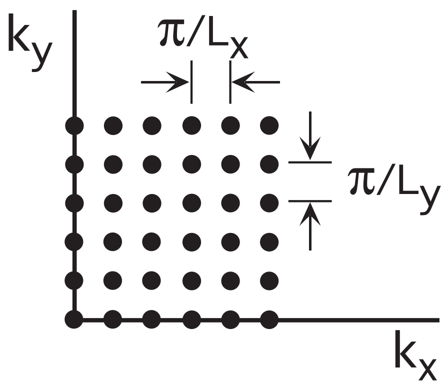
Particle in a Box

$0 < x < L_x, \quad 0 < y < L_y, \quad 0 < z < L_z$

$$\psi_{k_x,k_y,k_z}(\vec{r}) \propto \sin k_x x \sin k_y y \sin k_z z$$

$$\sin k_x L_x = 0 \Rightarrow k_x = n_x \left(\frac{\pi}{L_x}\right) \quad n_x = 1, 2, 3, \cdots$$



$$D(\vec{k})_{\text{wavevectors}} = \frac{L_x}{\pi}\frac{L_y}{\pi}\frac{L_z}{\pi} = \frac{V}{\pi^3}$$

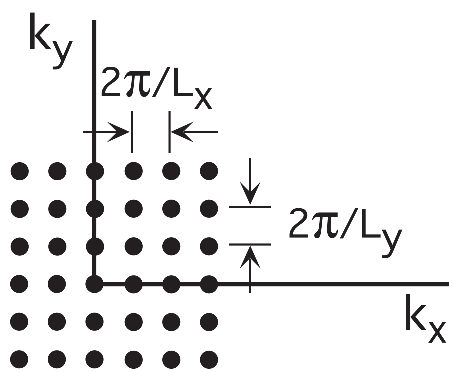
$$D(\vec{k})_{\text{states}} = (2S+1)\frac{V}{\pi^3}$$

<u>Plane Wave</u> $\psi_{\vec{k}}(\vec{r}) \propto \exp[i\vec{k}\cdot\vec{r}]$

Periodic Boundary Conditions

$$\psi_{\vec{k}}(\vec{r}+m_xL_x\hat{x}+m_yL_y\hat{y}+m_zL_z\hat{z}) = \psi_{\vec{k}}(\vec{r})$$

$$e^{ik_x(x+m_xL_x)} = e^{ik_xx} \Rightarrow k_x = n_x\left(\frac{2\pi}{L_x}\right) \quad n_x = \pm 1, \pm 2, \pm 3, \cdots$$



$$D(\vec{k})_{\text{wavevectors}} = \frac{L_x}{2\pi}\frac{L_y}{2\pi}\frac{L_z}{2\pi} = \frac{V}{(2\pi)^3}$$

$$D(\vec{k})_{\text{states}} = (2S+1)\frac{V}{(2\pi)^3}$$

The # of wavevectors with $|\vec{k}'| < k$ is the same in both cases.

$$\#_{\text{wavevectors}}(k) = \frac{1}{8}\left(\frac{4}{3}\pi k^3\right)\frac{V}{\pi^3} = \left(\frac{4}{3}\pi k^3\right)\frac{V}{(2\pi)^3}$$

