SSP 2014 ①

1). • α is the the coupling constant, a term dependent on the charges
• ρ is the term dependent on the materials scale and crystal lengths

$$U(r) = Ae^{-r/\rho} - \frac{\alpha z^2}{4\pi\epsilon_0 r}$$

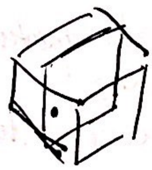
$$\frac{\partial u}{\partial r} = -\frac{1}{\rho}Ae^{-r/\rho} + \frac{\alpha z^2}{4\pi\epsilon_0 r^2} = 0 \quad \text{(at equilibrium)}$$

• Not Relevant

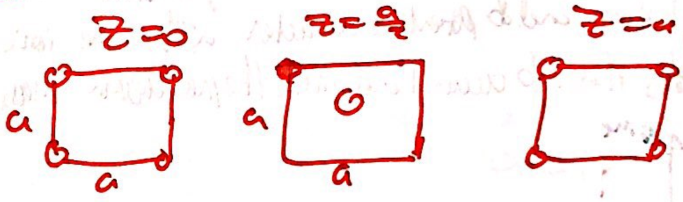
$$\frac{Ae^{-r/\rho}}{\rho} = \frac{\alpha z^2}{4\pi\epsilon_0 r^2}$$

$$A = \frac{\alpha z^2 \rho}{4\pi\epsilon_0 r^2 e^{-r/\rho}} = \frac{\alpha z^2 \rho e^{r/\rho}}{4\pi\epsilon_0 r^2}$$

2) BCC: $a(0,0,0), a(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})$



[001] direction



unit cross sections

$$\sqrt{a^2+a^2} = \sqrt{2}a$$

$$\sqrt{(\sqrt{2}a)^2+a^2} = \sqrt{3}a$$

$$\sqrt{3}a = 4r$$

$$r = \frac{\sqrt{3}a}{4}$$

$$\frac{2 \times \frac{4}{3}\pi r^3}{a^3} = \frac{2 \times \frac{4}{3} \times \frac{3^{3/2}}{4^3} \times a^3 \pi}{a^3} = \frac{2}{4^2} \times 3^{\frac{1}{2}} = \frac{\sqrt{3}}{8}\pi = \cancel{0.2165}$$

0.68

3) $\mathcal{E} = \dfrac{\hbar^2 k^2}{2M_e}$

$p = Mv = \hbar k$

$f = M\dfrac{dv}{dt} = \hbar\dfrac{dk}{dt} \Rightarrow M\dfrac{dv}{dt} = \hbar\dfrac{dk}{dt}$

$M\dfrac{d}{dt}\left(\dfrac{1}{\hbar}\dfrac{d\mathcal{E}}{dk}\right) = \hbar\dfrac{dk}{dt}$ $\quad v_g = \dfrac{d\omega}{dk} = \dfrac{1}{\hbar}\dfrac{d\mathcal{E}}{dk}$

$\mathcal{E} = \hbar\omega$

$d\mathcal{E} = \hbar d\omega$

$\dfrac{d\mathcal{E}}{dk} = \dfrac{2\hbar^2 k}{2M}$

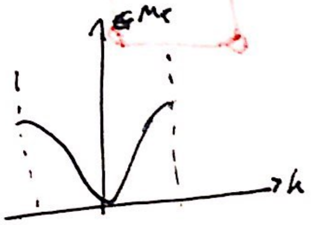
$= 2\left(\dfrac{\hbar^2}{2M}\right)^{\frac{1}{2}} \mathcal{E}^{\frac{1}{2}}$

$M\dfrac{d}{dt}\left(\dfrac{1}{\hbar}\dfrac{d\mathcal{E}}{dk}\right) = \hbar\dfrac{dk}{d\mathcal{E}}\dfrac{d\mathcal{E}}{dt}$

$M\dfrac{d}{dt}\dfrac{d\mathcal{E}}{dk} = \hbar^2\dfrac{dk}{d\mathcal{E}}\dfrac{d\mathcal{E}}{dt}$

$M = \dfrac{\hbar^2}{d^2\mathcal{E}/dk^2}$

- Effective electron mass is the mass of an electron in a lattice as its mass is also affected by holes and its potential interaction with the ionic lattice, so effective mass takes this into account and is not the free electron mass but rather, the band electron mass



4) Intrinsic:

$n = p$

$A(M_e^* T)^{3/2} e^{(\mu - \mathcal{E}_G)/k_BT} = A(M_h^* T)^{3/2} e^{-\mu/k_BT}$

