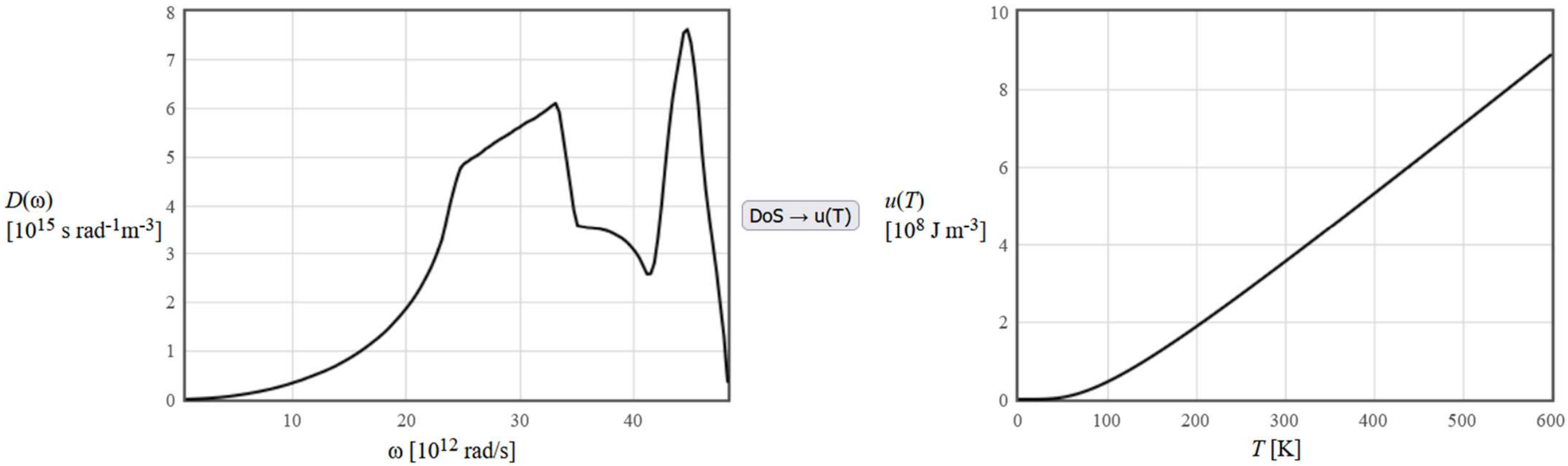
Phonons / Electrons

Density of states → Internal energy density

$$u(T) = \int_0^\infty \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} d\omega$$



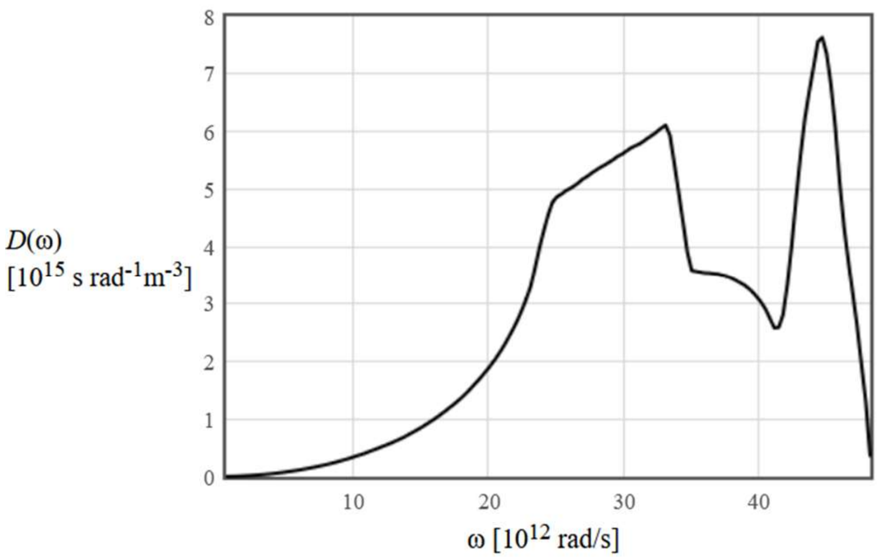
http://lampx.tugraz.at/~hadley/ss1/phonons/table/dos2ut.html

Specific Heat

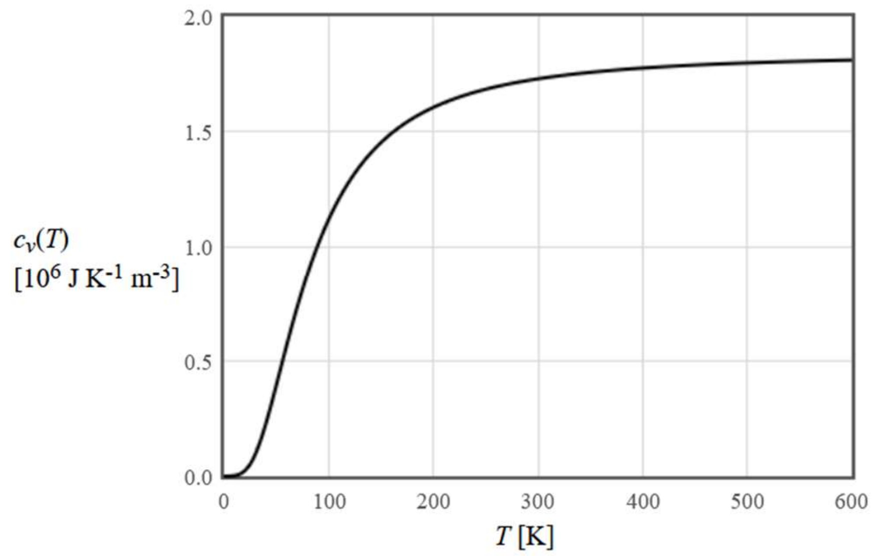
$$c_v = \left(\frac{\partial u}{\partial T}\right)_{N,V}$$

$$c_v = \int \hbar\omega D(\omega)\frac{\partial}{\partial T}\left(\frac{1}{e^{\frac{\hbar\omega}{k_BT}}-1}\right)d\omega$$

$$c_v = \int \left(\frac{\hbar\omega}{T}\right)^2 \frac{D(\omega)e^{\frac{\hbar\omega}{k_BT}}}{k_B\left(e^{\frac{\hbar\omega}{k_BT}}-1\right)^2}d\omega$$