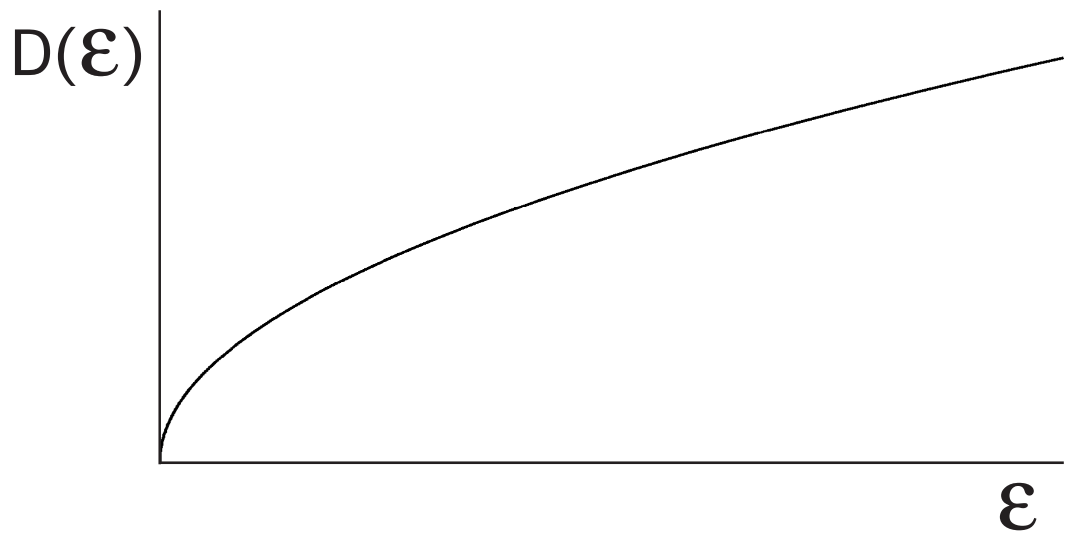
For free particles; $\epsilon = \dfrac{\hbar^2 k^2}{2m} \rightarrow k(\epsilon) = \sqrt{\dfrac{2m}{\hbar^2}}\sqrt{\epsilon}$

$$\#\text{wv}(\epsilon) = \left(\frac{4}{3}\pi k(\epsilon)^3\right)\frac{V}{(2\pi)^3} = \frac{V}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{3/2}$$

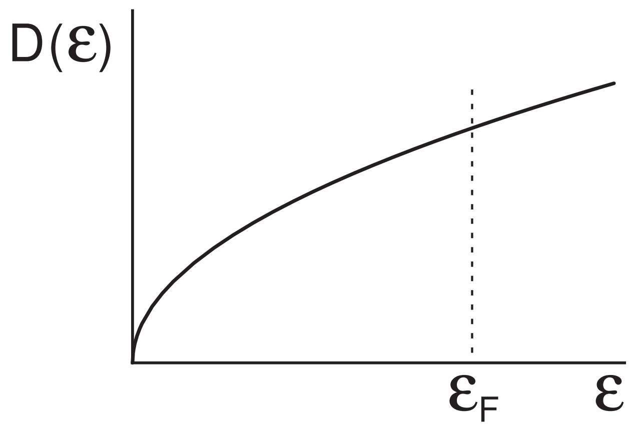
$$D_{\text{wv}}(\epsilon) = \frac{d}{d\epsilon}\#\text{wv}(\epsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{1/2}$$

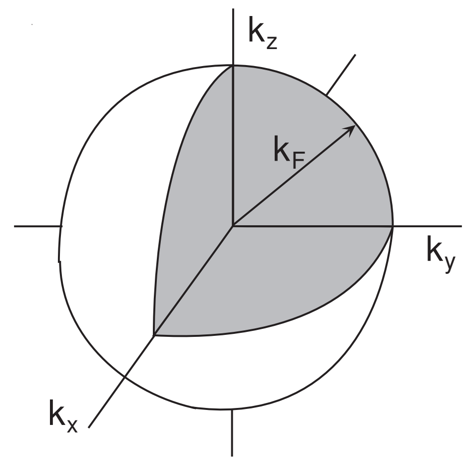
For free particles

$$D_{\text{states}}(\epsilon) = (2S+1)\frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{1/2}$$



Fermions: Non-interacting, free, spin 1/2, $T = 0$





Fermi sea

Fermi surface

Fermi wave vector k_F

Fermi energy $\epsilon_F = \hbar^2 k_F^2 / 2m$

$$N = 2 \times D_{\text{wavevectors}}(k) \times \frac{4}{3}\pi k_F^3 = \frac{8}{3}\pi \frac{V}{(2\pi)^3} k_F^3$$

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

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3} \propto (N/V)^{2/3}$$

$$D(\epsilon) = a\,\epsilon^{1/2}$$

$$N = \int_0^{\epsilon_F} D(\epsilon)\,d\epsilon = \tfrac{2}{3} a\,\epsilon_F^{3/2}$$

$$U = \int_0^{\epsilon_F} \epsilon D(\epsilon)\,d\epsilon = \tfrac{2}{5} a\,\epsilon_F^{5/2} = \underline{\tfrac{3}{5} N \epsilon_F} \quad \propto N(N/V)^{2/3}$$

