

# Free electron Fermi gas

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Kittel, chapter 6

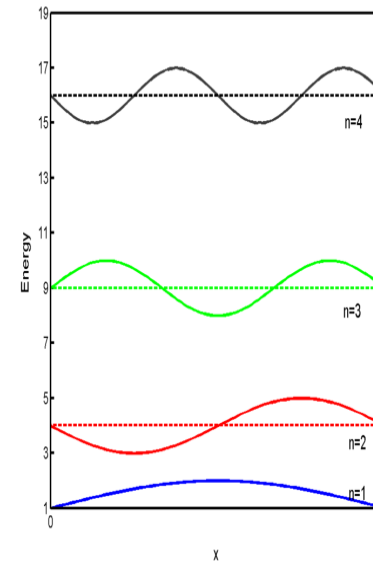
A simple model for a metal is electrons confined to box with periodic boundary conditions.

# Free particles in 1-d

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

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



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

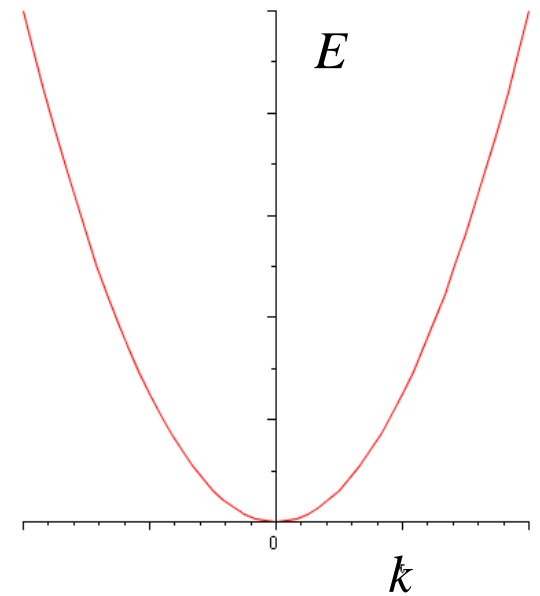
# Free particles

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

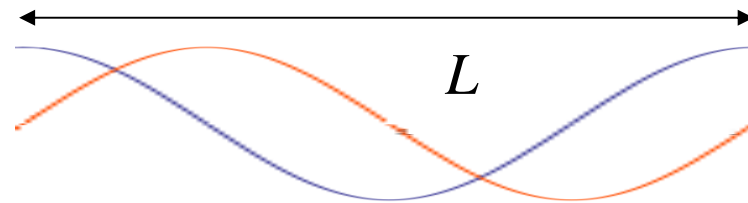
Eigen function solutions:  $\psi_k = A_k e^{i(kx - \omega t)}$

