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QM 115B Lec 10

Free Electron Gas ignore interactions

box $V = \begin{cases} 0 & 0 < x < l_x, 0 < y < l_y, 0 < z < l_z \\ \infty & \text{otherwise} \end{cases}$

inside $-\frac{\hbar^2 \nabla^2 \psi}{2m} = E \psi$

$$\psi(x, y, z) = \bar{X}(x) \bar{Y}(y) \bar{Z}(z)$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \bar{X}}{dx^2} = E \bar{X}$$

$$\frac{d^2 \bar{X}}{dx^2} = k_x^2 \bar{X}$$

$$\bar{X}(x) = A_x \sin(k_x x) + B_x \cos(k_x x)$$

$$\bar{X}(0) = 0 \Rightarrow B_x = 0$$

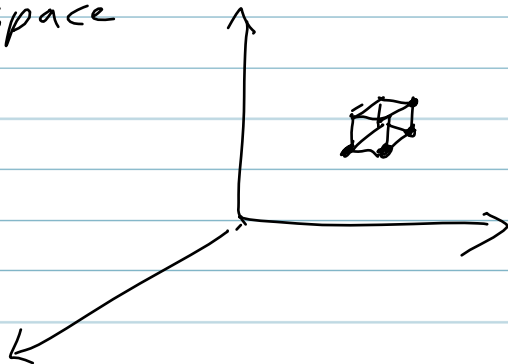
$$\bar{X}(x l_x) = 0 \Rightarrow k_x l_x = n_x \pi$$

$$\psi_{n_x n_y n_z} = \sqrt{\frac{8}{l_x l_y l_z}} \sin\left(\frac{n_x \pi x}{l_x}\right) \sin\left(\frac{n_y \pi y}{l_y}\right) \sin\left(\frac{n_z \pi z}{l_z}\right)$$

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_y^2} + \frac{n_z^2}{l_z^2} \right) = \frac{\hbar^2 k^2}{2m}$$

$$\vec{k} = (k_x, k_y, k_z) = \left(\frac{n_x \pi}{l_x}, \frac{n_y \pi}{l_y}, \frac{n_z \pi}{l_z} \right)$$

k-space



8 corners / box

each corner has 8 neighboring boxes

associate 1 box per state

Volume in k-space $\frac{\pi^3}{l_x l_y l_z} = \frac{\pi^3}{V}$

N atoms, each atom contribute g free electrons
N ~ 6x10²³ g = 1, 2

bigger g harder metal higher melting temp Na g=1 Mg g=2
only two electrons per state $\uparrow\downarrow$
states filled $\frac{Ng}{2}$

ground state fill up 1/8 sphere in k-space

radius k_F
 $\frac{1}{8} \left(\frac{4}{3} \pi k_F^3 \right) = \frac{Ng}{2} \left(\frac{\pi^3}{V} \right)$

$k_F = \left(\frac{3 Ng \pi^3}{4 \pi V} \right)^{1/3}$
 $= \left(\frac{Ng}{V} 3\pi^2 \right)^{1/3}$ $\rho = \frac{Ng}{V}$
density of free electrons

boundary of sphere is called Fermi surface

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

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Total energy of electron gas shell of thickness dk

$$\text{shell volume} = \frac{1}{8} (4\pi k^2) dk$$

$$\begin{aligned} \# \text{ electron states in shell} &= \frac{\text{shell vol.}}{\text{vol./state}} \frac{2}{\text{state}} \\ &= \frac{2}{8} \frac{(4\pi k^2) dk}{\pi^3/V} = \frac{V k^2 dk}{\pi^2} \end{aligned}$$

$$\text{each state has energy} = \frac{\hbar^2 k^2}{2m}$$

$$dE = \frac{\hbar^2 k^2}{2m} \frac{V}{\pi^2} k^2 dk$$

$$E_{\text{tot}} = \frac{\hbar^2 V}{2\pi^2 m} \int_0^{k_F} k^4 dk = \frac{\hbar^2 V}{2\pi^2 m} \frac{k_F^5}{5}$$

$$= \frac{\hbar^2 V}{10\pi^2 m} \left(\frac{3N_g \pi^2}{V} \right)^{5/3} \quad k_F = \left(\frac{3N_g \pi^2}{V} \right)^{1/3}$$

$$= \frac{\hbar^2}{10\pi^2 m} (3\pi^2 N_g)^{5/3} V^{-2/3}$$

$$\frac{dE}{dV} < 0$$

positive quantum degeneracy pressure

$$5.16 \text{ Cu: } E_F = 7\text{eV} = k_B T_F$$

$$T_F = 8 \times 10^4 \text{ K}$$

melting point of Cu is $1.3 \times 10^3 \text{ K}$