DoS → cv(T)



http://lampx.tugraz.at/~hadley/ss1/phonons/table/dos2cv.html

Heat capacity / specific heat

Heat capacity is the measure of the heat energy required to increase the temperature of an object by a certain temperature interval.

Specific heat is the measure of the heat energy required to increase the temperature of a unit quantity of a substance by a certain temperature interval.

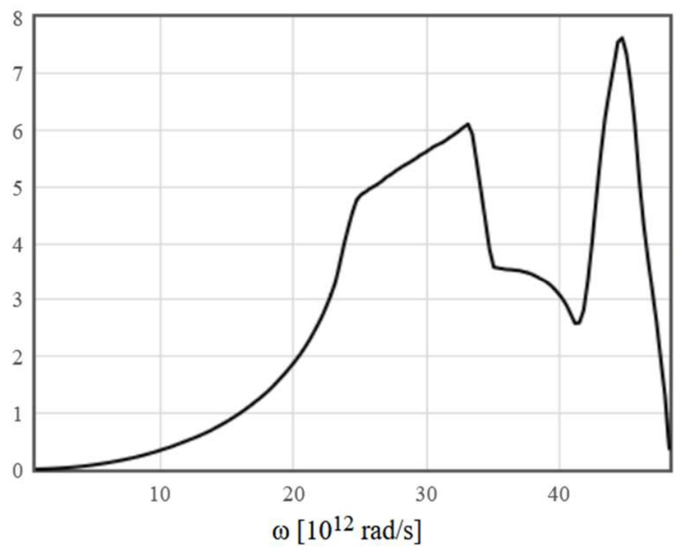
For solids, the heat capacity at constant volume and heat capacity at constant pressure are almost the same.

The heat capacity was historically important for understanding solids.

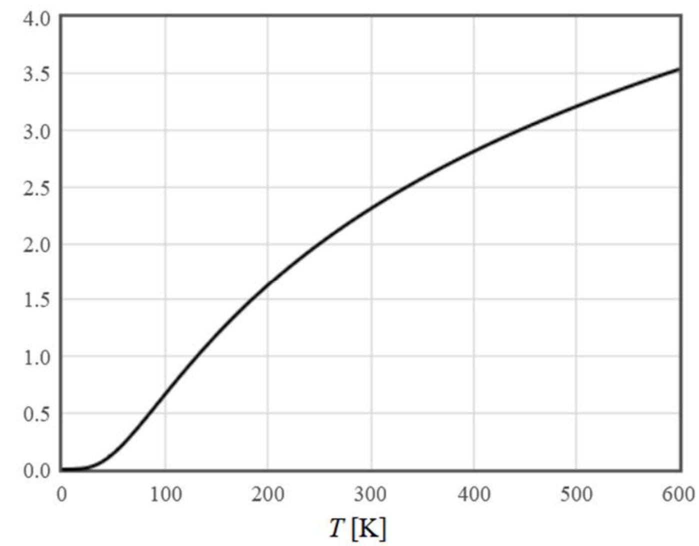
Density of states → entropy density

$$s = \int \frac{c_v}{T} dT$$

$$s = -\frac{\partial f}{\partial T} = -k_B \int_0^\infty D(\omega) \left(\ln\left(1 - e^{-\hbar\omega/k_BT}\right) + \frac{\hbar\omega}{k_BT\left(1 - e^{\hbar\omega/k_BT}\right)} \right) d\omega$$



DoS → s(T)



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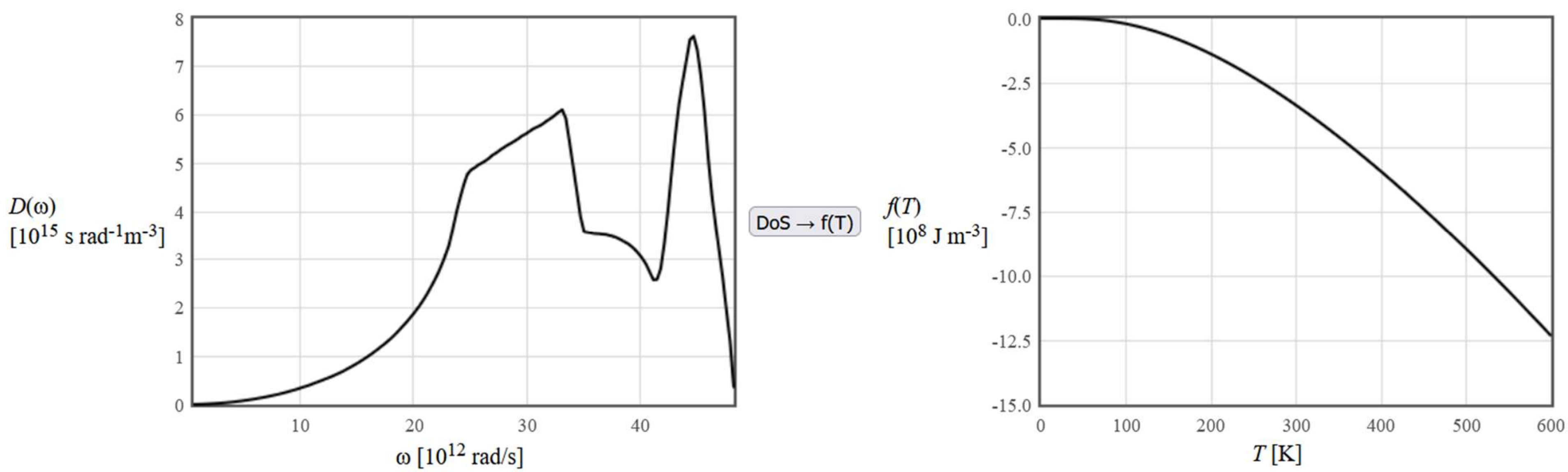
Density of states →
Helmholtz free energy density

