PHY 140A HW # 6

1.

(a)

Debye sphere has the same # of states (same volume) as BZ:

$V_{cell} = a^3/4$ for fcc structure.

$$\frac{4\pi}{3} k_D^3 = V_{BZ} = \frac{(2\pi)^3}{a^3/4} \Rightarrow k_D = \frac{2}{a}\sqrt[3]{3\pi^2}$$

(b)

$$v(k) = \frac{d\omega}{dk} = \Omega \cdot \frac{\pi}{2k_D} \cos\left(\frac{\pi}{2}\frac{k}{k_D}\right) = \frac{\pi\Omega}{2k_D}\cos\left(\frac{\pi k}{2k_D}\right)$$

$$c = \lim_{k\to 0} v(k) = \frac{\pi\Omega}{2k_D}$$

(c) $\omega - \omega(k) = 0$

$$\omega - \Omega \sin\left(\frac{\pi}{2}\frac{k}{k_D}\right) = 0$$

$$\Rightarrow k = \frac{2k_D}{\pi}\sin^{-1}\left(\frac{\omega}{\Omega}\right) = k(\omega)$$

(d)

$$N = 3 \times \frac{a^3/4}{(2\pi)^3} \times \frac{4}{3}\pi k^3 = \frac{a^3 k^3}{8\pi^2}$$

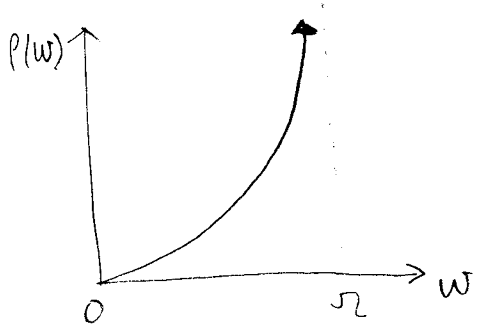
3 branches

$$\rho(\omega) = \frac{dN}{d\omega} = \frac{a^3}{8\pi^2} \cdot 3k^2 \frac{dk}{d\omega}$$

$$= \frac{3a^3}{8\pi^2} \cdot \left(\frac{2k_D}{\pi}\sin^{-1}\left(\frac{\omega}{\Omega}\right)\right)^2 \Big/ \frac{\pi\Omega}{2k_D}\sqrt{1-\left(\frac{\omega}{\Omega}\right)^2}$$

(e) at $\omega \to 0$, $\rho(\omega) \longrightarrow 0$

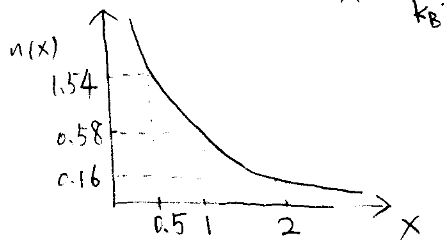
$\omega \to \Omega$, $\rho(\omega) \longrightarrow \infty$



$$x = \frac{\hbar\omega}{k_B T}$$

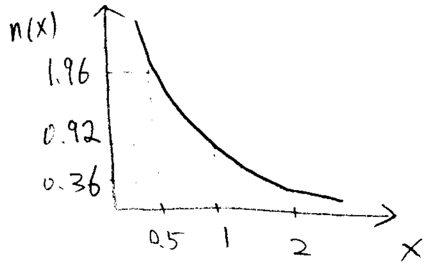
2.