Consequences: Motion at $T = 0$

$\vec{p} = \hbar\vec{k}$ $\qquad$ $\vec{p}_F = \hbar\vec{k}_F$ $\qquad$ $v_F = \frac{\hbar}{m}k_F$

Copper, one valence electron beyond a filled d shell

$$N/V = 8.45 \times 10^{22} \text{ atoms-cm}^{-3}$$

$$k_F = 1.36 \times 10^{8} \text{ cm}^{-1} \qquad v_F = 1.57 \times 10^{8} \text{ cm-s}^{-1}$$

$$p_F = 1.43 \times 10^{-19} \text{ g-cm-s}^{-1} \qquad \epsilon_F/k_B = 81,000K$$

Consequences: $P(T=0)$

$$U = \tfrac{3}{5} N \epsilon_F \qquad\qquad \epsilon_F \propto (N/V)^{2/3}$$

$$P = -\left(\frac{\partial U}{\partial V}\right)_{N,S} = -\tfrac{3}{5} N \underbrace{\left(\frac{\partial \epsilon_F}{\partial V}\right)_N}_{-\frac{2}{3}\frac{\epsilon_F}{V}} = \underline{\tfrac{2}{5}(N/V)\epsilon_F}$$

$$\propto (N/V)^{5/3}$$

$$\left(\frac{\partial P}{\partial V}\right)_{N,T} = -\tfrac{5}{3}\,(P/V) \text{ at } T = 0$$

$$\mathcal{K}_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{N,T} = \frac{3}{5}\frac{1}{P} = \frac{3}{2}\frac{1}{(N/V)\epsilon_F}$$

For potassium

$$\epsilon_F = 2.46 \times 10^4 K = 3.39 \times 10^{-12} \text{ ergs}$$

$$(N/V)_{\text{conduction}} = 1.40 \times 10^{22} \text{ cm}^{-3}$$

$$\mathcal{K}_T = \frac{1.5}{1.40 \times 10^{22} \times 3.39 \times 10^{-12}} = 31.6 \times 10^{-12} \text{ cm}^3\text{-ergs}^{-1}$$

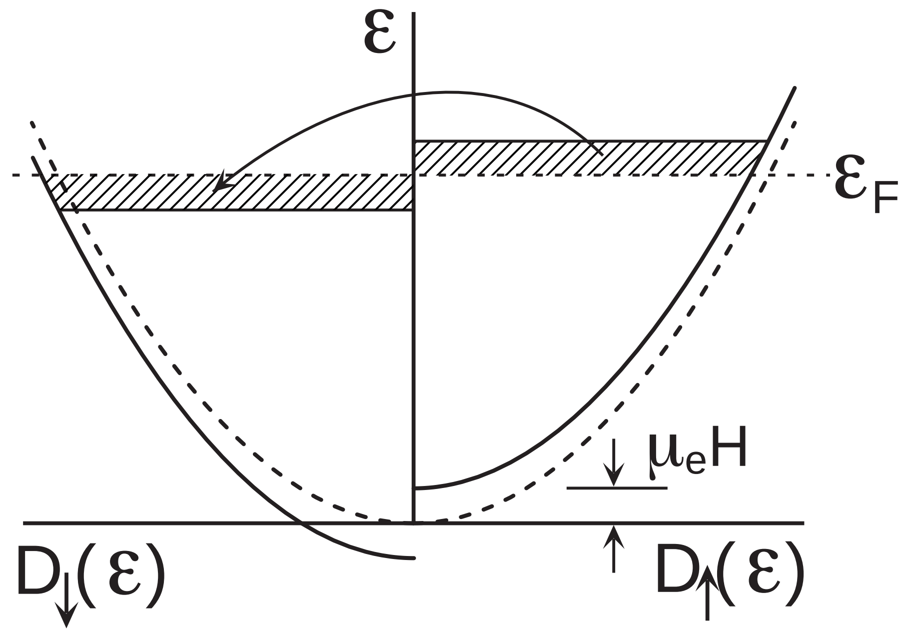
The measued value is 31×10^{-12} !