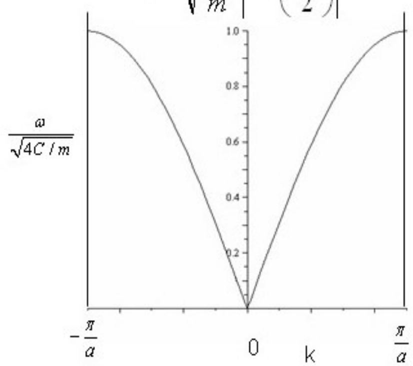
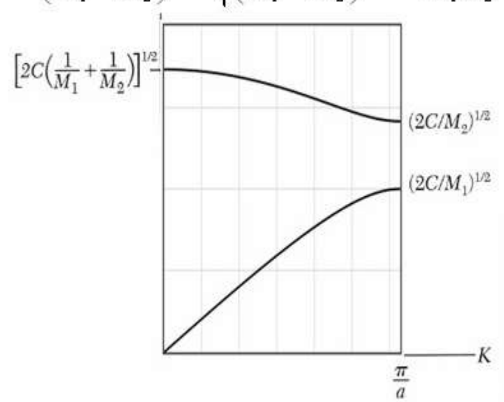
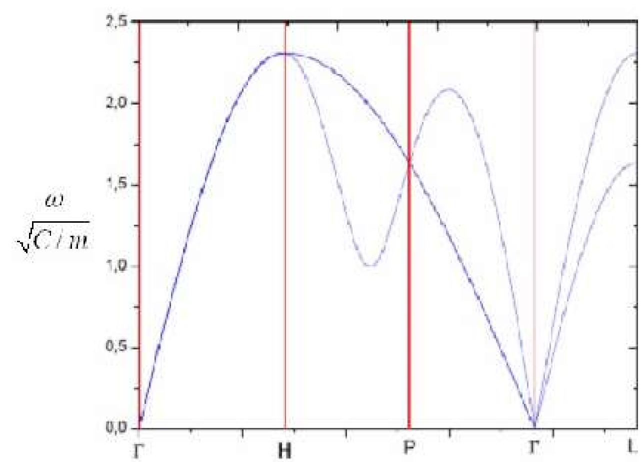
$$f(T) = k_B T \int_0^{\infty} D(\omega) \ln\left(1 - \exp\left(\frac{-\hbar\omega}{k_B T}\right)\right) d\omega.$$

$$f = u - Ts$$



http://lampx.tugraz.at/~hadley/ss1/phonons/table/dos2h.html

Phonons

	Linear Chain $m\frac{d^2u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1})$	Linear chain 2 masses $M_1\frac{d^2u_s}{dt^2} = C(v_{s-1} - 2u_s + v_s)$ $M_2\frac{d^2v_s}{dt^2} = C(u_s - 2v_s + u_{s+1})$	body centered cubic $\frac{d^2u^x_{lmn}}{dt^2} = \frac{C}{\sqrt{3}\,m}[(u^x_{l+1m+1n+1} - u^x_{lmn}) + (u^x_{l-1m+1n+1} - u^x_{l\ldots}$ $+(u^x_{l+1m-1n+1} - u^x_{lmn}) + (u^x_{l+1m+1n-1} - u^x_{lmn}) + (u^x_{l-1m+\ldots}$ $+(u^x_{l+1m-1n-1} - u^x_{lmn}) + (u^y_{l+1m+1n+1} - u^y_{lmn}) - (u^y_{l-1m+\ldots}$ $+(u^y_{l+1m-1n+1} - u^y_{lmn}) - (u^y_{l+1m+1n-1} - u^y_{lmn}) + (u^y_{l-1m+\ldots}$ $+(u^y_{l+1m-1n-1} - u^y_{lmn}) + (u^z_{l+1m+1n+1} - u^z_{lmn}) - (u^z_{l-1m+\ldots}$ $+(u^z_{l+1m-1n+1} - u^z_{lmn}) - (u^z_{l+1m+1n-1} - u^z_{lmn}) + (u^z_{l-1m+\ldots}$ $-(u^z_{l+1m-1n-1} - u^z_{lmn})]$ And similar expressions for the *y* and *z* (
Eigenfunction solutions	$u_s = A_k e^{i(ksa - \omega t)}$	$u_s = ue^{i(ksa-\omega t)}$ $v_s = ve^{i(ksa-\omega t)}$	$u^x_{lmn} = u^x_{\vec{k}} e^{i(l\vec{k}\cdot\vec{a_1} + m\vec{k}\cdot\vec{a_2} + n\vec{k}\cdot\vec{a_3})} = u^x_{\vec{k}} e^{i(\frac{(-l\ldots}{}}$ And similar expressions for the *y* and *z* (
Dispersion relation	$\omega = \sqrt{\frac{4C}{m}}\left\|\sin\left(\frac{ka}{2}\right)\right\|$ 	$\omega^2 = C\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2\left(\frac{ka}{2}\right)}{M_1M_2}}$  Calculate ω(k)	The dispersio $\begin{bmatrix} 4 - \cos(\frac{a}{2}(k_x + k_y + k_z)) - \cos(\frac{a}{2}(3k_x - k_y - k_z)) & -\cos(\frac{a}{2}(k_x + k_y \ldots \\ -\cos(\frac{a}{2}(-k_x + 3k_y - k_z)) - \cos(\frac{a}{2}(-k_x - k_y + 3k_z)) - \frac{m\omega^2}{\sqrt{3}C} & +\cos(\frac{a}{2}(-k_x + 3 \ldots \\ -\cos(\frac{a}{2}(k_x + k_y + k_z)) + \cos(\frac{a}{2}(3k_x - k_y - k_z)) & 4 - \cos(\frac{a}{2}(k_x + \ldots \\ +\cos(\frac{a}{2}(-k_x + 3k_y - k_z)) - \cos(\frac{a}{2}(-k_x - k_y + 3k_z)) & -\cos(\frac{a}{2}(-k_x + 3 \ldots \\ -\cos(\frac{a}{2}(k_x + k_y + k_z)) + \cos(\frac{a}{2}(3k_x - k_y - k_z)) & -\cos(\frac{a}{2}(k_x + k_y \ldots \\ -\cos(\frac{a}{2}(-k_x + 3k_y - k_z)) + \cos(\frac{a}{2}(-k_x - k_y + 3k_z)) & +\cos(\frac{a}{2}(-k_x + 3 \ldots \end{bmatrix}$ 
Density of states $D(k)$	$D(k) = \frac{1}{\pi}$	$D(k) = \frac{1}{\pi}$	$D(k) = \frac{3k^2}{2\pi^2}$

