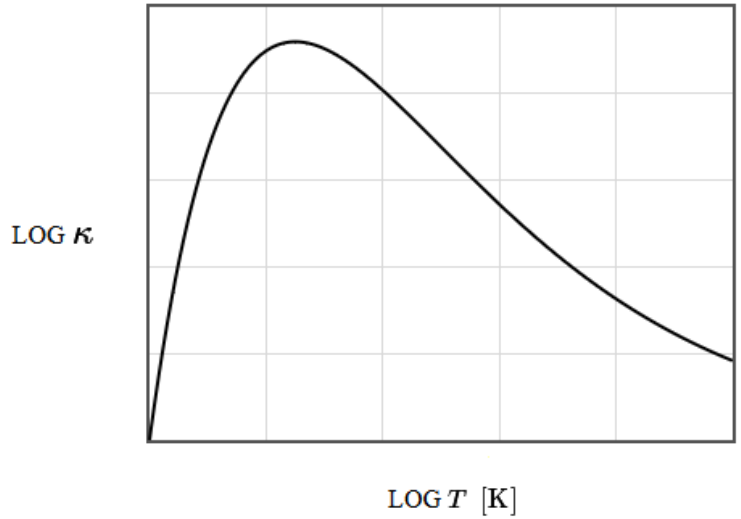


Fig. 2.69 Temperature dependence of the thermal conductivity coefficient for sapphire: (**a**) low temperatures; (**b**) high temperatures

Thermal conductivity

$$\vec{j}_U = -K\nabla T$$

Material	Thermal conductivity W/(m·K)
Glass	1.1
Concrete, stone	1.7
Ice	2
Sandstone	2.4
Sapphire	35
Stainless steel	12.11 ~ 45.0
Lead	35.3
Aluminum	237
Aluminum alloys	120—180
Gold	318
Copper	401
Silver	429
Diamond	900 - 2320
Graphene	(4840±440) - (5300±480)



Phonon student projects

Calculate a dispersion relation including next nearest neighbors.

Write a javascript program that plots the phonon dispersion relation in an arbitrary direction.

Calculate one column of the phonon table: hcp, NaCl, CsCl, ZnS, diamond, ...

Calculate the temperatures at which ZnO goes through a phase transition.

Free electron Fermi gas

Kittel, chapter 6

A simple model for a metal is electrons confined to box with periodic boundary conditions.

Like the problem of photons in a box except:

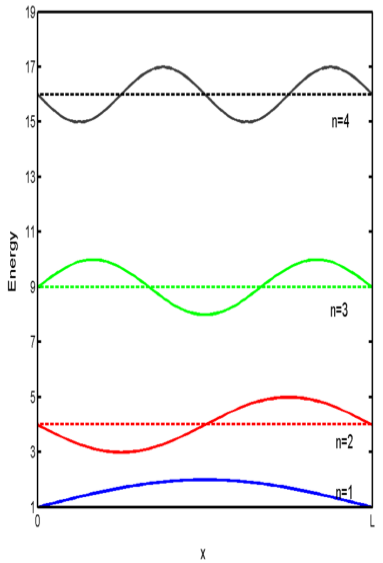
Solve the Schrödinger equation instead of the wave equation.

Electrons are fermions not bosons.

Free particles in 1-d

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad V = 0$$

$$E = \frac{n^2h^2}{8mL^2} = \frac{h^2}{2m\lambda^2} = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m} = \frac{mv^2}{2}$$