Magnetic Susceptibility

$$\vec{H} = H\hat{z}$$

$$\epsilon_{k,\uparrow} = \epsilon(k) + \mu_e H$$

$$\epsilon_{k,\downarrow} = \epsilon(k) - \mu_e H$$



$$N_\downarrow - N_\uparrow = \left(\frac{N}{2} + \mu_e H \, \frac{D(\epsilon_F)}{2}\right) - \left(\frac{N}{2} - \mu_e H \, \frac{D(\epsilon_F)}{2}\right)$$

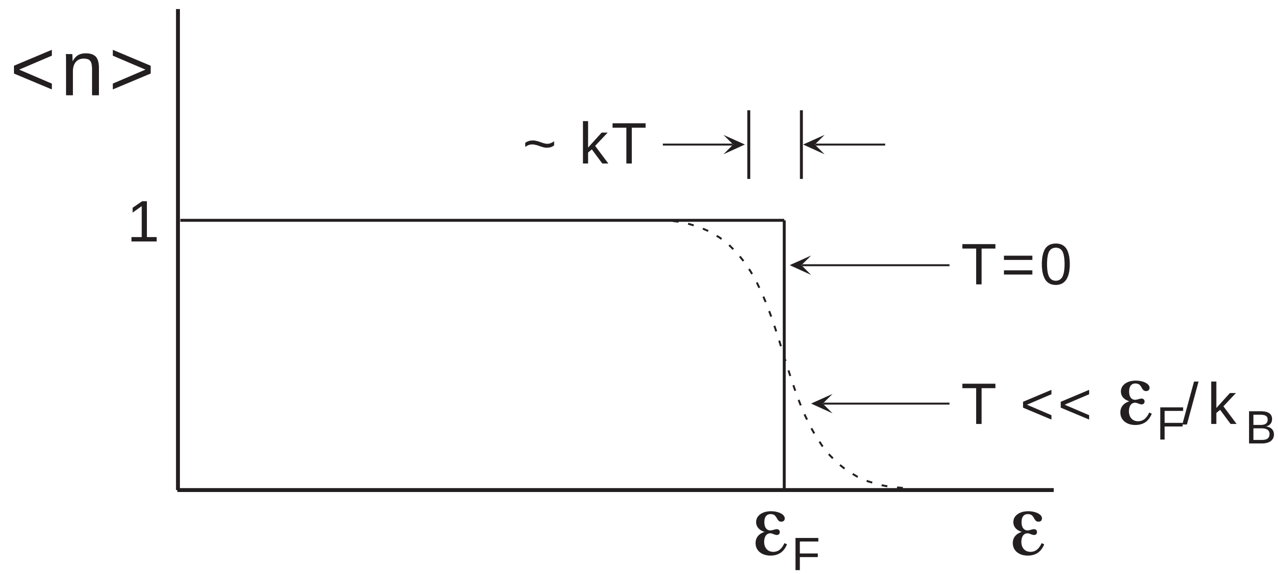
$$= \mu_e H D(\epsilon_F) \quad \Rightarrow \quad M = \mu_e^2 H D(\epsilon_F) \equiv \chi H$$

$$\underline{\chi = \mu_e^2 D(\epsilon_F)}$$

This expression holds as long as $kT \ll \epsilon_F$, so χ is temperature independent in this region. This is <u>not</u> Curie law behavior. It is called Pauli paramagnetism.

Temperature Dependence of $< n_{\vec{k},m_s} >$

$< n_{\vec{k},m_s} >= f(\epsilon)$ only, as in the Canonical Ensemble



Estimate C_V

	Classical	Quantum
# electrons	N	N
# electrons influenced	N	$\sim N \times \frac{kT}{\epsilon_F}$
$\Delta\epsilon$	$\frac{3}{2}kT$	$\sim kT$
ΔU	$\frac{3}{2}NkT$	$\sim N\,\frac{(kT)^2}{\epsilon_F}$
C_V	$\frac{3}{2}Nk$	$\sim 2Nk\,\frac{kT}{\epsilon_F}$