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

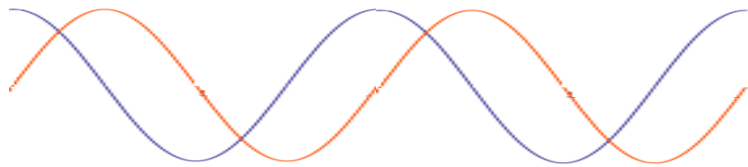


# Periodic boundary conditions

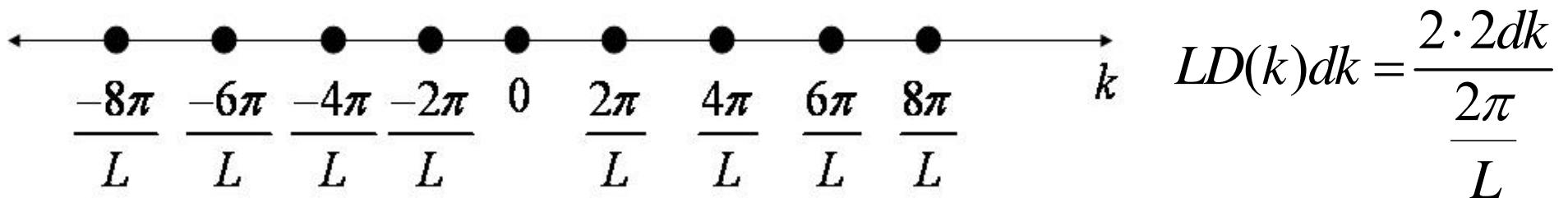
$$\psi = A_k e^{i(kx - \omega t)}$$



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



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



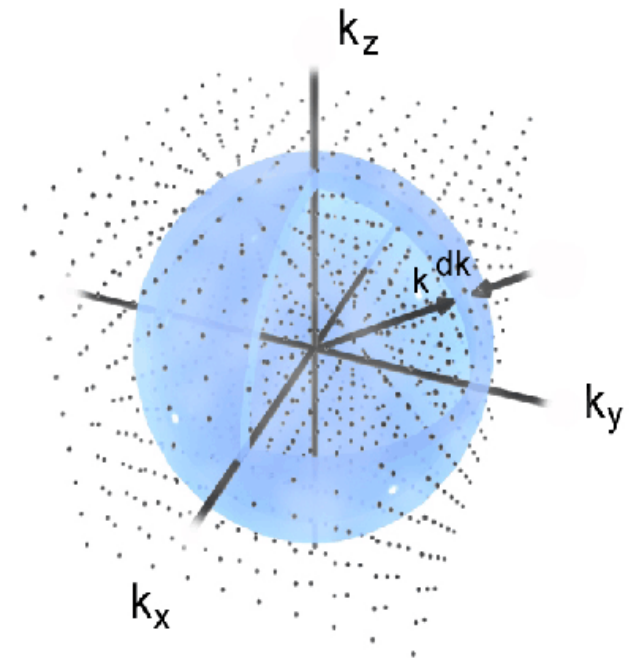
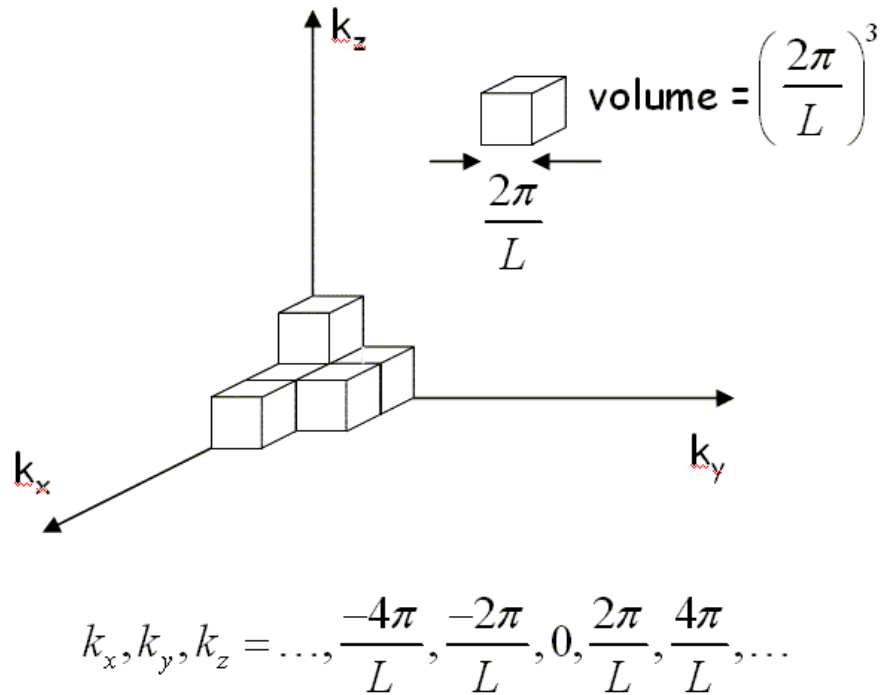
Density of states:

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

Spin

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

# Density of states



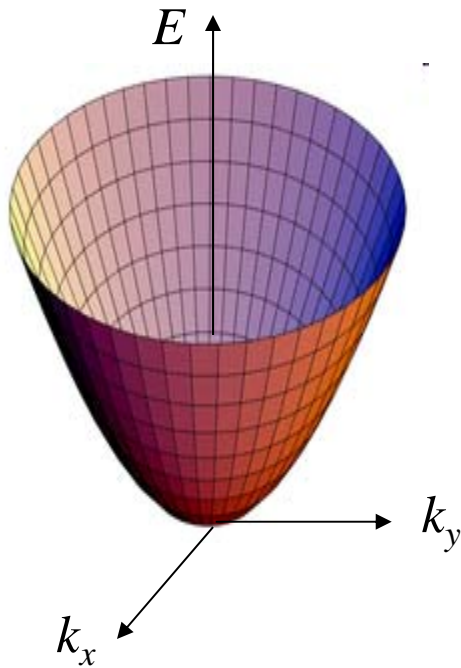
Number of states  
 between  $k$  and  $k+dk$  =  $2 \frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3} = \frac{k^2 L^3}{\pi^2} dk = L^3 D(k) dk$   
 for a box of size  $L^3$ .

spin

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

