2. Free electrons

Oct 4, 2018

TU Graz

Advanced Solid State Physics

Solid-state physics, the largest branch of condensed matter physics, is the study of rigid matter, or solids. The bulk of solid-state physics theory and research is focused on crystals, largely because the periodicity of atoms in a crystal, its defining characteristic, facilitates mathematical modeling, and also because crystalline materials often have electrical, magnetic, optical, or mechanical properties that can be exploited for engineering purposes. The framework of most solid-state physics theory is the Schrödinger (wave) formulation of non-relativistic quantum mechanics.

- Solid state physics in Wikipedia

The most remarkable thing is the great variety of *qualitatively different* solutions to Schrödinger's equation that can arise. We have insulators, semiconductors, metals, superconductors—all obeying different macroscopic laws: an electric field causes an electric dipole moment in an insulator, a steady current in a metal or semiconductor and a steadily accelerated current in a superconductor. Solids may be transparent or opaque, hard or soft, brittle or ductile, magnetic or non-magnetic.

From *Solid State Physics* by H. E. Hall

To a large extent, our success in understanding solids is a consequence of nature's kindness in organizing them for us... By the term solid we shall really always mean crystalline solid, and, moreover, infinite perfect crystalline solid at that.

From *States of Matter* by David L. Goodstein

http://lampx.tugraz.at/~hadley/ss2/

TUG -> Institute of Solid State Physics -> Courses

Student projects

Something that will help other students pass this course

2VO + 1UE

Derivation
Example calculations (phonon dispersion relation for GaAs)
Javascript calculations
Lecture videos

Examination

1 hour written exam

One page of handwritten notes

Oral exam

- Student project
- Mistakes on written exam
- General questions about the course