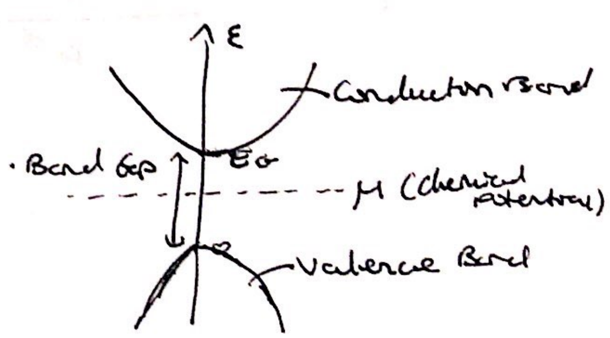
$\left(\dfrac{M_e^*}{M_h^*}\right)^{3/2} e^{(2\mu - \mathcal{E}_G)/k_BT} = 1$

$\left(\dfrac{M_e^*}{M_h^*}\right)^{3/2} = e^{(\mathcal{E}_G - 2\mu)/k_BT}$

$\dfrac{3}{2}\ln\left(\dfrac{M_e^*}{M_h^*}\right) k_BT = \mathcal{E}_G - 2\mu$

$2\mu = \mathcal{E}_G - \dfrac{3}{2}\ln\left(\dfrac{M_e^*}{M_h^*}\right) k_BT$

$\mu = \dfrac{\mathcal{E}_G}{2} + \dfrac{3}{4}\ln\left(\dfrac{M_H^*}{M_e^*}\right) k_BT$



②

5) $K = \frac{1}{3} v l c$

- The ~~mean~~ average velocity of the ~~particles~~ phonons in given
- The mean free path ~~for particles~~ between phonon collisions
- The specific Heat capacity per unit volume

- Normal occurs when phonon scattering ~~is~~ occurs and remains in a brillouin zone boundary → Two phonons collide, total momentum conserved, Doesn't limit thermal conducting → $T \ll \Theta_D$
- Umklapp phonon scattering occurs when a resultant of phonon following scattering lies outside the brillouin zone boundary and requires the addition / subtraction of a lattice constant to become normal. → Total momentum not conserved, k_3 in opposite direction. → k_1 & k_2 need to be close to BZB

They can help understand the graph as normal occur at a relatively low temperature with smaller momenta and so rises according to $\sim T^3$ at low temperature, ↳ Also limits thermal conductivity whereas at high temperature, a lot of scattering occurs with a temperature dependence of $\sim \frac{1}{T}$.

High T: $T \geq \Theta_D$
→ Lots of events, a lot of scattering
→ ~~Goa~~ $l \propto \frac{1}{T}$.

6) $n\lambda = 2d\sin\theta$

$\underline{G} = h b_1 + k b_2 + l b_3$

$|\underline{G}|^2 = h^2 + k^2 + l^2$

$d_{hkl} = \frac{a}{|\underline{G}|}$

$d_{hkl}^2 = \frac{a^2}{|\underline{G}|^2} = \frac{a^2}{h^2+k^2+l^2}$

- $T \sim \Theta_D$ Freezes. $\propto e^{-\Theta_D/T}$ $\sim \frac{1}{l}$ $l \propto e^{\Theta_D/T}$

$d^2 = \left(\frac{n\lambda}{2\sin\theta}\right)^2$

- low T. $\omega \to \left(\frac{T}{\Theta_D}\right)^3$

$$\boxed{\frac{n^2\lambda^2}{4\sin^2\theta} = \frac{a^2}{h^2+k^2+l^2}}$$

For $n=1$, max $\theta = 90°$, ∴ $\sin\theta = 1$

$$\Rightarrow \frac{\lambda^2}{4} \leq \frac{a^2}{h^2+k^2+l^2}$$

$$\therefore \frac{4a^2}{\lambda^2} \geq h^2+k^2+l^2$$

$$\frac{4a^2}{\lambda^2} = \frac{4 \times (0.3)^2}{(0.34)^2} = 3.114$$

$3.114 \geq h^2+k^2+l^2$

Allowed indices:

$\{100\}, \{110\}, \{111\}$, ~~$\{200\}$~~

Highest Miller Indice!

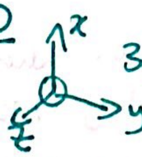
7a) • As there are Nk_B contributions per dimension, ~~a~~ half correspond to spatial freedoms, $\frac{Nk_B}{2}$ (kinetic energy) and the rest correspond to potential energy.