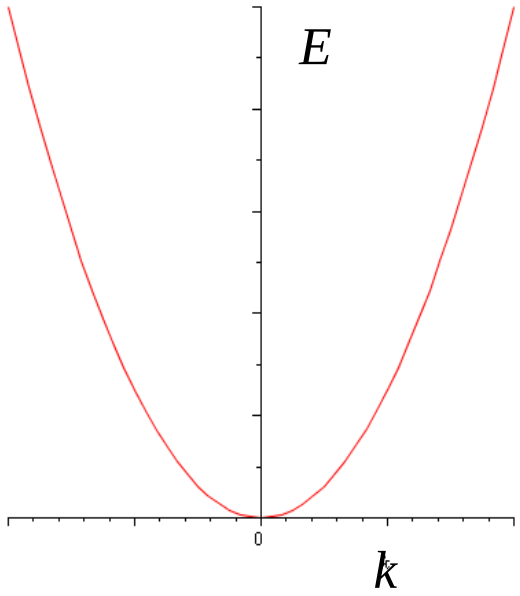
$$\lambda = \frac{2L}{n}$$

Free particles in 1-d

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} \qquad V = 0$$

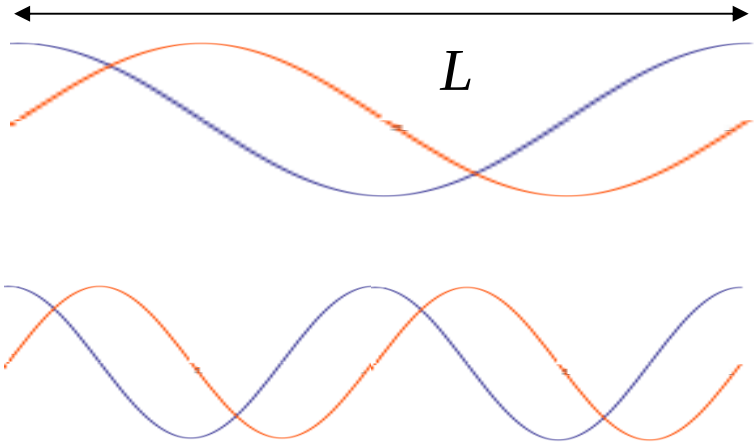
Eigen function solutions: $\psi_k = A_k e^{i(kx-\omega t)}$

Dispersion relation: $E = \hbar\omega = \frac{\hbar^2 k^2}{2m} = \frac{1}{2}mv^2$