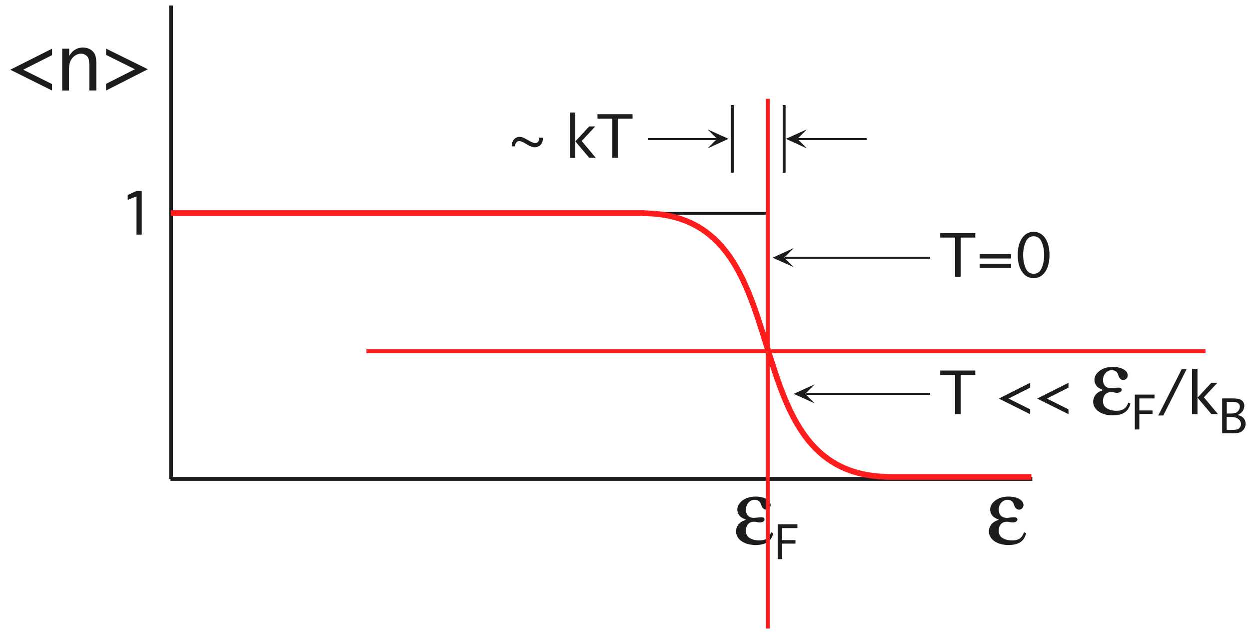
Exact result: $C_V = \frac{\pi^2}{2}\,Nk\,\frac{kT}{\epsilon_F}$

$$N = \int_0^\infty < n(\epsilon, \mu(T), T) > D(\epsilon)\, d\epsilon$$

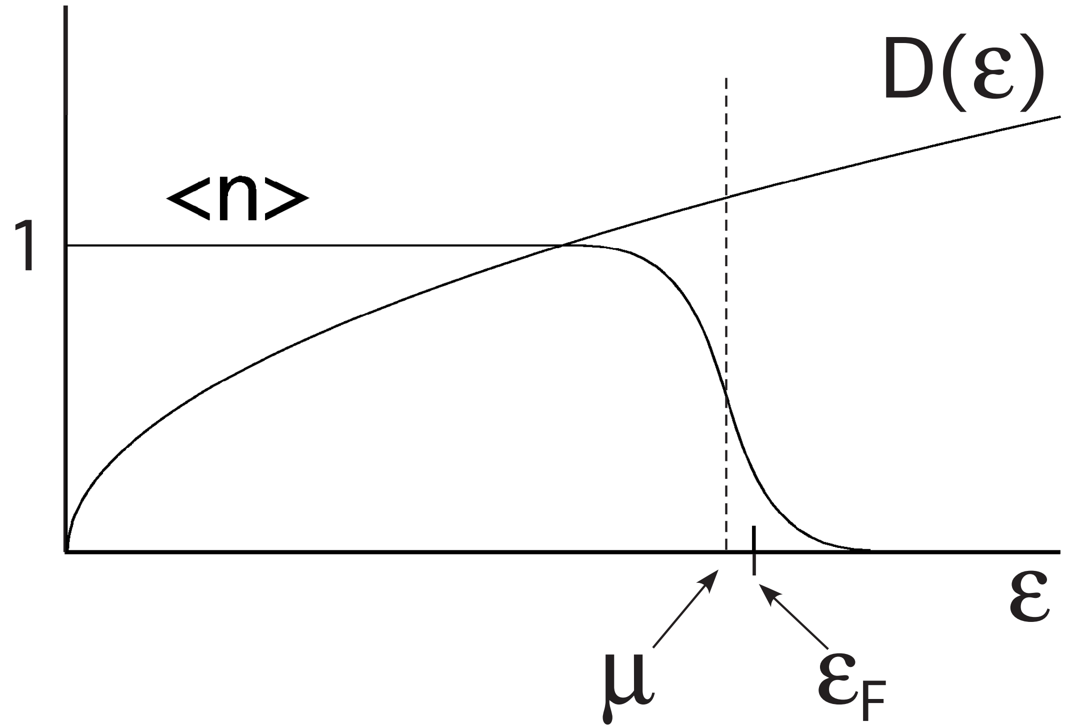
This expression implicitly determines $\mu = \mu(T)$.