Thermal properties

internal energy density $u = \int_0^\infty u(\omega) d\omega = \int_0^\infty \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} d\omega \quad \left[\text{J/m}^3\right]$

specific heat $c_v = \frac{du}{dT} = \int \left(\frac{\hbar\omega}{T}\right)^2 \frac{D(\omega)\exp\left(\frac{\hbar\omega}{k_B T}\right)}{k_B\left(\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1\right)^2} d\omega \quad [\text{J K}^{-1}\ \text{m}^{-3}]$

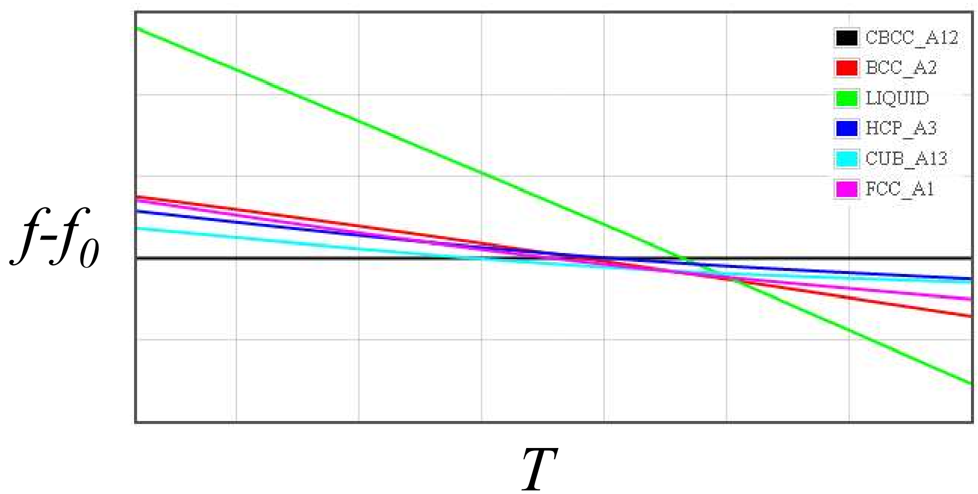
entropy density $s(T) = \int \frac{c_v}{T} dT = \frac{1}{T}\int_0^\infty \frac{\hbar\omega D(\omega)}{\exp\left(\frac{\hbar\omega}{k_B T}\right) - 1} d\omega \quad [\text{J K}^{-1}\ \text{m}^{-3}]$

Helmholtz free energy density

$$f(T) = u - Ts = k_B T \int_0^\infty D(\omega) \ln\left(1 - \exp\left(\frac{-\hbar\omega}{k_B T}\right)\right) d\omega \quad \left[\text{J/m}^3\right]$$

Quartz

α-Quartz
trigonal
2.65 g/cm³ $\rightarrow$ 573°C $\rightarrow$ β-Quartz
hexagonal
2.53 g/cm3 $\rightarrow$ 870°C $\rightarrow$ β-Tridymite
hexagonal
2.25 g/cm³ $\rightarrow$ 1470°C $\rightarrow$ β-Cristobalite
cubic
2.20 g/cm3 $\rightarrow$ 1705°C $\rightarrow$ Silica Melt