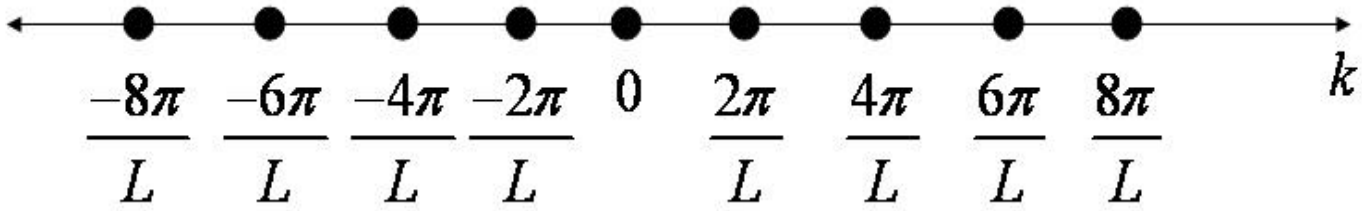
Periodic boundary conditions

$$\psi = A_k e^{i(kx-\omega t)}$$



$$\frac{2\pi}{L}$$

$$\frac{4\pi}{L}$$

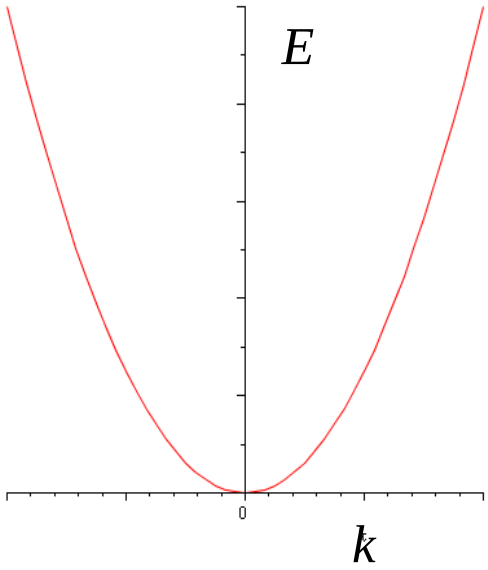


$$LD(k)dk = \frac{2 \cdot 2dk}{\frac{2\pi}{L}}$$

Density of states: $\boxed{D(k) = \frac{2}{\pi}}$ ← Spin

Number of states between $|k|$ and $|k|+dk$ is $LD(k)dk$

Free particles in 1-d



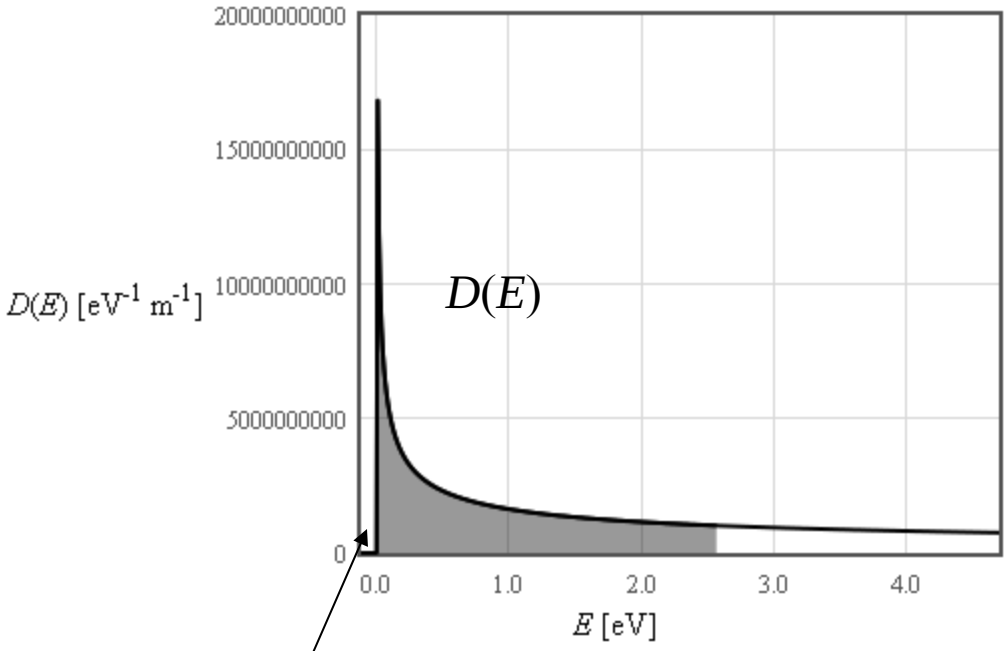
$$D(k) = \frac{2}{\pi} \longleftarrow \text{Spin}$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$\frac{dk}{dE} = \frac{1}{2\hbar}\sqrt{\frac{2m}{E}}$$

$$D(E) = D(k)\frac{dk}{dE} = \frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}$$