$$U = \int_0^\infty < n(\epsilon, \mu(T), T) > \epsilon\, D(\epsilon)\, d\epsilon$$

To determine C_V from this expression one must take into account the temperature dependence of μ in addition to the explicit dependence of $< n >$ on T.



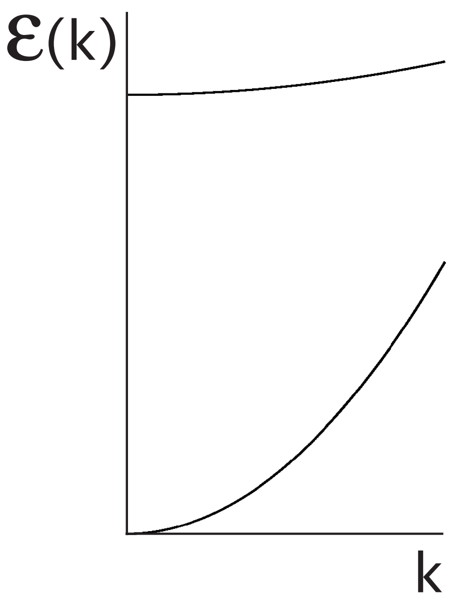
$$\underbrace{[< n > -1/2]}_{\text{at } \epsilon = \mu + \delta} = -\underbrace{[< n > -1/2]}_{\text{at } \epsilon = \mu - \delta}$$



Because $D(\epsilon)$ is an increasing function of ϵ, μ must decrease with increasing temperature.

Elementary Excitations Excitations out of the ground state in interacting many-body systems.

For a 3D Coulomb gas of electrons



Plasma oscillations (plasmons)