Free electron Fermi gas

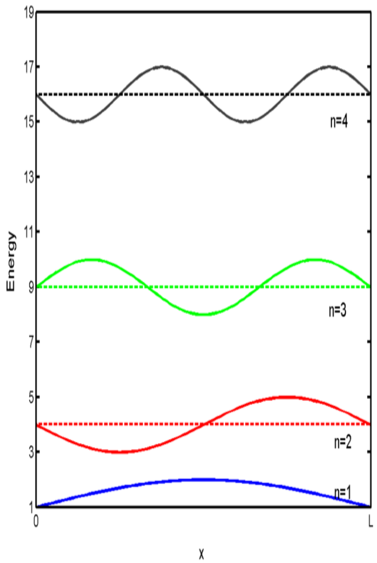
Kittel, chapter 6

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

Free particles in 1-d

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

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

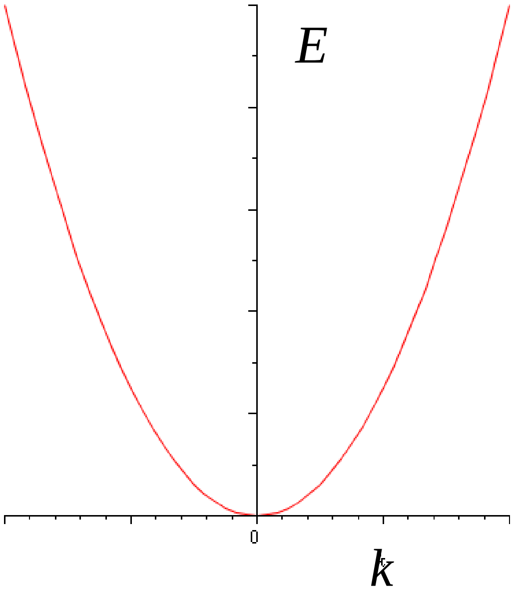


$$\lambda = \frac{2L}{n}$$

Free particles

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

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

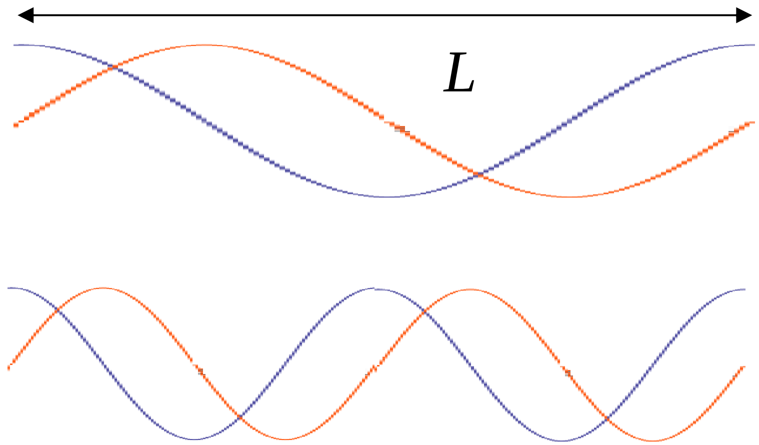


Dispersion relation: $E = \hbar\omega = \frac{\hbar^2 k^2}{2m} = \frac{1}{2}mv^2$

Eigenvalues of T:

$$T\psi_k = A_k e^{i(k(x+a)-\omega t)} = A_k e^{ika} e^{i(kx-\omega t)} = e^{ika}\psi_k$$