Density of states



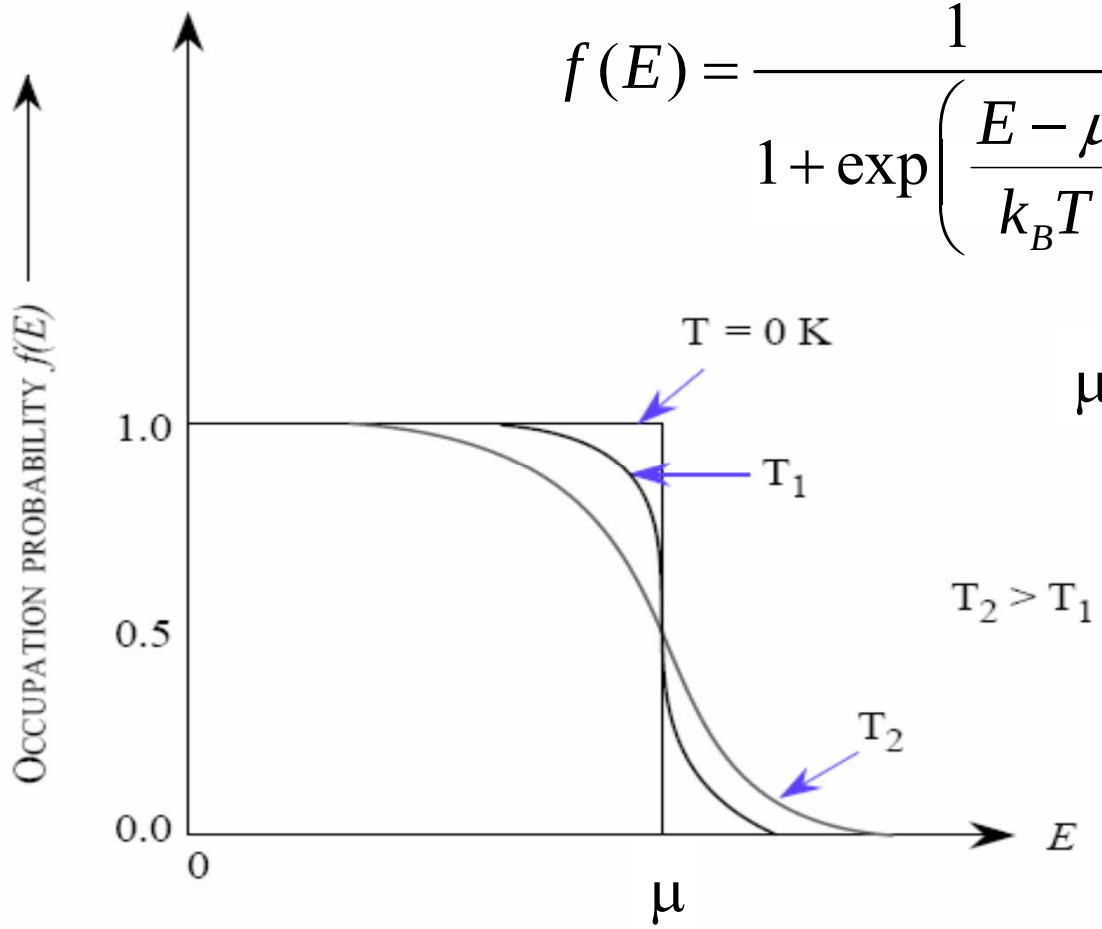
Van Hove singularity

E

Fermi function

$f(E)$ is the probability that a state at energy E is occupied.

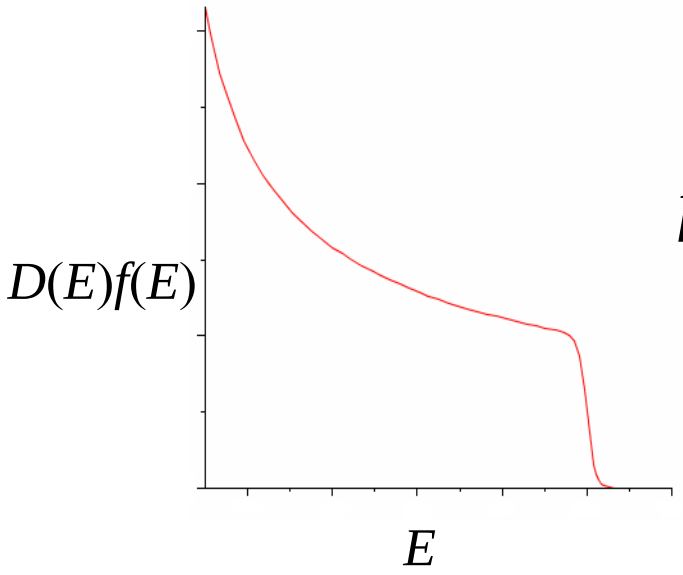
$$f(E) = \frac{1}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)}$$