• ~~In~~ In 2D there are only x and y spatial dimensions

• And only interacts with 2 potentials, so the total contribution is $Nk_B + Nk_B = 2Nk_B$, corresponding to the number of atoms

b)
• The medium is dispersionless ($\omega = V_s k$)
• The solids obey is harmonic potential
• There is a high frequency cut-off at ω_D
• the crystal is isotropic (identical at all angles)

3D



$3(\frac{1}{2})$ translational

$3(\frac{1}{2})$ rotational

$\Leftrightarrow 2(\frac{1}{2})$ vibrational

$3Nk$

2D: $2(\frac{1}{2})$ translational

$\Leftrightarrow 2(\frac{1}{2})$ vibrational

c) ~~$g(k)dk =$~~

Annulus: $A = 2\pi k\, dk$

$$g(k)\,dk = \boxed{2\pi k\, dk \left(\frac{L}{2\pi}\right)^2} = \frac{2\pi k L^2}{2\,4\pi^2} dk$$

$$= \frac{k A^2}{2\pi} dk$$

$$g(\omega) = \frac{\omega L^2}{2\pi V_s^2}$$

$$g(k)dk = g(\omega)d\omega$$

$$\frac{kA^{\cancel{2}}}{2\pi} dk = g(\omega)d\omega$$

$$\frac{kA^{\cancel{2}}}{2\pi}\frac{dk}{d\omega} = g(\omega)$$

$$\omega = V_s k \Rightarrow \frac{d\omega}{dk} = V_s$$

$$k = \frac{\omega}{V_s}$$

$$N = \int^{\omega_D} g(\omega)\, d\omega$$

$$\frac{\omega}{V_s}\frac{A}{2\pi}\frac{1}{V_s} = \boxed{\frac{\omega A}{2\pi V_s^2} = g(\omega)}$$

$$\frac{2N}{\omega_D^2} = \frac{L^2}{2\pi}\frac{1}{V_s^2}$$

$$\omega_D = \frac{V_s}{2\sqrt{\pi}}\left(\frac{A}{N}\right)^{\frac{1}{2}}$$

$$g(\omega) = \frac{2N}{\omega_D^2}\omega$$

d)
$$E = \int_0^{\omega_D} \varepsilon(\omega)\, g(\omega)\, d\omega$$

$$\varepsilon(\omega) = \hbar\omega\left(n(\omega) + \tfrac{1}{2}\right), \quad n(\omega) = \frac{1}{e^{\hbar\omega/k_BT} - 1}$$

$$\Rightarrow E = \hbar\omega \frac{2N\omega}{\omega_D^2}\int_0^{\omega_D} n(\omega) + \tfrac{1}{2}\; d\omega$$

$$= 2\hbar N\frac{\omega^2}{\omega_D^2}\int_0^{\omega_D} \frac{1}{e^{\hbar\omega/k_BT} - 1} + \frac{1}{2}\; d\omega$$

$$= \frac{2N}{\omega_D^2}\int_0^{\omega_D} \frac{\hbar\omega^2}{e^{\hbar\omega/k_BT} - 1}\, d\omega + 2N\int^{\omega_D} \frac{\omega^2}{\omega_D^2}\,\frac{1}{2}\, d\omega \rightarrow \frac{u_z}{2}$$

(3)

theory only accounts for half of total energy, include spin also

$$\Rightarrow U = U_Z + \frac{4N}{\omega_D^2}\int_0^{\omega_D} \frac{\hbar\omega^2}{e^{\hbar\omega/kT}-1}\,d\omega$$

e) $$C_V = \left.\frac{\partial U}{\partial T}\right|_V = \frac{4N}{\omega_D^2}\int_0^{\omega_D} \hbar\omega^2 \frac{\partial}{\partial T}\left(e^{\hbar\omega/kT}-1\right)^{-1} d\omega$$

$$= \frac{4N}{\omega_D^2}\int_0^{\omega_D} \hbar\omega^2 \times \frac{\hbar\omega}{kT^2} \times \left(e^{\hbar\omega/kT}-1\right)^{-2} e^{\hbar\omega/kT}\,d\omega$$

$$= \frac{4N\hbar^2}{\omega_D^2 T^2 k}\int_0^{\omega_D} \frac{\omega^3 e^{\hbar\omega/kT}}{\left(e^{\hbar\omega/kT}-1\right)^2}\,d\omega$$

$x = \frac{\hbar\omega}{kT}$, $x = \frac{\hbar\omega_D}{kT} = \frac{\Theta_D}{T}$ $\Rightarrow \Theta_D = \frac{\hbar\omega_D}{k}$

