SPECIFIC HEAT

$$C_V = \left(\frac{\Delta U}{\Delta T}\right)_V \longrightarrow \Delta T = \frac{\Delta U}{C_V}$$

specific heat coefficient

T = temperature

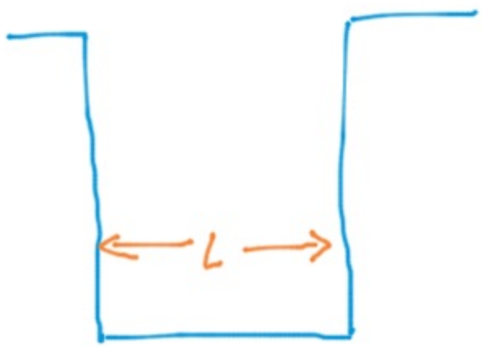
U = Energy of system

$$C_V = C_{LATTICE} + C_{ELECTRONIC} + \ldots\ldots$$

LAST TIME

TODAY

FREE ELECTRON GAS: N-electrons in a box



Schrödinger Equation

$$\mathcal{H}\psi = \frac{-\hbar^2}{2m}\cdot\frac{d^2}{dx^2}\psi = E\psi$$

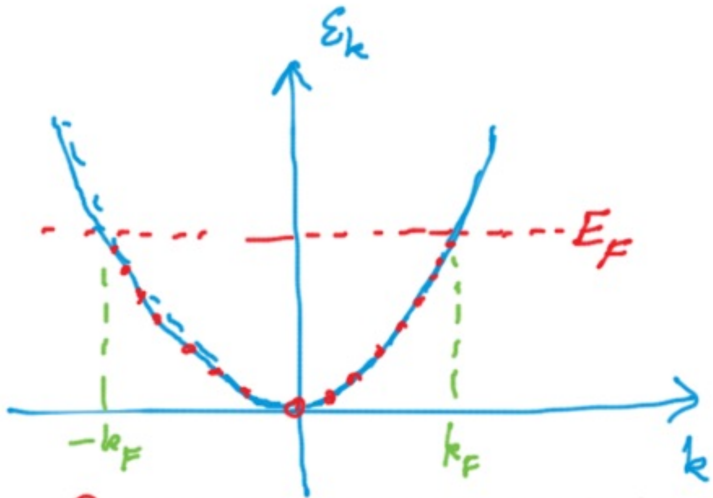
Hamiltonian   wavefunction   Eigen Energy

$$\psi(x) \propto e^{ikx} \quad \& \quad E = \frac{(\hbar k)^2}{2m}$$

PERIODIC BOUNDARY CONDITION

$$k = 0;\ \pm\frac{2\pi}{L};\ \pm\frac{4\pi}{L};\ \ldots$$

DISPERSION RELATION:



PAULI EXCLUSION PRINCIPLE

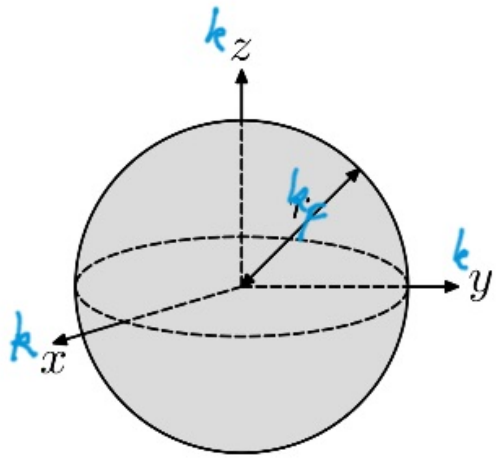
FERMI ENERGY E_F

FERMI MOMENTUM k_F

FERMI TEMPERATURE T_F

$$E_F = \frac{(\hbar k_F)^2}{2m} = k_B T_F$$

Estimation of FERMI ENERGY



ELECTRON SPIN

$$N = 2 \, \frac{4\pi k_F^3}{3} \cdot \frac{1}{\left(\frac{2\pi}{L}\right)^3} = \frac{V}{3\pi^2} k_F^3$$

$$\Downarrow \quad k_F = \left(3\pi^2 \frac{N}{V}\right)^{1/3} = \left(3\pi^2 n\right)^{1/3}$$