# Free particles in 3-d

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



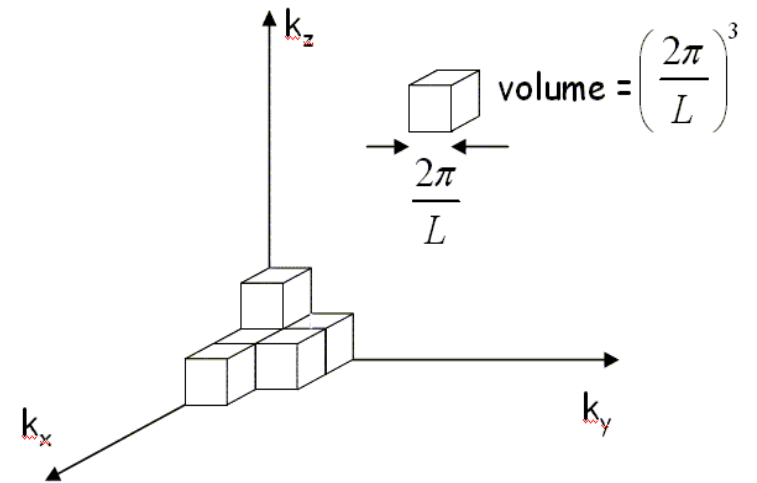
Density of states

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

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

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

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



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