Collective modes: H.O.s

Quasi-particles

('dressed' electrons) $\epsilon = \frac{\hbar^2 k^2}{2m^*}$

Other collective modes

Phonons, lattice vibrations in solids

Spin waves, in Ferromagnets

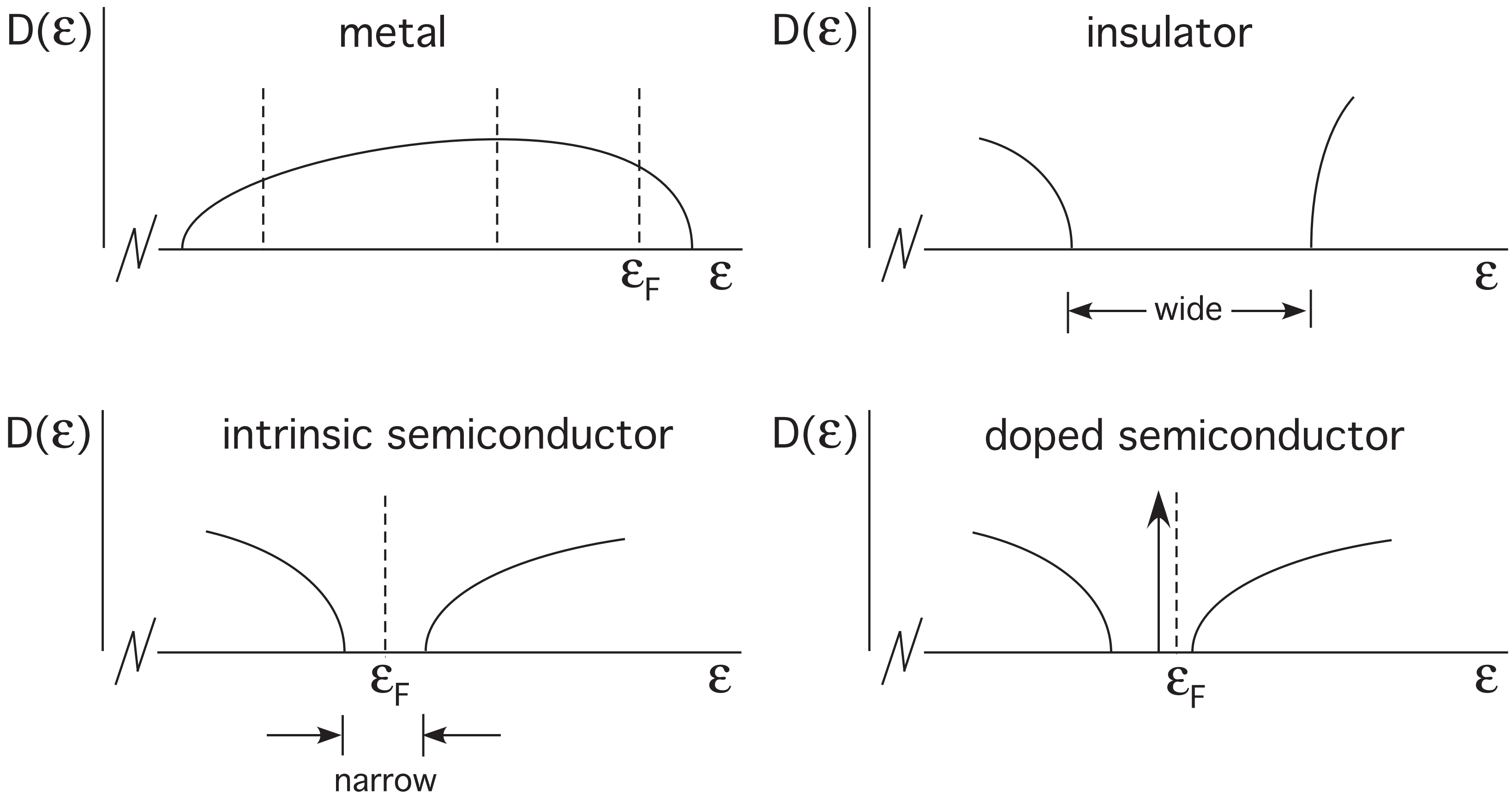
Ripplons, waves on surfaces

Other quasi-particles

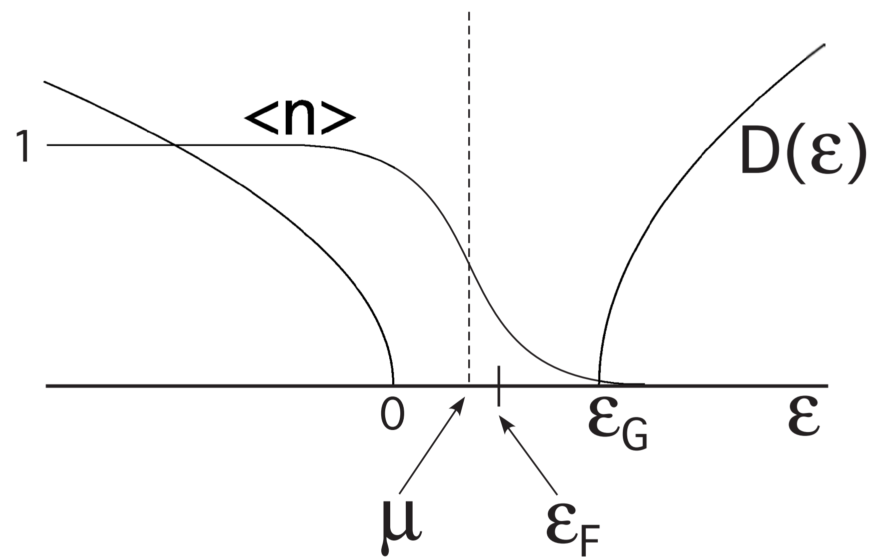
Polarons, (electron+lattice distortion)