where $n = \frac{N}{V}$ = electron density

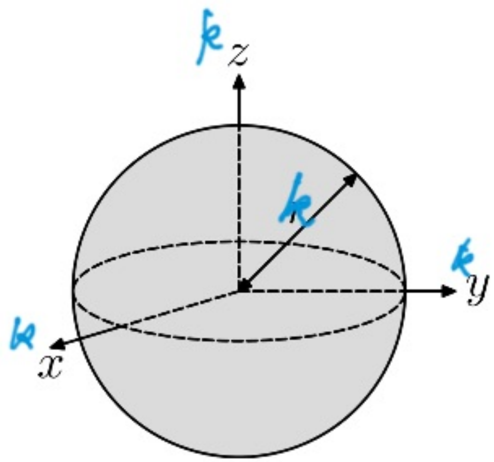
$$E_F = \frac{\hbar^2}{2m} \left(3\pi^2 n\right)^{2/3}$$

BACK-ON-THE-ENVELOPPE ESTIMATION:

Assume 1 electron per unit cell $V_{cell} = 10^{-30} m^3$

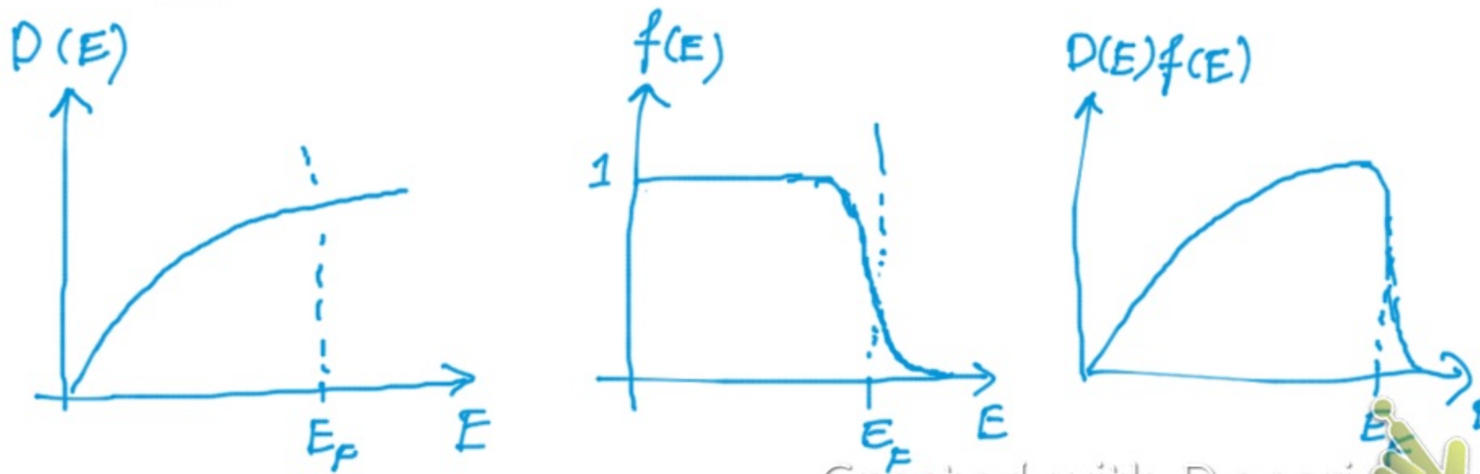
$n =$ $\quad$ $E_F =$ $\quad$ $T_F =$

DENSITY-OF-STATES:



$$N = \frac{V}{3\pi^2} k^3 = \frac{V}{3\pi^2} \cdot \left(\frac{2m}{\hbar^2} E \right)^{3/2}$$

$$D(E) \equiv \frac{dN}{dE} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E} \quad (3D)$$