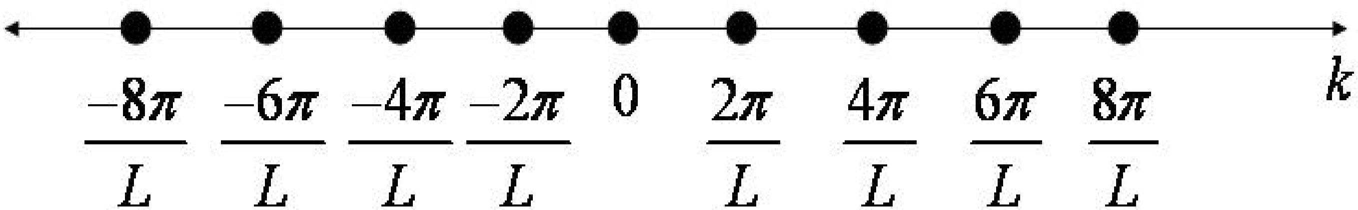
Periodic boundary conditions



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

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

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

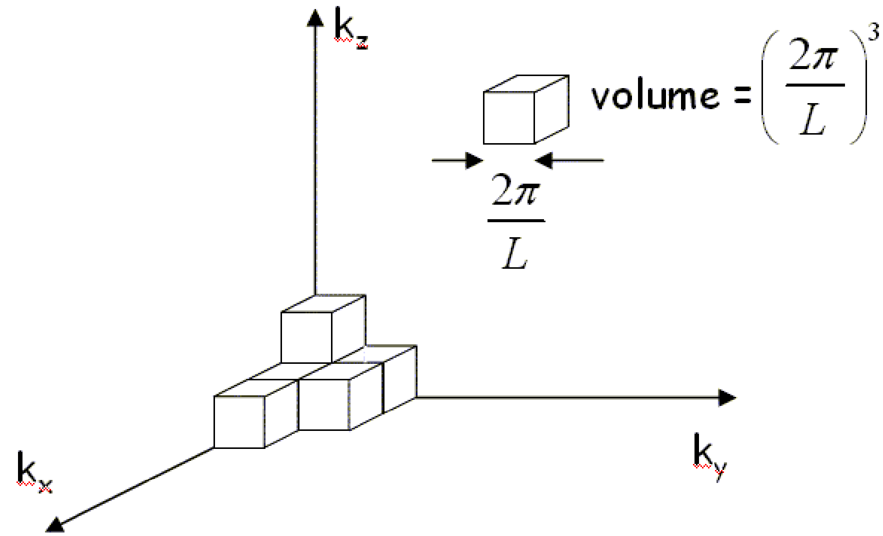


$$LD(k)dk = \frac{2\cdot 2dk}{\frac{2\pi}{L}}$$

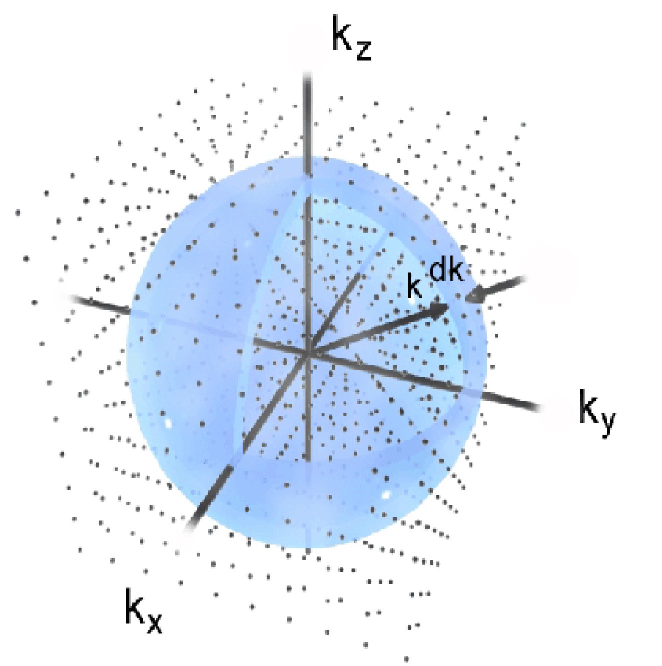
Density of states: $D(k) = \frac{2}{\pi}$ ← Spin

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

Density of states



$$k_x, k_y, k_z = \ldots, \frac{-4\pi}{L}, \frac{-2\pi}{L}, 0, \frac{2\pi}{L}, \frac{4\pi}{L}, \ldots$$



Number of states between k and $k+dk$ for a box of size L^3. =

$$2\frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3} = \frac{k^2 L^3}{\pi^2} dk = L^3 D(k) dk$$

spin

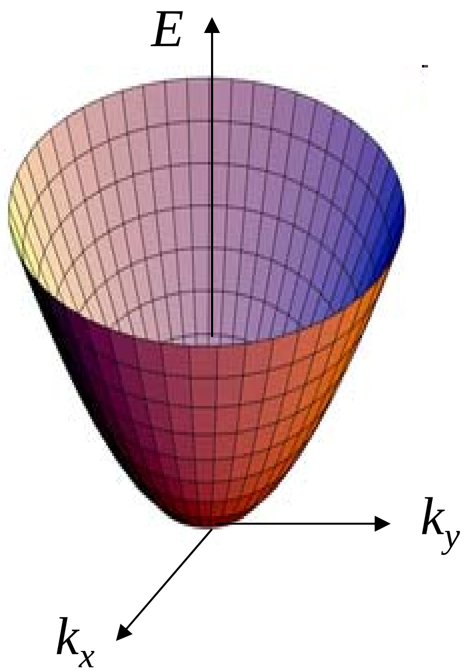
$D(k) = k^2/\pi^2$ = density of states/m^3