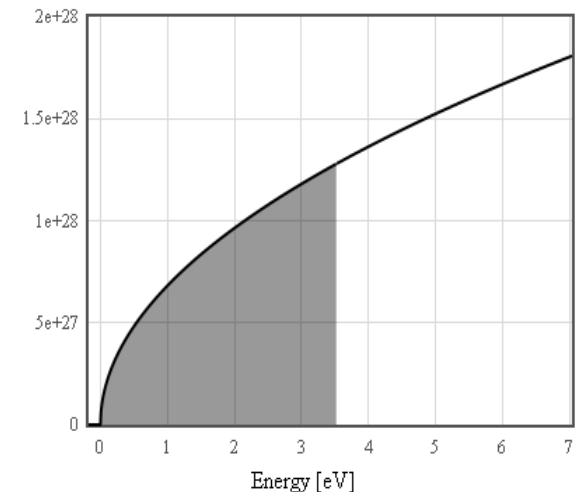
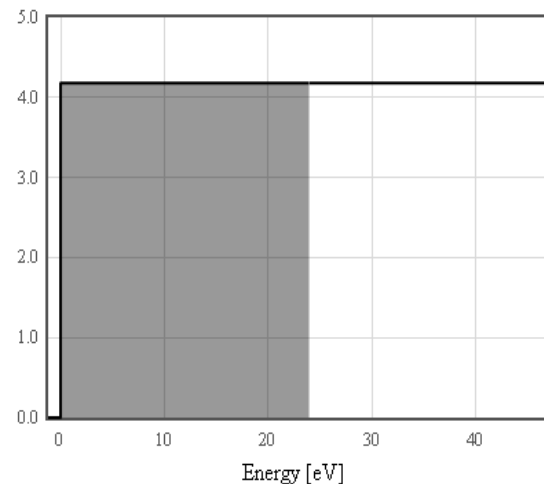
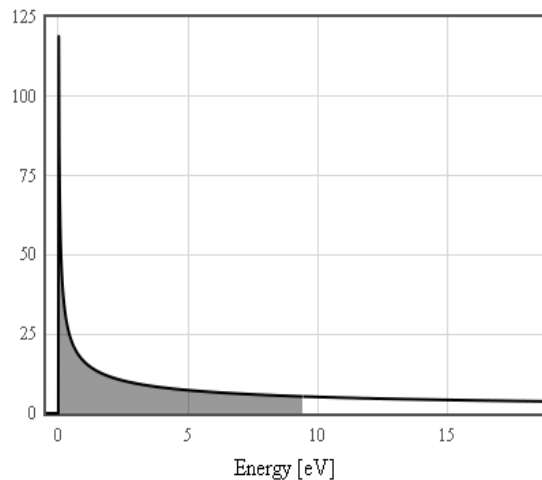
$$D(E) = \frac{(2m)^{\frac{3}{2}}}{2\pi^2 \hbar^3} \sqrt{E}$$

# Free electron Fermi gas

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

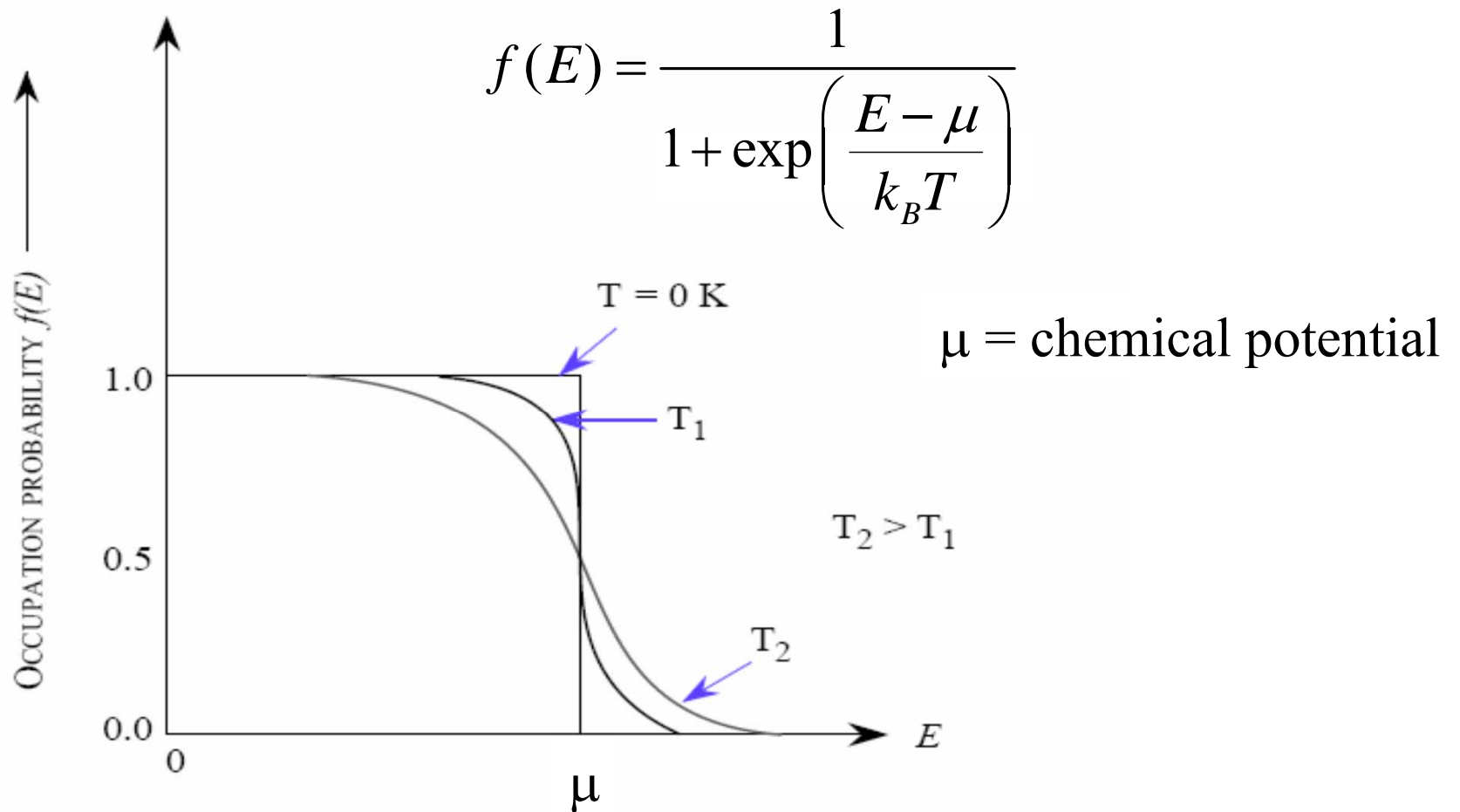
$$2 - d \quad D(E) = \frac{m}{\hbar^2 \pi} = \frac{n}{E_F} \quad \text{J}^{-1} \text{m}^{-2}$$