μ = chemical potential

Chemical potential

$$D(E) = \frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}$$



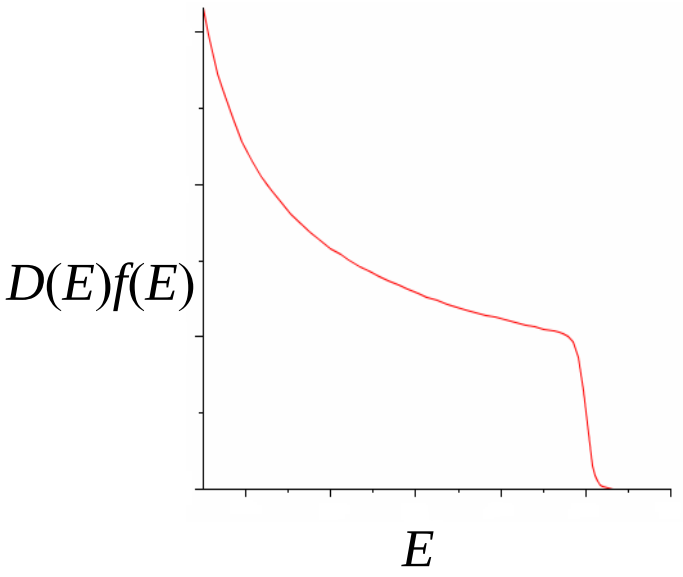
$$f(E) = \frac{1}{1+\exp\left(\dfrac{E-\mu}{k_B T}\right)}$$

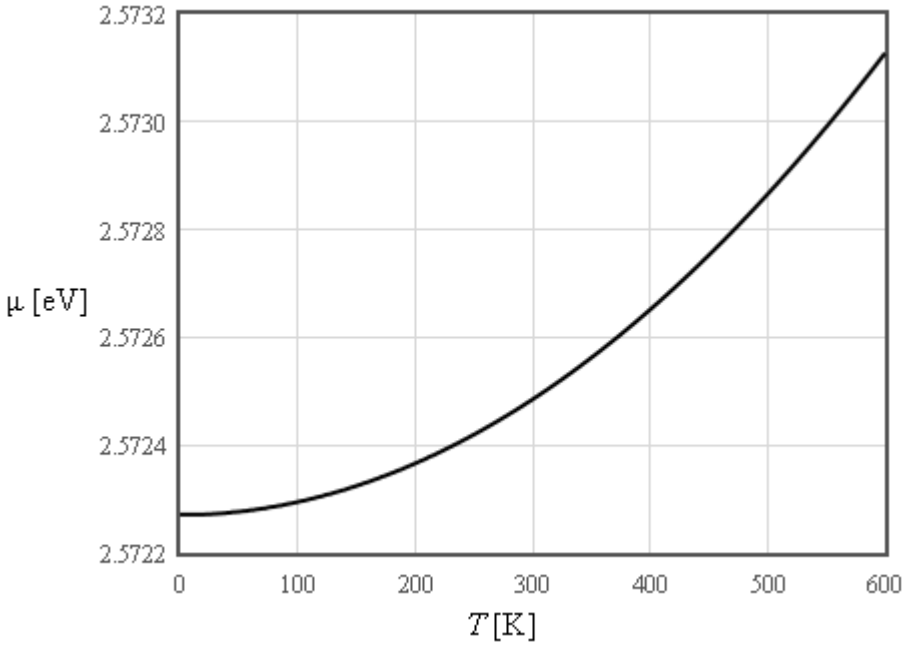
The chemical potential is implicitly defined as the energy that solves the following equation.

$$n = \frac{N}{L} = \int_{-\infty}^{\infty} D(E)\, f(E) dE = \int_{-\infty}^{\infty} \frac{D(E)dE}{1+\exp\left(\dfrac{E-\mu}{k_B T}\right)}$$

Here N is the total number of electrons.

Chemical potential





μ is temperature dependent

Fermi energy

$$E_F = \mu(T=0)$$

In semiconductor books, $E_F(T) = \mu(T)$.

At $T = 0$ $$n = \int_{-\infty}^{E_F} D(E)dE$$

In one dimension,

$$n = \int_0^{E_F} \frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}dE = \frac{2}{\pi\hbar}\sqrt{2mE_F}$$