(a) $$n\left(\frac{\hbar\omega}{k_B T}\right) = \frac{1}{e^{\left(\frac{\hbar\omega}{k_B T}\right)} - 1}$$



$$n(x) = \frac{1}{e^x - 1}$$

(b) $$\frac{dn\left(\frac{\hbar\omega}{k_B T}\right)}{dT} = \frac{\frac{\hbar\omega}{k_B T^2}\, e^{\left(\frac{\hbar\omega}{k_B T}\right)}}{\left(e^{\left(\frac{\hbar\omega}{k_B T}\right)} - 1\right)^2}$$



$$n(x) = \frac{x e^x}{(e^x - 1)^2}$$

3. (a)

1-D

$$N = 2 \times \frac{L}{2\pi} \times 2k_F \Rightarrow k_F = \frac{N\pi}{2L}$$

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{N\pi}{2L}\right)^2$$

$$\rho(\epsilon) = \frac{dN}{d\epsilon} = \frac{2L}{\pi}\frac{dk}{d\epsilon} = \frac{2L}{\pi}\frac{m}{\hbar^2}\frac{\hbar}{\sqrt{2m\epsilon}} = \frac{N}{2}\epsilon^{-1/2}\epsilon_F^{-1/2}$$

2-D

$$N = 2 \times \frac{L^2}{(2\pi)^2} \times \pi k_F^2 \Rightarrow k_F = \left(\frac{2\pi N}{L^2}\right)^{1/2}$$

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\frac{2\pi N}{L^2} = \frac{\pi N \hbar^2}{m L^2}$$

$$\rho(\epsilon) = \frac{dN}{d\epsilon} = \frac{L^2}{2\pi}\cdot 2k\frac{dk}{d\epsilon} = \frac{k}{\pi}L^2\cdot\frac{m}{\hbar^2 k} = \frac{L^2 m}{\pi\hbar^2} = \frac{N}{\epsilon_F}$$

3-D

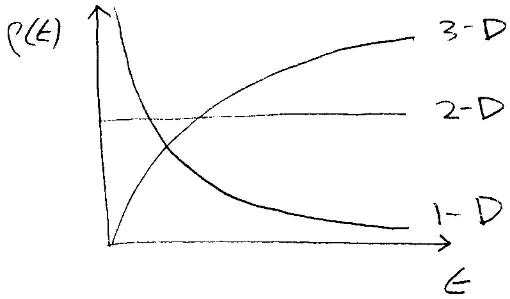
$$N = 2 \times \frac{L^3}{8\pi^3} \times \frac{4}{3}\pi k_F^3 \Rightarrow k_F = \left(\frac{3N\pi^2}{L^3}\right)^{1/3}$$

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

$$\rho(\epsilon) = \frac{dN}{d\epsilon} = \frac{L^3}{3\pi^2}3k^2\frac{dk}{d\epsilon} = \frac{L^3}{3\pi^2}\cdot 3\cdot\frac{2m\epsilon}{\hbar^2}\cdot\frac{m}{\hbar^2}\cdot\frac{\hbar}{\sqrt{2m\epsilon}}$$

$$= \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{1/2} = \frac{3}{2}\frac{N}{\epsilon_F}\left(\frac{\epsilon}{\epsilon_F}\right)^{1/2}$$

OR:



$$\rho(\epsilon) = 2\sum_k \delta(\epsilon - \epsilon_k)$$

$$= 2\left(\frac{L}{2\pi}\right)^d \int d^d k\ \delta(\epsilon - \epsilon_k)$$

$\boxed{d = 1, 2, 3}$

$$= 2\left(\frac{L}{2\pi}\right)^d \int_{S(\epsilon)} \frac{d^{d-1}S}{|\nabla \epsilon_k|}$$

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

$$\nabla\epsilon = \frac{\hbar^2 k}{m}$$

$$k = \sqrt{\frac{2m\epsilon}{\hbar^2}}$$

$$= 2\left(\frac{L}{2\pi}\right)^d \int_{S(\epsilon)} \frac{d^{d-1}S\ \ m}{\hbar^2 \cdot k(\epsilon)}$$

$$= 2\left(\frac{L}{2\pi}\right)^d \frac{m}{\hbar^2} \begin{cases} 2/k(\epsilon), & d = 1 \\ 2\pi, & d = 2 \\ 4\pi\, k(\epsilon), & d = 3 \end{cases}$$

(b)