ELECTRONIC ENERGY

EXERCISE

$$T=0: \qquad U(0) = \int_0^\infty f(\varepsilon)\,\varepsilon\, D(\varepsilon)\, d\varepsilon = \int_0^{\varepsilon_F} \varepsilon\, D(\varepsilon)\, d\varepsilon =$$

$$T\neq 0: \qquad U(T) = \int_0^\infty f(\varepsilon, T, \mu(T))\,\varepsilon\, D(\varepsilon)\, d\varepsilon$$

$$y = \frac{\varepsilon}{k_B T} \qquad = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2} \int_0^\infty \frac{\varepsilon^{3/2}}{e^{(\varepsilon-\mu)/k_B T}+1}\, d\varepsilon$$

$$y_0 = \frac{\mu}{k_B T}$$

$$\mu \gg k_B T \qquad = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2} (k_B T)^{5/2} \int_0^\infty \frac{y^{3/2}}{e^{y-y_0}+1}\, dy$$

$$\Downarrow$$

$$y_0 \to \infty \qquad = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2} \frac{\mu^{5/2}}{5/2}\left\{1 + \frac{5}{8}\left(\frac{\pi k_B T}{\mu}\right)^2\right\}$$

$$F_j(y_0) = \int_0^\infty \frac{y^j}{e^{y-y_0}+1}\, dy \overset{y_0\to\infty}{\approx} \frac{y_0^{j+1}}{j+1}\left(1 + \frac{\pi^2 j(j+1)}{6 y_0^2} + \dots\right)$$

Temperature dependence of chemical potential:

$$N = \int_0^\infty f(\varepsilon) D(\varepsilon)\, d\varepsilon = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\sqrt{\varepsilon}}{e^{\frac{\varepsilon-\mu}{k_B T}}+1}\, d\varepsilon$$

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

$$y = \frac{\varepsilon}{k_B T}$$

$$y_0 = \frac{\mu}{k_B T}$$

$$= \alpha (k_B T)^{3/2} \int_0^\infty \frac{\sqrt{y}}{e^{y-y_0}+1}\, dy$$

$$= \alpha \cdot (k_B T)^{3/2} \cdot \frac{y_0^{3/2}}{3/2}\left(1 + \frac{\pi^2\, 1/2 \cdot 3/2}{6 y_0^2}\right)$$

$$= \frac{2}{3}\alpha\, \mu^{3/2}\left(1 + \frac{\pi^2}{8}\left(\frac{k_B T}{\mu}\right)^2\right)$$

$$\Downarrow$$

$$\mu(T) = \left(\frac{3}{2}\frac{N}{\alpha}\right)^{2/3}\left(1 + \frac{\pi^2}{8}\left(\frac{k_B T}{\mu}\right)^2\right)^{2/3} \simeq \varepsilon_F\left(1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\mu}\right)^2\right)$$

$$F_j(y_0) = \int_0^\infty \frac{y^j}{e^{y-y_0}+1}\, dy \overset{y_0 \to \infty}{\approx} \frac{y_0^{j+1}}{j+1}\left(1 + \frac{\pi^2 j(j+1)}{6 y_0^2} + \dots\right)$$

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

Combine Our Results

$$\mu(T) = \mathcal{E}_F\left(1 - \frac{\pi^2}{12}\left(\frac{k_BT}{\mu}\right)^2\right) \Rightarrow \mu^{5/2}(T) = \mathcal{E}_F^{5/2}\cdot\left\{1 - \frac{5\pi^2}{24}\left(\frac{k_BT}{\mu}\right)^2\right\}$$

$$U(T) = \frac{2}{5}\mu^{5/2}\left\{1 + \frac{5}{8}\left(\frac{\pi k_BT}{\mu}\right)^2\right\}\cdot\frac{V}{2\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2}$$

$$= \frac{2}{5}\mathcal{E}_F^{3/2}\left\{1 - \frac{5\pi^2}{24}\left(\frac{k_BT}{\mu}\right)^2\right\}\left\{1 + \frac{5}{8}\left(\frac{\pi k_BT}{\mu}\right)^2\right\}\cdot\frac{V}{2\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2}$$

$$\simeq \frac{2}{5}\mathcal{E}_F^{5/2}\frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left\{1 + \frac{5}{12}\left(\frac{\pi k_BT}{\mu}\right)^2\right\}$$

$$\simeq \frac{2}{5}\mathcal{E}_F^{5/2}\frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left\{1 + \frac{5}{12}\left(\frac{\pi k_BT}{\mathcal{E}_F}\right)^2\right\} \qquad E_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