Electrons

Free particles in 1-d

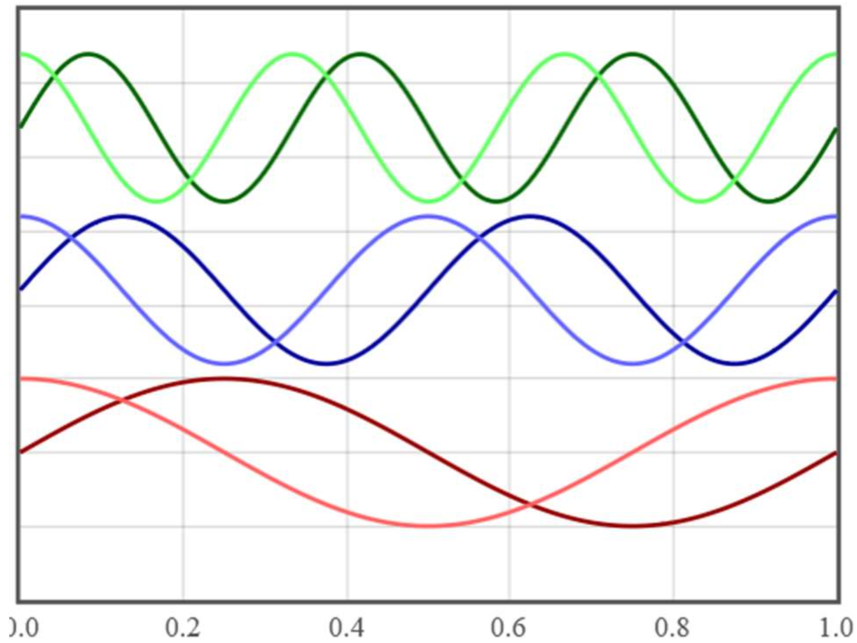
Fill the electrons states like in an atom.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

$$V(x) = 0$$

$$\psi_k = \frac{e^{i(kx-\omega t)}}{\sqrt{L}}$$

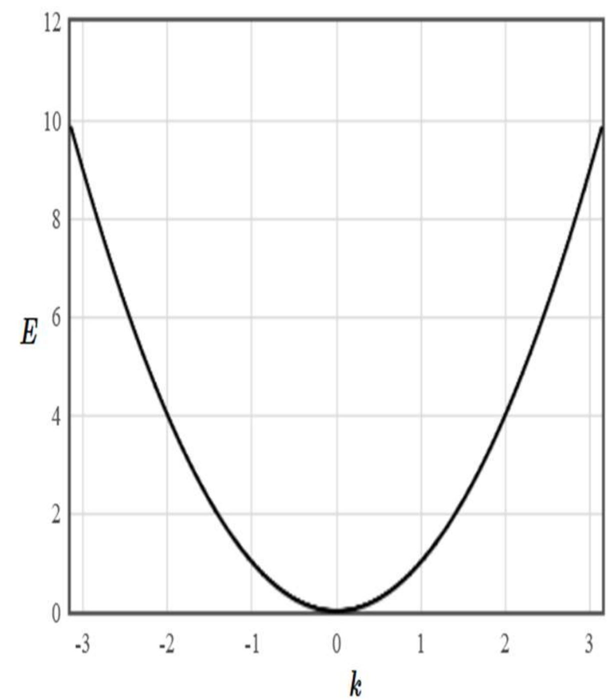
$$\psi_k{}^{*}\psi_k = \frac{1}{L}$$



Free particles in 1-d

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

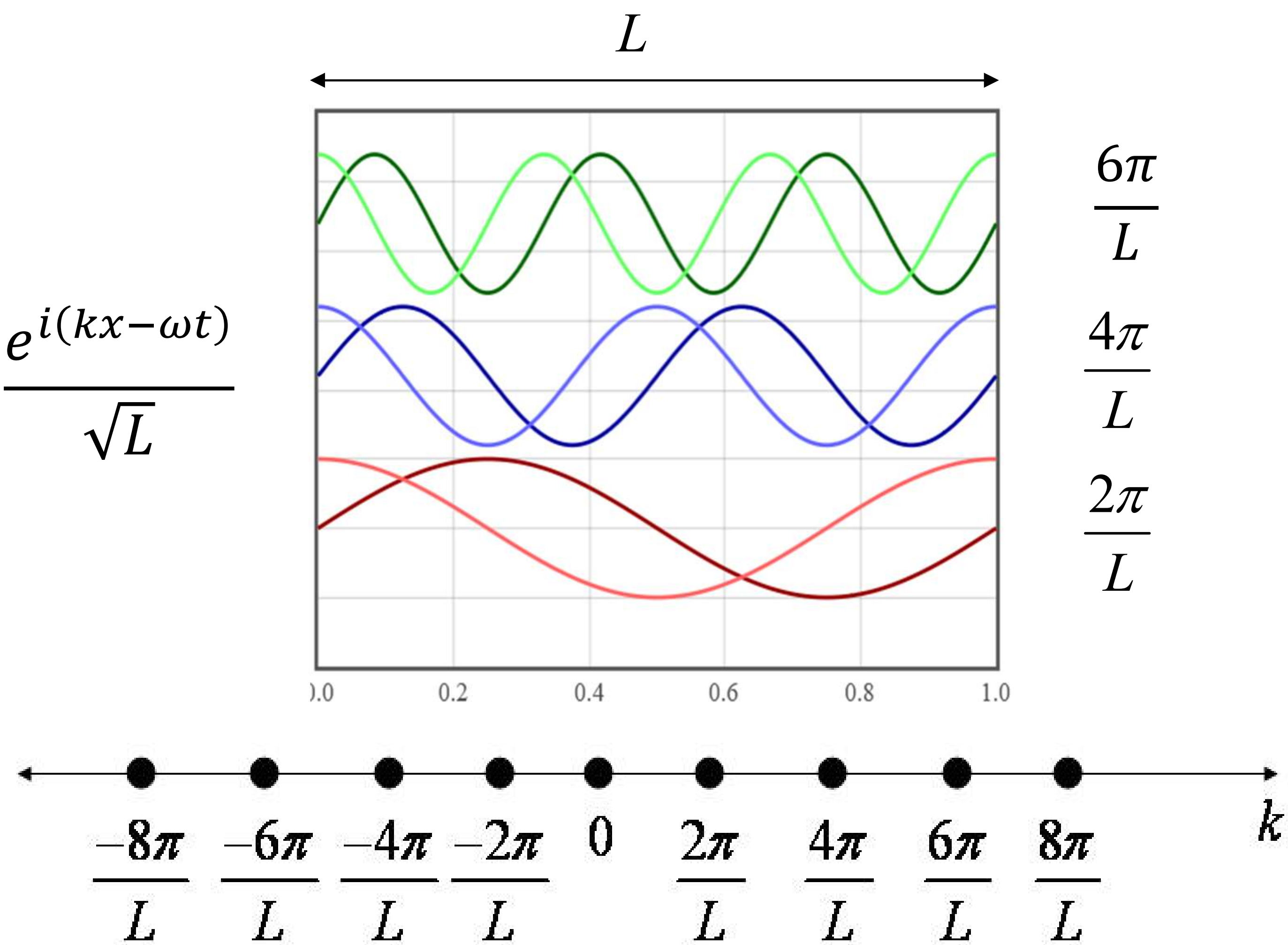
Eigen function solutions: $\psi_k = \dfrac{e^{i(kx-\omega t)}}{\sqrt{L}}$