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



# Fermi function

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





# Fermi energy

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In solid state physics books,

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

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

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

In three dimensions,

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

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

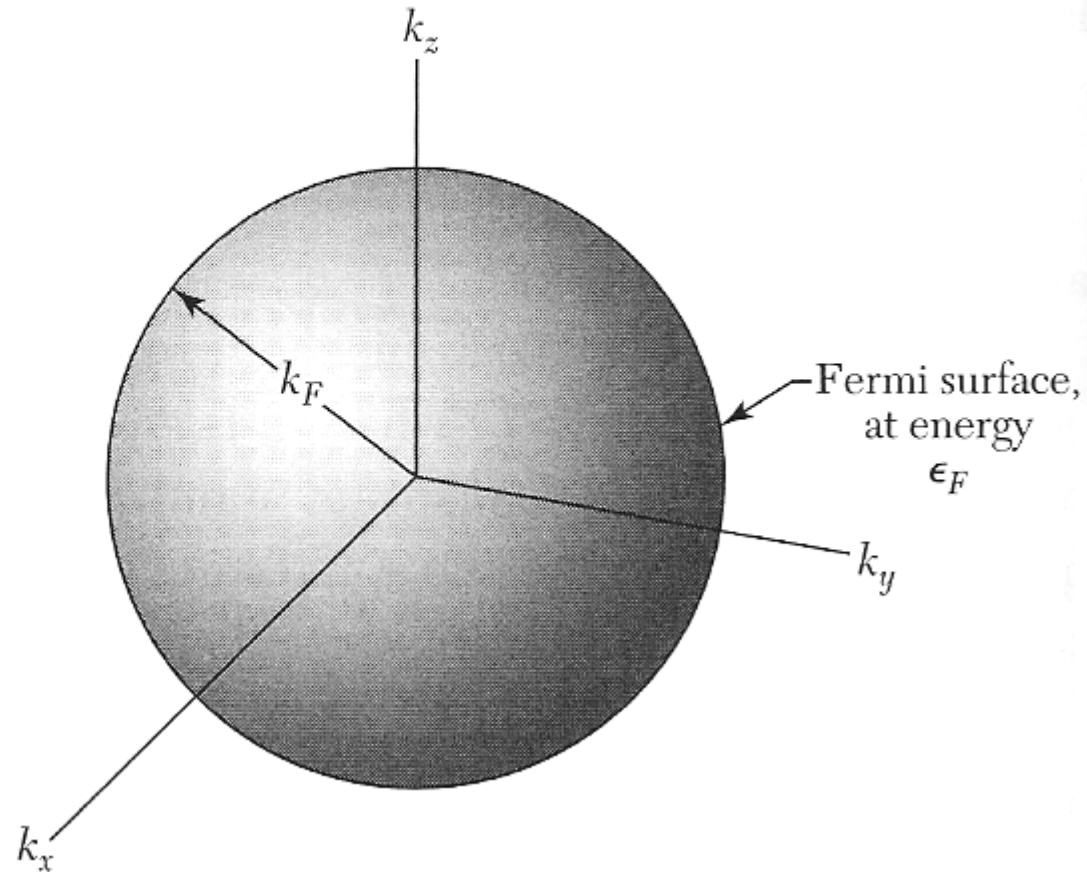
# Fermi sphere

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

spin

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

$n$  = electron density



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

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

# Free particles in 1-d

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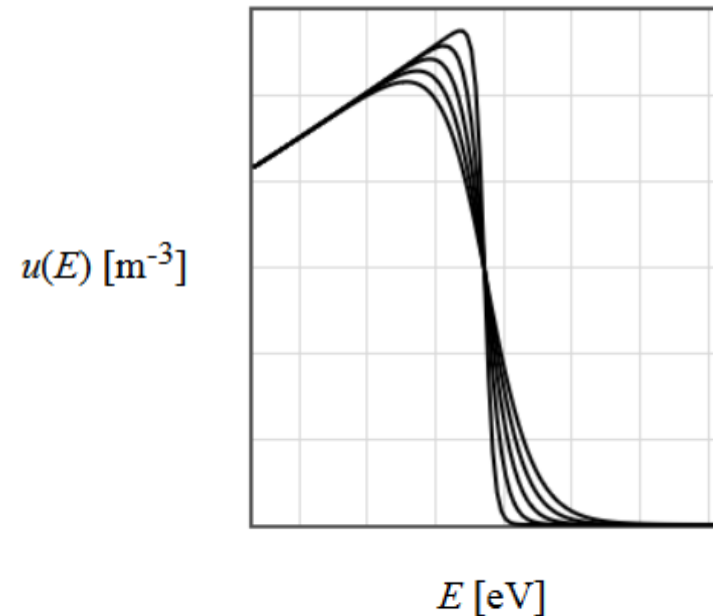
internal energy spectral density