<u>1-D</u>

$$\langle\epsilon\rangle = \frac{\int_0^{\epsilon_F} \rho(\epsilon)\,\epsilon\, d\epsilon}{\int_0^{\epsilon_F} \rho(\epsilon)\, d\epsilon}$$

$$= \frac{\int_0^{\epsilon_F} \epsilon^{1/2}\, d\epsilon}{\int_0^{\epsilon_F} \epsilon^{-1/2}\, d\epsilon}$$

$$= \frac{\frac{2}{3}\epsilon_F^{\frac{3}{2}}}{2\ \epsilon_F^{1/2}} = \frac{1}{3}\epsilon_F$$

<u>2-D</u>

$$\langle\epsilon\rangle = \frac{\int_0^{\epsilon_F} \epsilon\, d\epsilon}{\int_0^{\epsilon_F} 1\, d\epsilon}$$

$$= \frac{\frac{1}{2}\epsilon_F^2}{\epsilon_F} = \frac{1}{2}\epsilon_F$$

3-D
$$\langle \epsilon \rangle = \frac{\int_0^{\epsilon_F} \epsilon^{1/2} \epsilon \, d\epsilon}{\int_0^{\epsilon_F} \epsilon^{1/2} \, d\epsilon} = \frac{\frac{2}{5}\epsilon_F^{5/2}}{\frac{2}{3}\epsilon_F^{3/2}} = \frac{3}{5}\epsilon_F$$

4.

(a)

$\langle 100 \rangle$: ZB at $|\vec{k}| = \frac{2\pi}{a}$

$\langle 110 \rangle$: ZB at $|\vec{k}| = \sqrt{2}\frac{\pi}{a}$

$\langle 111 \rangle$: ZB at $|\vec{k}| = \sqrt{3}\frac{\pi}{a}$

Refer to text book <u>p.p. 73 , Figure 3.3</u>

(b)

$$\epsilon_{100} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{a}\right)^2 = \frac{2\hbar^2\pi^2}{ma^2}$$

$$\epsilon_{110} = \frac{\hbar^2}{2m}\left(\sqrt{2}\frac{\pi}{a}\right)^2 = \frac{\hbar^2\pi^2}{ma^2} = \frac{1}{2}\epsilon_{100}$$

$$\epsilon_{111} = \frac{\hbar^2}{2m}\left(\sqrt{3}\frac{\pi}{a}\right)^2 = \frac{3\hbar^2\pi^2}{2ma^2} = \frac{3}{4}\epsilon_{100}$$

$a = 3\times10^{-10}$ m , $m = 9.1\times10^{-31}$ kg , $\hbar = 1.055\times10^{-34}$ J/s

$$\epsilon_{100} = \frac{2\times(1.055)^2\times10^{-68}\times\pi^2}{9.1\times10^{-31}\times9\times10^{-20}}\times\frac{1}{1.6\times10^{-19}} \sim 16.7 \text{ eV}$$

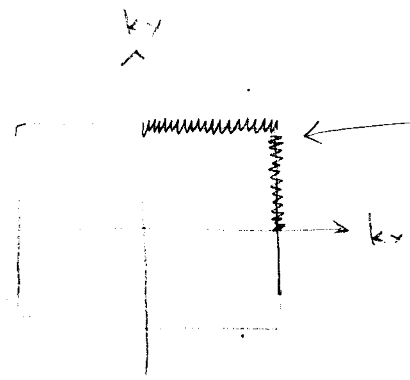
$$\epsilon_{110} = \frac{1}{2}\epsilon_{100} \sim 8.3 \text{ eV}$$

$$\epsilon_{111} = \frac{3}{4}\epsilon_{100} \sim 12.5 \text{ eV}$$

(c)

Gap at 1D zone boundary results in a true gap.

2D



must have gap along all of zone boundary

specifically at $(\frac{\pi}{a}, 0)$ & $(\frac{\pi}{a}, \frac{\pi}{a})$

$\downarrow \quad \epsilon_{100}$ $\qquad \downarrow \quad \epsilon_{110} = 2\epsilon_{100}$

3D must have gap over 3D region & even more zone boundaries $\Rightarrow$ tougher criterion.