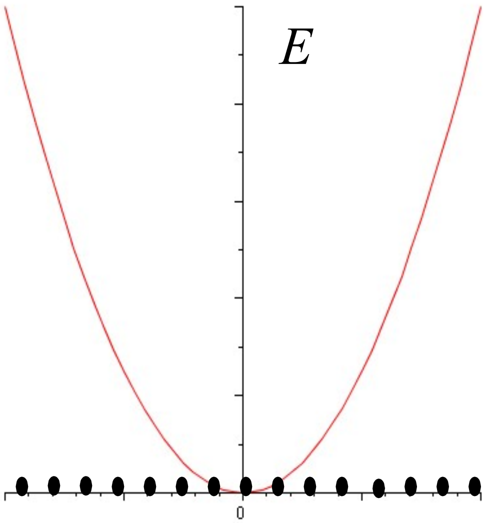
Dispersion relation: $E = \hbar\omega = \dfrac{\hbar^2 k^2}{2m} = \dfrac{1}{2}mv^2$

Periodic boundary conditions

$$\psi_k = \frac{e^{i(kx-\omega t)}}{\sqrt{L}}$$



Free particles in 1-d

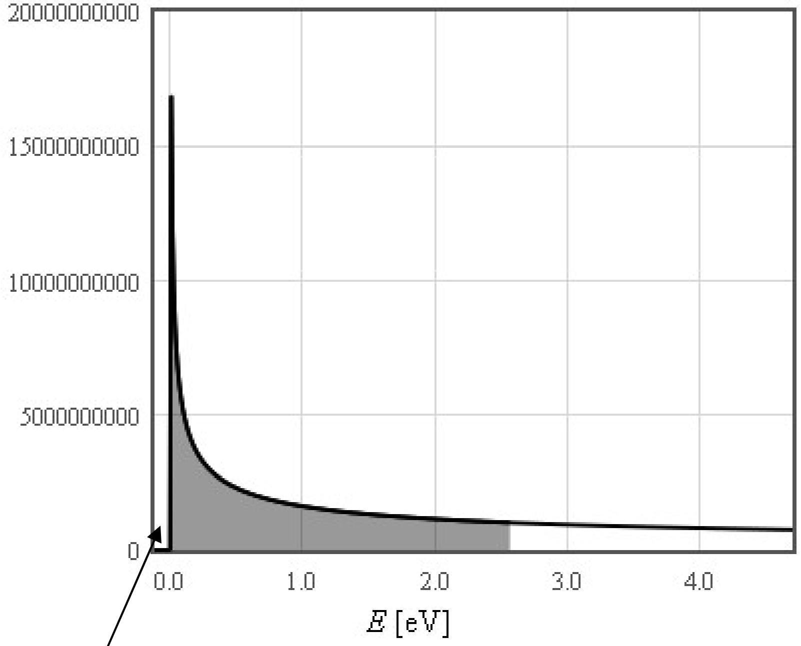


E

k

Density of states

$D(E)$



E

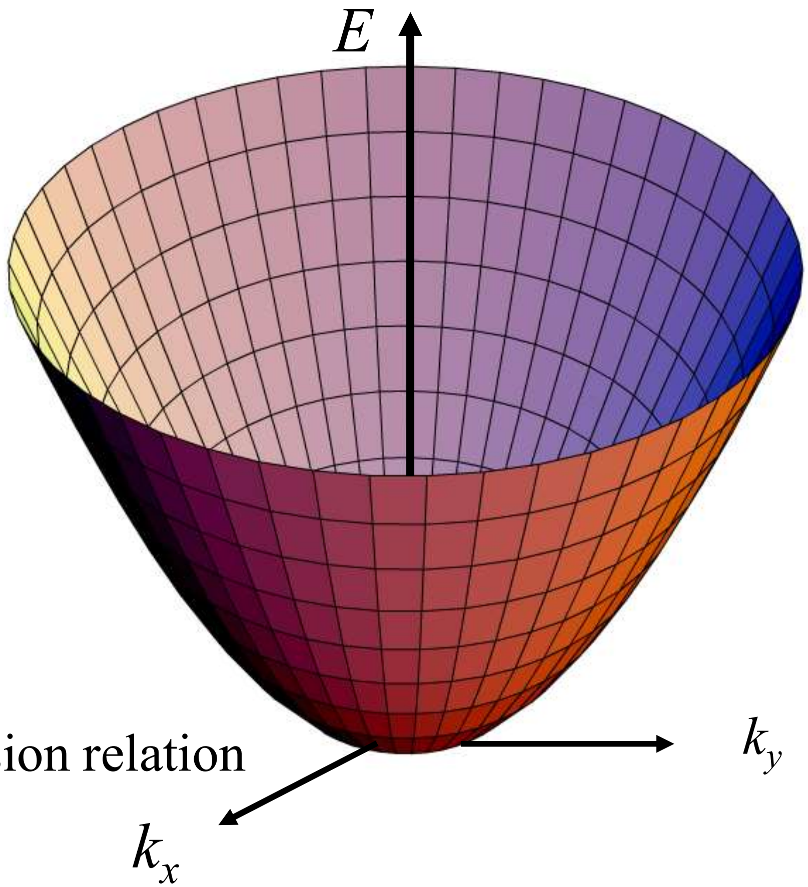
Van Hove singularity

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

free electrons (simple model for a metal)

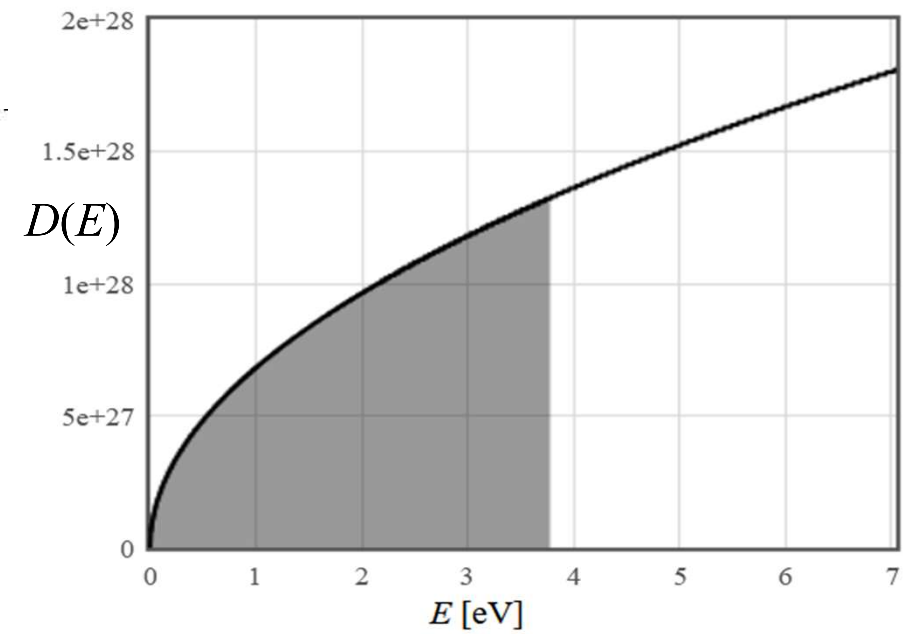
$$\vec{p} = \hbar \vec{k}$$

$$E(\vec{k}) = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$$