$$E_F = \frac{\pi^2\hbar^2 n^2}{8m}$$

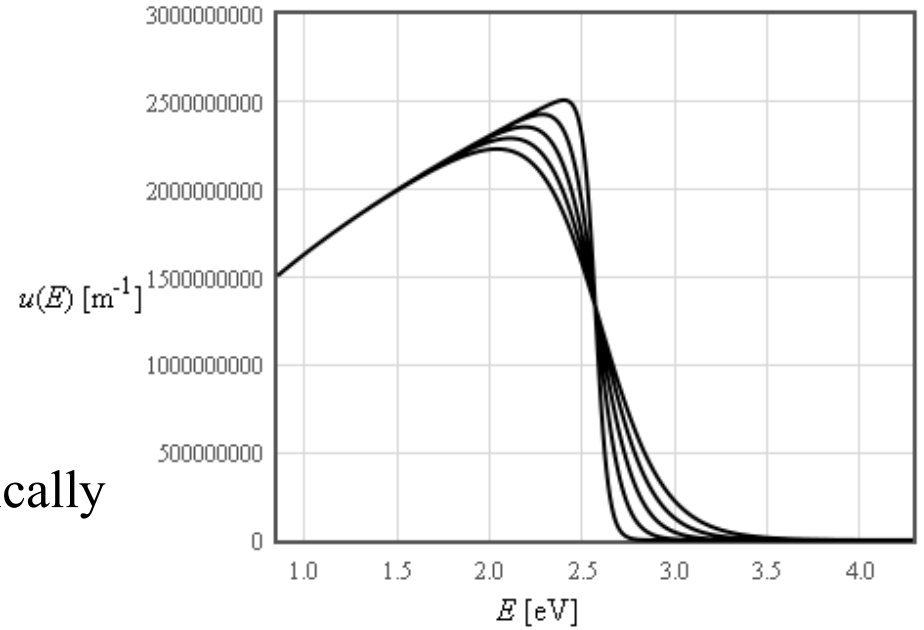
Free particles in 1-d

internal energy spectral density

$$u(E) = ED(E)f(E) = \frac{\sqrt{2mE}}{\pi\hbar}\frac{1}{\exp\left(\frac{E-\mu}{k_B T}\right)+1}$$

$$u = \int_{-\infty}^{\infty} u(E)dE$$

$$c_v = \frac{du}{dT}$$



Not possible to do this integral analytically

analog to the Planck curve for electrons in 1-d

Thermodynamic properties

$$D(E) = \frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}$$

From the density of states, the thermodynamic properties can be calculated.

Internal energy $u = \int_{-\infty}^{\infty} ED(E)f(E)dE$	$u \approx \frac{1}{3}nE_F + \frac{\pi^2 D(E_F)}{6}(k_B T)^2$ J m^{-1} $\approx \frac{\pi^2\hbar^2 n^3}{24m} + \frac{2m}{3\hbar^2 n}(k_B T)^2$ J m^{-1}
Specific heat $c_v = \left(\frac{\partial u}{\partial T}\right)_{V=const}$	$c_v \approx \frac{\pi^2 D(E_F)}{3}k_B^2 T$ J K^{-1}m^{-1} $\approx \frac{4m}{3\hbar^2 n}k_B^2 T$ J K^{-1}m^{-1}
Entropy $s = \int \frac{c_v}{T}dT$	$s \approx \frac{\pi^2 D(E_F)}{3}k_B^2 T$ J K^{-1}m^{-1} $\approx \frac{4m}{3\hbar^2 n}k_B^2 T$ J K^{-1}m^{-1}
Helmholtz free energy $f = u - Ts$	$f \approx \frac{1}{3}nE_F - \frac{\pi^2 D(E_F)}{6}(k_B T)^2$ J m^{-1} $\approx \frac{\pi^2\hbar^2 n^3}{24m} - \frac{2m}{3\hbar^2 n}(k_B T)^2$ J m^{-1}
Pressure $P = -\left.\frac{\partial F}{\partial V}\right\|_{N,T}$	$P \approx \frac{2}{3}nE_F + \frac{\pi^2 D(E_F)}{3}(k_B T)^2$ N $P \approx \frac{\pi^2\hbar^2 n^3}{12m} + \frac{4m}{3\hbar^2 n}(k_B T)^2$ N
Bulk modulus $B = -V\frac{\partial P}{\partial V}$	$B \approx 2nE_F - \frac{\pi^2 D(E_F)}{3}(k_B T)^2$ N $B \approx \frac{\pi^2\hbar^2 n^3}{4m} - \frac{4m}{3\hbar^2 n}(k_B T)^2$ N