Free particles in 3-d

Density of states

$$E = \frac{\hbar^2 k^2}{2m}$$

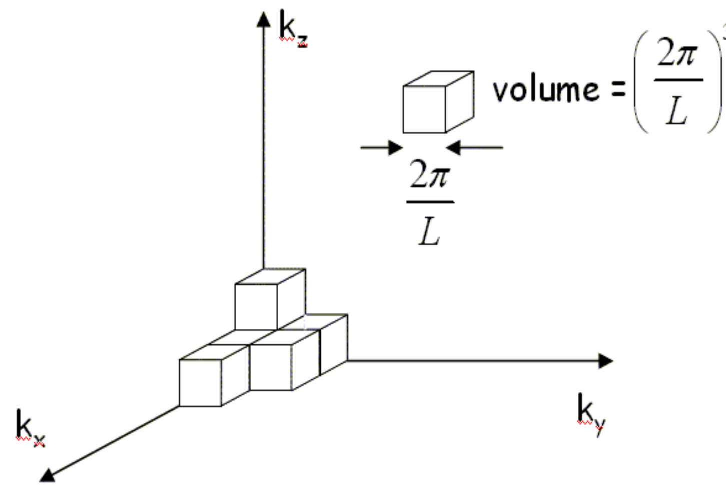
$$D(k) = \frac{k^2}{\pi^2}$$



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

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

$$D(E) = D(k)\frac{dk}{dE}$$



$$k_x, k_y, k_z = \ldots, \frac{-4\pi}{L}, \frac{-2\pi}{L}, 0, \frac{2\pi}{L}, \frac{4\pi}{L}, \ldots$$

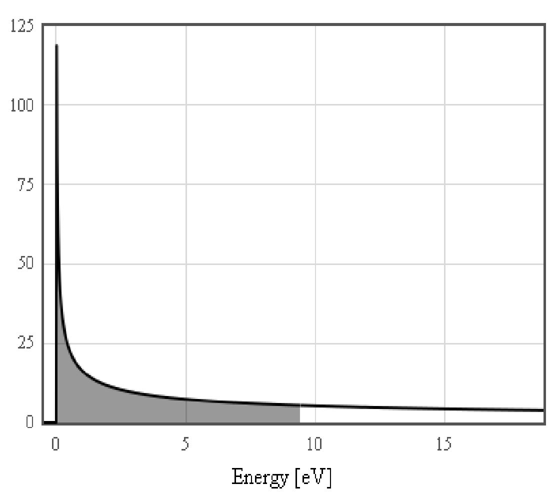
$$D(E) = \frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E}$$

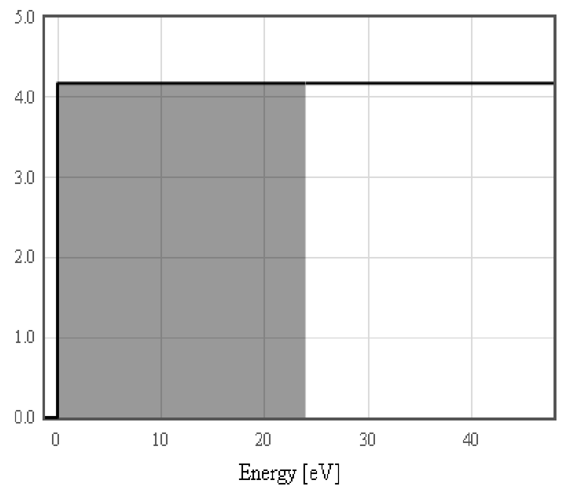
Free electron Fermi gas

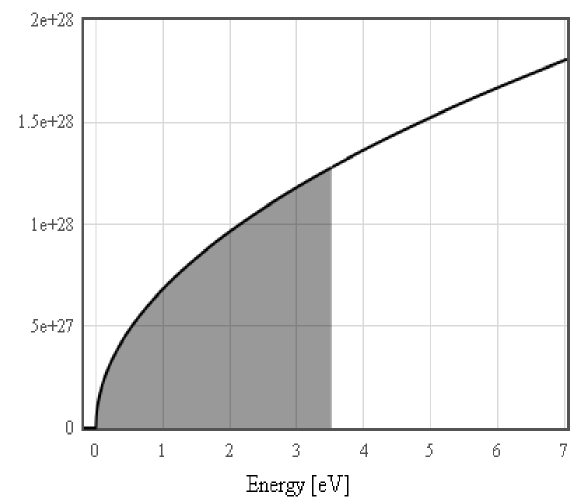
1 - d $$D(E)=\sqrt{\frac{2m}{\hbar^2\pi^2 E}}=\frac{n}{2\sqrt{E_F E}} \quad \text{J}^{-1}\text{m}^{-1}$$