$dx = \frac{\hbar\,d\omega}{kT}$, $\omega = \frac{kTx}{\hbar}$, $\omega_D = \frac{k\Theta_D}{\hbar}$

$$= \frac{4N\cancel{\hbar^2}}{\left(\frac{k\Theta_D}{\hbar}\right)^2 T^2 k}\int_0^{\Theta_D/T} \frac{k^3T^3x^3}{\hbar^3}\frac{e^x}{(e^x-1)^2}\,\frac{kT}{\hbar}\,dx$$

$$= \frac{4NT^2k}{\Theta_D^2}\int_0^{\Theta_D/T} \frac{x^3e^x}{(e^x-1)^2}\,dx = 4Nk\left(\frac{T}{\Theta_D}\right)^2\int_0^{\Theta_D/T}\frac{x^3e^x}{(e^x-1)^2}\,dx$$

f) $T \to 0$, $\frac{\Theta_D}{T} \to \infty$

$$\Rightarrow 4Nk\left(\frac{T}{\Theta_D}\right)^2\int_0^{\infty}\frac{x^3e^x}{(e^x-1)^2}\,dx \simeq 4Nk\left(\frac{T}{\Theta_D}\right)^2 \times 7.21$$

∴ This is expected as 3D is proportional to $\left(\frac{T}{\Theta_D}\right)^3$

f) $T \to \infty$, $e^x \simeq 1 + x + \dots$

$$\Rightarrow 4Nk\left(\frac{T}{\Theta_D}\right)^2\int_0^{\Theta_D/T}\frac{x^3(1+x+\dots)}{(1+x+\dots-1)^2}\,dx = 4Nk\left(\frac{T}{\Theta_D}\right)^2\int_0^{\Theta_D/T} x^2\,dx$$

$$= 4Nk\left(\frac{T}{\Theta_D}\right)^2 \cdot \left[\frac{x^2}{2}\right]_0^{\Theta_D/T} = 4Nk\cancel{\left(\frac{T}{\Theta_D}\right)^2}\cancel{\left(\frac{\Theta_D}{T}\right)^2} = \frac{4Nk}{2} = 2Nk$$

(2D)

∴ Matches classical limit!

8)

$S_G = \sum_i^N f_i e^{i\underline{G}\cdot\underline{r}}$

- S_G = ~~structure~~ unit structure factor
- f_i = atomic form factor
- $\underline{G}$ = lattice vector $\underline{G} = h\underline{b}_1 + k\underline{b}_2 + l\underline{b}_3$ — Reciprocal wave vector
- $\underline{r}$ = Position of atom in crystal

⇒ Generally non zero when terms do not cancel each other out, more likely in a pure crystal than alloy as in alloy all have the same atomic form factor.

Laue condition : $\Delta = G$

c) fcc: $a(0,0,0), a(\frac{1}{2},\frac{1}{2},0), a(\frac{1}{2},0,\frac{1}{2}), a(0,\frac{1}{2},\frac{1}{2})$

$\underline{G} = \frac{2\pi}{a}\{h\,k\,l\}$

⇒ Assume all have the same f

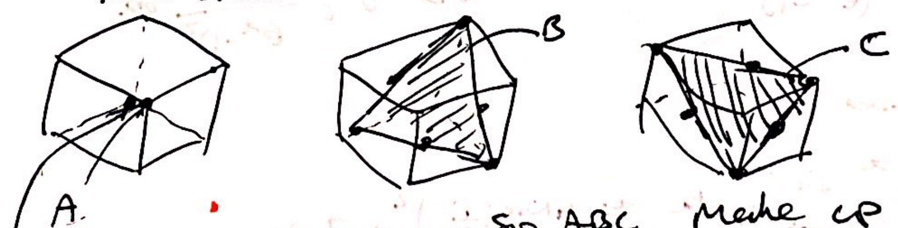
$$S_G = f\left[e^0 + e^{i\frac{2\pi}{a}\cdot a(\frac{1}{2},\frac{1}{2},0)\cdot(h,k,l)} + e^{i\frac{2\pi}{a}\cdot a(\frac{1}{2},0,\frac{1}{2})(hkl)} + e^{i\frac{2\pi}{a}(0,\frac{1}{2},\frac{1}{2})(hkl)}\right]$$

$$= f\left[1 + (-1)^{(h+k)} + (-1)^{(h+l)} + (-1)^{(k+l)}\right]$$

$$= \begin{cases} 4f & \text{when } h,k,l \text{ all odd/even} \\ 0 & \text{otherwise} \end{cases}$$