dispersion relation

3-d density of states

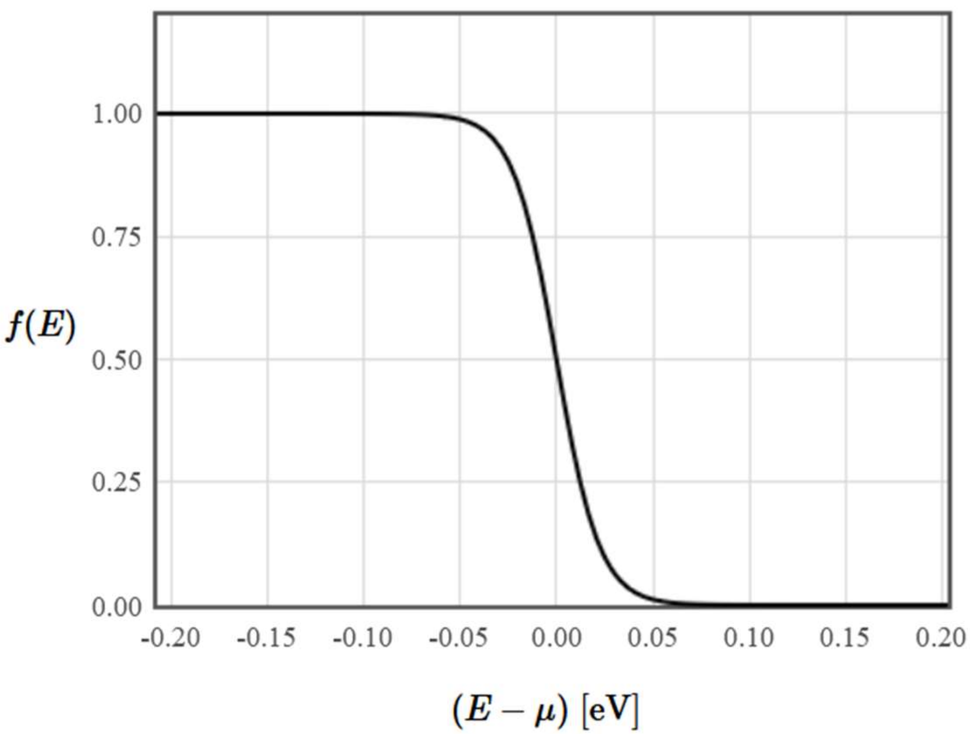


$$D(E) = \begin{cases} 0 & \text{for} \quad E < 0 \\ \dfrac{(2m)^{3/2}}{2\pi^2\hbar^3}\sqrt{E} & \text{for} \quad E > 0 \end{cases}$$

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

http://lampx.tugraz.at/~hadley/ss1/materials/thermo/gp/gp/Fermi-function.html

Chemical potential

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

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

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

Here n is the electron density.