2 - d $$D(E)=\frac{m}{\hbar^2\pi}=\frac{n}{E_F} \quad \text{J}^{-1}\text{m}^{-2}$$

3 - d $$D(E)=\frac{\pi}{2}\left(\frac{2m}{\hbar^2\pi^2}\right)^{3/2}\sqrt{E}=\frac{3n}{2E_F^{3/2}}\sqrt{E} \quad \text{J}^{-1}\text{m}^{-3}$$



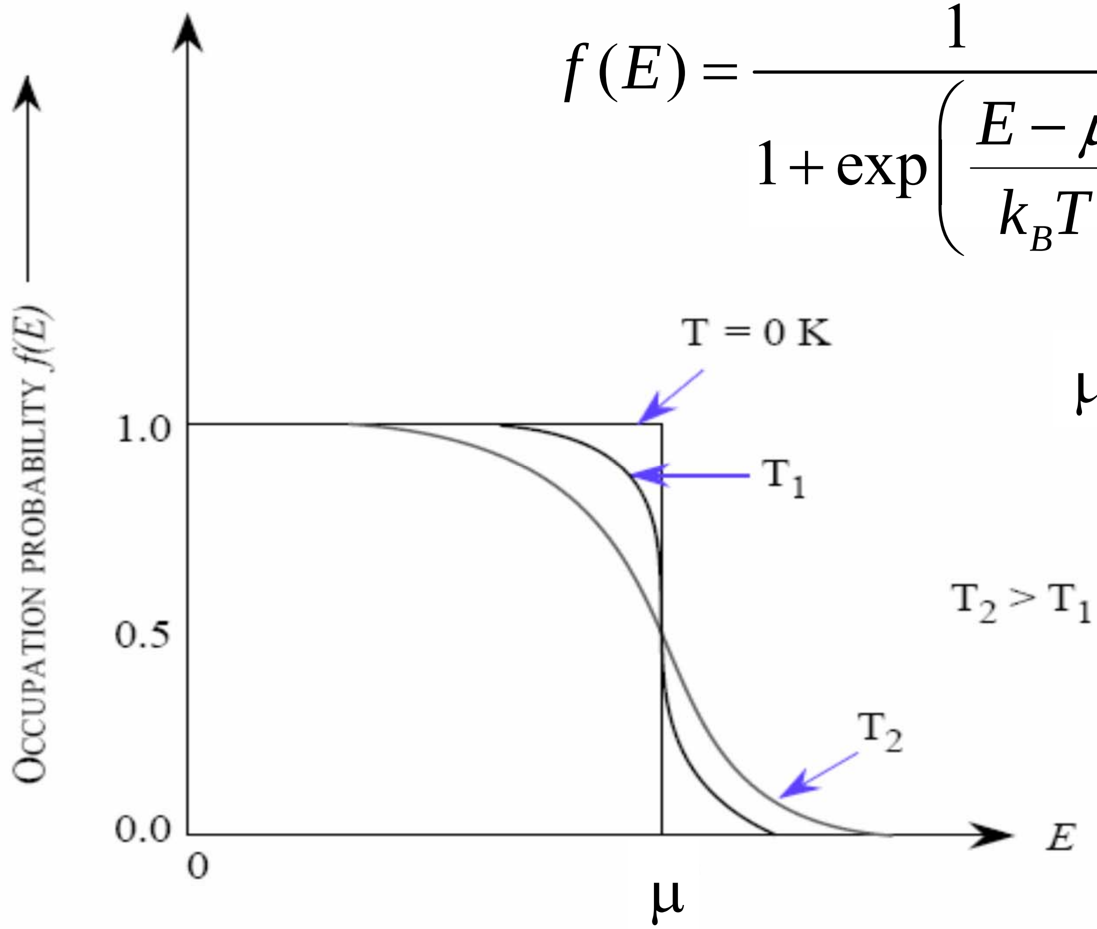




Fermi function

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

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



μ = chemical potential

Fermi energy

In solid state physics books,

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

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

At $T = 0$

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

In three dimensions,

$$n = \frac{N}{L^3} = \frac{\sqrt{2}m^{3/2}}{\pi^2\hbar^3}\int_0^{E_F}\sqrt{E}\,dE = \frac{(2m)^{3/2}}{3\pi^2\hbar^3}E_F^{3/2}$$