CALCULATION OF SPECIFIC HEAT

$$U(T) \approx \frac{2}{5}\varepsilon_F^{5/2}\frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left\{1+\frac{5}{12}\left(\frac{\pi k_B T}{\varepsilon_F}\right)^2\right\}$$

$$\Downarrow$$

$$C_V = \frac{dU(T)}{dT} = \frac{V}{6}\varepsilon_F^{3/2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\cdot\frac{k_B^2 T}{\varepsilon_F} = \frac{\pi^2}{3}D(\varepsilon_F)\cdot k_B^2 T$$

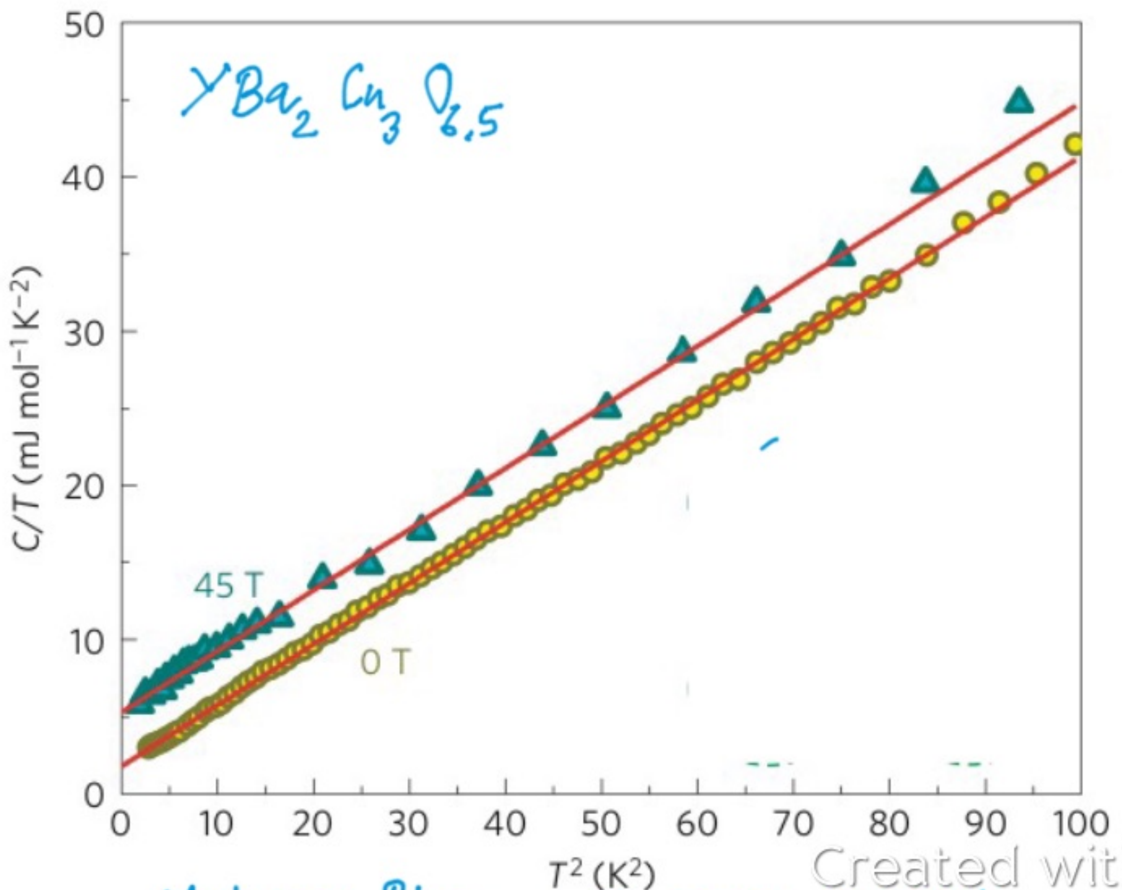
$$= \frac{V}{2}\frac{(\pi k_B)^2}{\varepsilon_F}n\cdot T$$

$$= \frac{\pi^2}{2}\cdot N\cdot k_B\cdot\frac{T}{T_F}$$

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

$$\Downarrow \quad \varepsilon_F^{3/2} = \left(\frac{\hbar^2}{2m}\right)^{3/2}\cdot 3\pi^2 n$$

REAL DATA: $C_V = \gamma \cdot T + \alpha T^3 \Rightarrow \frac{C_V}{T} = \gamma + \alpha T^2$



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