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

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

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

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	$\psi_k = A_k \exp(i(kx - \alpha t))$	$\psi_k = A_k \exp(i(\vec{k} \cdot \vec{r} - \alpha t))$	$\psi_k = A_k \exp(i(\vec{k} \cdot \vec{r} - \alpha t))$
Eigenvalues of the translation operator $T\psi_k(\vec{r}) = \psi_k(\vec{r} + \vec{R}) = \lambda_k \psi_k(\vec{r})$	$\lambda_k = \exp(ikR)$	$\lambda_{\vec{k}} = \exp(i\vec{k} \cdot \vec{R})$	$\lambda_{\vec{k}} = \exp(i\vec{k} \cdot \vec{R})$
Dispersion relation	$E = \hbar\omega = \frac{\hbar^2 k^2}{2m} \quad \text{J}$	$E = \hbar\omega = \frac{\hbar^2 k^2}{2m} \quad \text{J}$	$E = \hbar\omega = \frac{\hbar^2 k^2}{2m} \quad \text{J}$
Density of states	$D(k) = \frac{2}{\pi}$	$D(k) = \frac{k}{\pi} \quad \text{m}^{-1}$	$D(k) = \frac{k^2}{\pi^2} \quad \text{m}^2$
Density of states $D(E) = D(k) \frac{dk}{dE}$	$D(E) = \frac{1}{\pi\hbar} \sqrt{\frac{2m}{E}} = \frac{n}{2\sqrt{E_F E}} \quad \text{J}^{-1}\text{m}^{-1}$	$D(E) = \frac{m}{\pi\hbar^2} = \frac{n}{E_F} \quad \text{J}^{-1}\text{m}^{-2}$	$D(E) = \frac{(2m)^{3/2}}{2\pi^2\hbar^3} \sqrt{E} = \frac{3n}{2E_F^{3/2}} \sqrt{E} \quad \text{J}^{-1}\text{m}^{-3}$
Fermi energy $E_F$ $n = \int_{-\infty}^{E_F} D(E) dE$	$E_F = \frac{\pi^2 \hbar^2 n^2}{8m} \quad \text{J}$	$E_F = \frac{\pi \hbar^2 n}{m} \quad \text{J}$	$E_F = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} \quad \text{J}$
$D(E_F)$	$D(E_F) = \frac{4m}{\pi^2 \hbar^2 n} \quad \text{J}^{-1}\text{m}^{-1}$	$D(E_F) = \frac{m}{\pi \hbar^2} \quad \text{J}^{-1}\text{m}^{-2}$	$D(E_F) = \frac{m(3n)^{1/3}}{\pi^3 \hbar^2} \quad \text{J}^{-1}\text{m}^{-3}$
$D'(E_F) = \frac{dD}{dE} \Big _{E=E_F}$	$D'(E_F) = \frac{-16m^2}{\pi^4 \hbar^4 n^3} \quad \text{J}^2\text{m}^{-1}$	$D'(E_F) = 0 \quad \text{J}^2\text{m}^{-2}$	$D'(E_F) = \frac{m^2}{\hbar^4 \sqrt[3]{3\pi^8 n}} \quad \text{J}^2\text{m}^{-3}$
Chemical potential $\mu$ $n = \int_{-\infty}^{\mu} D(E) f(E) dE$	$\mu \approx E_F - \frac{\pi^2}{6} (k_B T)^2 \frac{D'(E_F)}{D(E_F)} \quad \text{J}$ $\approx \frac{\pi^2 \hbar^2 n^2}{8m} + \frac{2m}{3\hbar^2 n^2} (k_B T)^2 \quad \text{J}$	$\mu = k_B T \ln \left( \exp \left( \frac{E_F}{k_B T} \right) - 1 \right) \quad \text{J}$ $= k_B T \ln \left( \exp \left( \frac{\pi \hbar^2 n}{m k_B T} \right) - 1 \right) \quad \text{J}$	$\mu \approx E_F - \frac{\pi^2}{6} (k_B T)^2 \frac{D'(E_F)}{D(E_F)} \quad \text{J}$ $\approx \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} - \frac{\pi^2 m}{2\hbar^2 3^{1/3} n^{1/3}} (k_B T)^2 \quad \text{J}$
Internal energy distribution $u(E) = E \frac{D(E)}{\exp \left( \frac{E - \mu}{k_B T} \right) + 1}$	$u(E) = \frac{n}{2} \sqrt{\frac{E}{E_F}} \frac{1}{\exp \left( \frac{E - \mu}{k_B T} \right) + 1} \quad \text{m}^{-1}$ $= \frac{1}{\pi \hbar} \sqrt{2mE} \frac{1}{(E - \mu)} \quad \text{m}^{-1}$	$u(E) = \frac{n}{E_F} \frac{E}{\exp \left( \frac{E - \mu}{k_B T} \right) + 1} \quad \text{m}^{-2}$ $= \frac{m}{\pi \hbar^2} \frac{E}{(E - \mu)} \quad \text{m}^{-2}$	$u(E) = \frac{3n}{2} \left( \frac{E}{E_F} \right)^{3/2} \frac{1}{\exp \left( \frac{E - \mu}{k_B T} \right) + 1} \quad \text{m}^{-3}$ $= \frac{1}{2\pi^2 \hbar^3} (2mE)^{3/2} \quad \text{m}^{-3}$