$$E_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3}$$

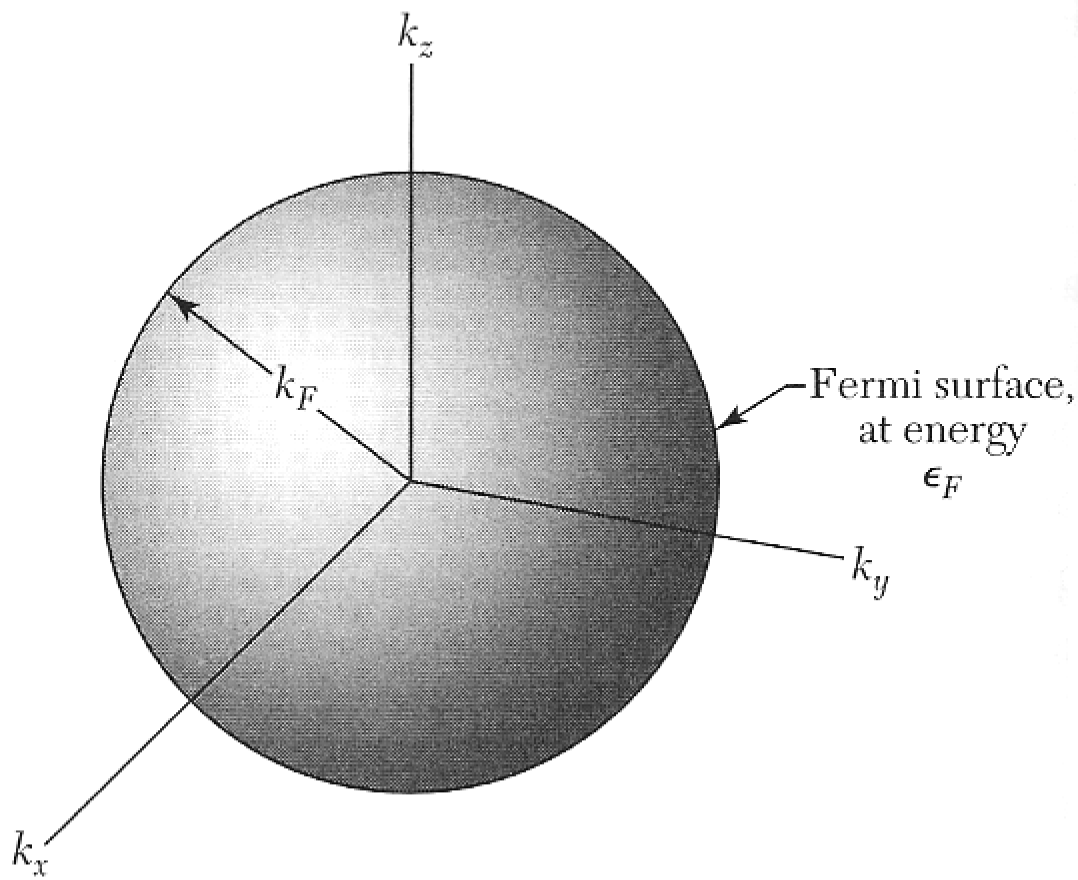
Fermi sphere

$$N = 2\frac{4\pi k_F^3}{3\left(\frac{2\pi}{L}\right)^3}$$

spin

$$k_F = \left(3\pi^2 n\right)^{1/3}$$

n = electron density



$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2\left(3\pi^2 n\right)^{2/3}}{2m}$$

The thermal and electronic properties depend on the states at the Fermi surface.