in ionic materials

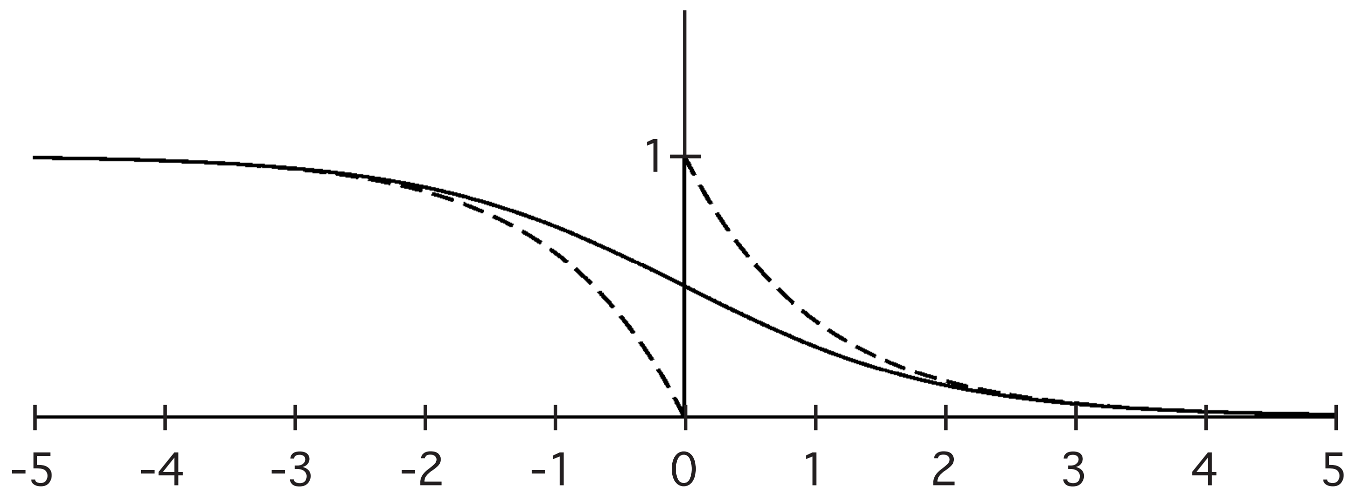
Some possible electronic densities of states in solids



Finding $\mu(T)$ in an intrinsic semiconductor



Assume the energy gap is $\gg k_B T$.



Comparison of $1/(e^x + 1)$ with e^{-x} when $x > 0$ and $1 - e^x$ when $x < 0$.

$$< n_e > \;\to\; e^{-(\epsilon-\mu)/k_BT} = e^{-(\epsilon_G-\mu)/k_BT}\; e^{-(\epsilon-\epsilon_G)/k_BT}$$

$$D_{\text{states},e}(\epsilon) \;=\; \frac{V}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}(\epsilon-\epsilon_G)^{1/2}$$

$$N_e \;=\; \int_{\epsilon_G}^{\infty} < n_e > D(\epsilon)\, d\epsilon$$

$$=\; \frac{V}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} e^{-(\epsilon_G-\mu)/k_BT}\int_0^{\infty}\sqrt{\delta}\, e^{-\delta/k_BT}\, d\delta$$

$$=\; \frac{V}{4}\left(\frac{2m_e k_B T}{\pi\hbar^2}\right)^{3/2} e^{-(\epsilon_G-\mu)/k_BT}$$

$$< n_h > \; = \; 1 - < n_e > \rightarrow \; e^{-(\mu-\epsilon)/k_B T}$$

$$D_{\text{states},h}(\epsilon) \; = \; \frac{V}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2}(-\epsilon)^{1/2}$$

$$N_h \; = \; \int_{-\infty}^{0} < n_h > D(\epsilon)\, d\epsilon$$

$$= \; \frac{V}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2} e^{-\mu/k_B T}\int_0^{\infty}\sqrt{\delta}\, e^{-\delta/k_B T}\, d\delta$$

$$= \; \frac{V}{4}\left(\frac{2m_h k_B T}{\pi\hbar^2}\right)^{3/2} e^{-\mu/k_B T}$$

$$N_h = N_e$$

$$m_h^{3/2}\, e^{-\mu/k_B T} = m_e^{3/2}\, e^{-(\epsilon_G - \mu)/k_B T}$$

$$(m_h/m_e)^{3/2} = e^{-\epsilon_G/k_B T}\; e^{2\mu/k_B T}$$

$$(3/2) k_B T \ln(m_h/m_e) = -\epsilon_G + 2\mu$$

$$\mu = \underline{\epsilon_G/2 - (3/4) k_B T \ln(m_e/m_h)}$$