Fermi energy

In solid state physics books,

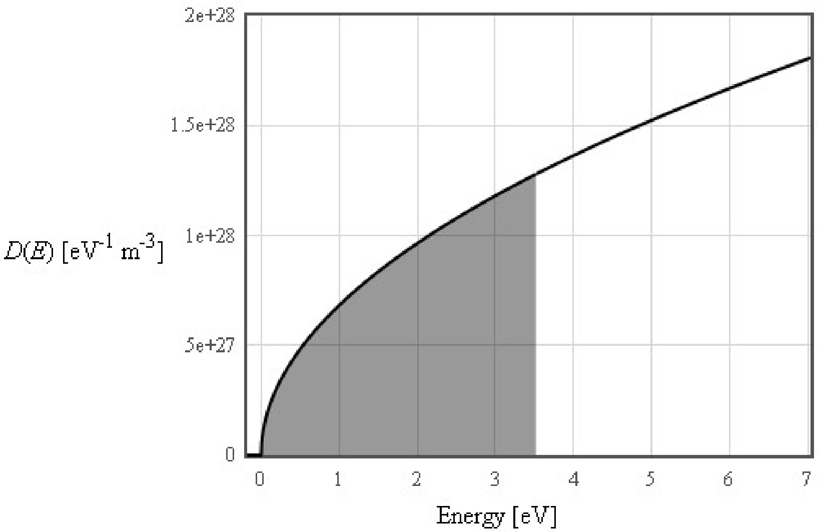
$$E_F = \mu(T=0).$$

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

At $T = 0$

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

Free particles in 3-d



At $T = 0$:

$$n = \int_0^{E_F} D(E)\,dE$$

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

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

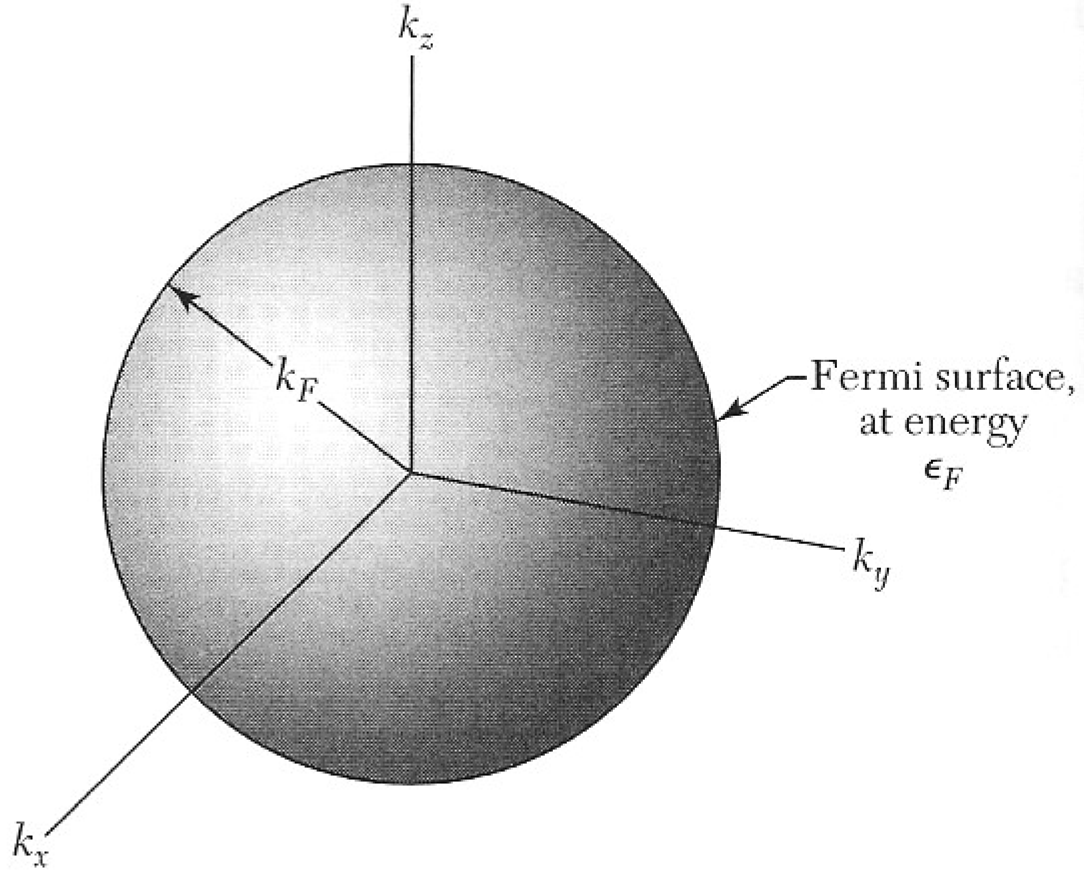
Fermi sphere

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

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.

Internal energy density at T = 0

$$u = \int_{-\infty}^{\infty} E D(E) dE = \int_{0}^{E_f} E D(E) dE$$

$$D(E) = \frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E} \quad \mathrm{J^{-1}\,m^{-3}}$$

$$u = \int_{0}^{E_f} \frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3} E^{3/2} dE = \frac{(2m)^{\frac{3}{2}}}{5\pi^2\hbar^3} E_f^{\frac{5}{2}}$$

$$E_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3} \qquad u(T=0) = \frac{3}{5} n E_F$$

$$u(T=0) = \frac{\pi^{\frac{4}{3}}\hbar^2}{10m}(3n)^{\frac{5}{3}} = \frac{\pi^{\frac{4}{3}}\hbar^2}{10m}\left(\frac{3N}{V}\right)^{\frac{5}{3}}$$