Free particles in 1-d

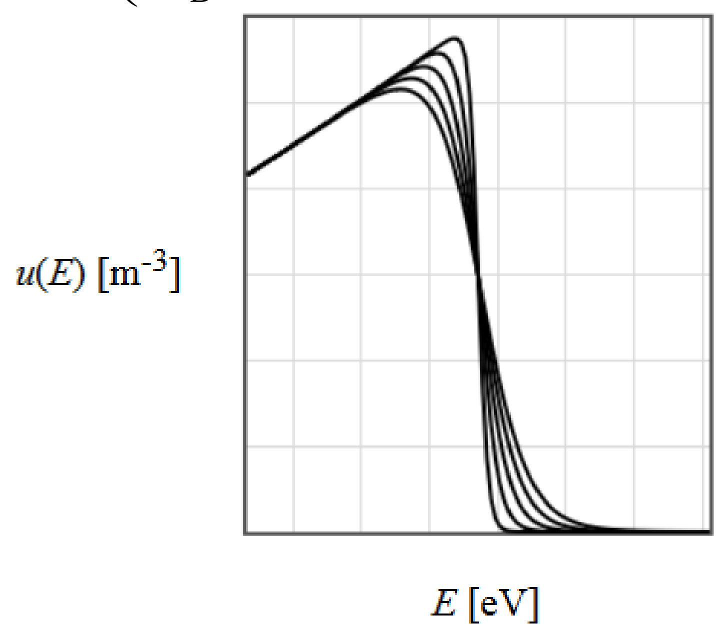
internal energy spectral density

$$u(E) = ED(E)f(E) = \frac{\pi}{2}\left(\frac{2m}{\hbar^2\pi^2}\right)^{3/2} \frac{1}{\exp\left(\frac{E-\mu}{k_B T}\right)+1} E^{\frac{3}{2}}$$

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

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

Not possible to do this integral analytically



analog to the Planck curve for electrons in 1-d

The free electron model is a one parameter model

	1-D Schrödinger equation for a free particle $i\hbar\frac{d\psi}{dt}=-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$	**2-D Schrödinger equation for a free particle** $i\hbar\frac{d\psi}{dt}=-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dx^2}+\frac{d^2\psi}{dy^2}\right)$	**3-D Schrödinger equation for a free particle** $i\hbar\frac{d\psi}{dt}=-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dx^2}+\frac{d^2\psi}{dy^2}+\frac{d^2\psi}{dz^2}\right)$
Eigenfunction solutions	$\psi_k=A_k\exp\left(i\left(kx-\omega t\right)\right)$	$\psi_k=A_{\vec{k}}\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)$	$\psi_k=A_{\vec{k}}\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)$
Eigenvalues of the translation operator $T\psi_k(\vec{r})=\psi_k(\vec{r}+\vec{R})=\lambda_k\psi_k(\vec{r})$	$\lambda_k=\exp\left(ikR\right)$	$\lambda_{\vec{k}}=\exp\left(i\vec{k}\cdot\vec{R}\right)$	$\lambda_{\vec{k}}=\exp\left(i\vec{k}\cdot\vec{R}\right)$
Dispersion relation	$E=\hbar\omega=\frac{\hbar^2k^2}{2m}$ J	$E=\hbar\omega=\frac{\hbar^2k^2}{2m}$ J	$E=\hbar\omega=\frac{\hbar^2k^2}{2m}$ J
Density of states	$D(k)=\frac{2}{\pi}$	$D(k)=\frac{k}{\pi}$ $\mathrm{m^{-1}}$	$D(k)=\frac{k^2}{\pi^2}$ $\mathrm{m^{-2}}$
Density of states $D(E)=D(k)\frac{dk}{dE}$	$D\left(E\right)=\frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}=\frac{n}{2\sqrt{E_FE}}$ $\mathrm{J^{-1}m^{-1}}$	$D\left(E\right)=\frac{m}{\pi\hbar^2}=\frac{n}{E_F}$ $\mathrm{J^{-1}m^{-2}}$	$D\left(E\right)=\frac{\left(2m\right)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E}=\frac{3n}{2E_F^{3/2}}\sqrt{E}$ $\mathrm{J^{-1}m^{-3}}$
Fermi energy E_F $n=\int_{-\infty}^{E_F}D(E)dE$	$E_F=\frac{\pi^2\hbar^2n^2}{8m}$ J	$E_F=\frac{\pi\hbar^2n}{m}$ J	$E_F=\frac{\hbar^2}{2m}\left(3\pi^2n\right)^{\frac{2}{3}}$ J
$D(E_F)$	$D\left(E_F\right)=\frac{4m}{\pi^2\hbar^2n}$ $\mathrm{J^{-1}m^{-1}}$	$D\left(E_F\right)=\frac{m}{\pi\hbar^2}$ $\mathrm{J^{-1}m^{-2}}$	$D\left(E_F\right)=\frac{m\left(3n\right)^{\frac{1}{3}}}{\pi^{\frac{4}{3}}\hbar^2}$ $\mathrm{J^{-1}m^{-3}}$
$D'(E_F)=\frac{dD}{dE}\Big\rvert_{E=E_F}$	$D'(E_F)=\frac{-16m^2}{\pi^4\hbar^4n^3}$ $\mathrm{J^{-2}m^{-1}}$	$D'(E_F)=0$ $\mathrm{J^{-2}m^{-2}}$	$D'(E_F)=\frac{m^2}{\hbar^4\sqrt[3]{3\pi^8n}}$ $\mathrm{J^{-2}m^{-3}}$
Chemical potential μ $n=\int_{-\infty}^{\infty}D(E)f(E)dE$	$\mu\approx E_F-\frac{\pi^2}{6}\left(k_BT\right)^2\frac{D'(E_F)}{D(E_F)}$ J $\approx\frac{\pi^2\hbar^2n^2}{8m}+\frac{2m}{3\hbar^2n^2}\left(k_BT\right)^2$ J	$\mu=k_BT\ln\left(\exp\left(\frac{E_F}{k_BT}\right)-1\right)$ J $=k_BT\ln\left(\exp\left(\frac{\pi\hbar^2n}{mk_BT}\right)-1\right)$ J	$\mu\approx E_F-\frac{\pi^2}{6}\left(k_BT\right)^2\frac{D'(E_F)}{D(E_F)}$ J $\approx\frac{\hbar^2}{2m}\left(3\pi^2n\right)^{\frac{2}{3}}-\frac{\pi^{\frac{2}{3}}m}{2\hbar^23^{\frac{10}{3}}n^{\frac{2}{3}}}\left(k_BT\right)^2$ J
Internal energy distribution $u\left(E\right)=E\frac{D(E)}{\exp\left(\frac{E-\mu}{k_BT}\right)+1}$	$u\left(E\right)=\frac{n}{2}\sqrt{\frac{E}{E_F}}\frac{1}{\exp\left(\frac{E-\mu}{k_BT}\right)+1}$ $\mathrm{m^{-1}}$ $=\frac{1}{\pi\hbar}\sqrt{2mE}\,\frac{1}{\left(E-\mu\right.\ldots}$ $\mathrm{m^{-1}}$	$u\left(E\right)=\frac{n}{E_F}\frac{E}{\exp\left(\frac{E-\mu}{k_BT}\right)+1}$ $\mathrm{m^{-2}}$ $=\frac{m}{\pi\hbar^2}\frac{E}{\left(E-\mu\right.\ldots}$ $\mathrm{m^{-2}}$	$u\left(E\right)=\frac{3n}{2}\left(\frac{E}{E_F}\right)^{3/2}\frac{1}{\exp\left(\frac{E-\mu}{k_BT}\right)+1}$ $\mathrm{m^{-3}}$ $=\frac{\frac{1}{2\pi^2\hbar^3}\left(2mE\right)^{3/2}}{\ldots}$ $\mathrm{m^{-3}}$