~~{200}, {112}~~, {111}, {200}, {220}

b) ABC structure is necessary to generate the fcc lattice



A Repeats itself on the opposite corner

So ABC Make up FCC

lattice + basis = fcc

lattice (0,0,0) + (basis)

↳ $\frac{a}{2}(1,1,0) + \frac{a}{2}(1,0,1) + \frac{a}{2}(0,1,1)$ ⇒ fcc!

d) $\lambda = 0.150\,nm$

$2\theta = 42.18°, 49.10°, 71.97°$

$\theta = 21.09°, 24.55°, 35.985°$

hkl	$h^2+k^2+l^2$	$\frac{(h^2+k^2+l^2)_n}{(h^2+k^2+l^2)_1}$	$\theta(°)$	$\sin^2\theta$	$\frac{\sin^2\theta_n}{\sin^2\theta_1}$
111	3	1	21.09	0.1294	1
200	4	4/3	24.55	0.1726	4/3
220	8	8/3	35.985	0.345	8/3

④

So angles ⟺ indices
(2θ) {hkl}

42.18° ⟺ {111}
49.10° ⟺ {200}
~~8~~ 71.97° ⟺ {220}

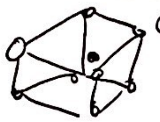
$n\lambda = 2d\sin\theta$

$$\frac{\lambda}{\sin\theta} = \frac{0.15}{\sin(21.09)} = d = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{a}{\sqrt{3}}$$

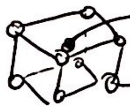
$$a = \frac{0.15 \times \sqrt{3}}{\sin(21.09)} = 0.\cancel{722}\,nm$$

3.61Å

e) Above Tc:



Below Tc:



Above Tc: $\cancel{S_G = \sum_j f_j e^{iG\cdot r}}$ $\quad S_G = \sum_j f_j e^{iG\cdot r}$

$\cancel{f_{Cu/Zn}}$ $f_{Cu/Zn} = f$

$$\cancel{S_G}\quad S_G = f\left(e^0 + e^{i\frac{2\pi}{a}(\frac{a}{2},\frac{a}{2},\frac{a}{2})(h,k,l)}\right) = f\left(1 + e^{i\pi(h+k+l)}\right)$$

$$= f\left(1 + (-1)^{h+k+l}\right)$$

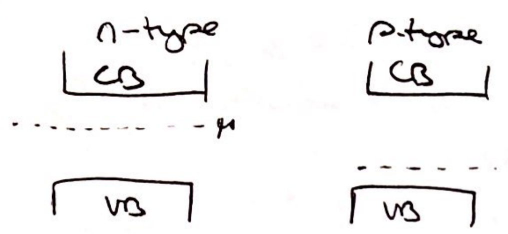
$$= \begin{cases} 2f & \text{if } h+k+l = \text{even} \\ 0 & \text{if } h+k+l = \text{odd} \end{cases}$$

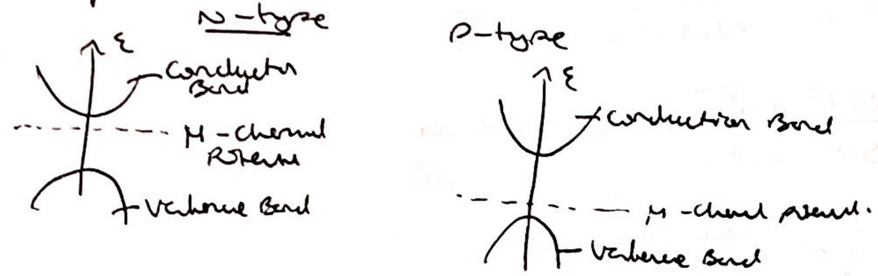
Below Tc: $S_G = f_{Zn}e^0 + f_{Cu}e^{i\pi(h+k+l)} = f_{Zn} + (-1)^{h+k+l} f_{Cu}$

$$= \begin{cases} f_{Zn} + f_{Cu} & \text{if } h+k+l = \text{even} \\ f_{Zn} - f_{Cu} & \text{if } h+k+l = \text{odd} \end{cases}$$

- $|S_G|^2 \propto$ Intensity, I, ∴ ~~B~~ upon x-ray scattering, the reflected intensity could be recorded. If it is fairly constant then we are above Tc. If there is a discrepancy then we have gone below Tc, hence Tc may be experimentally determined.

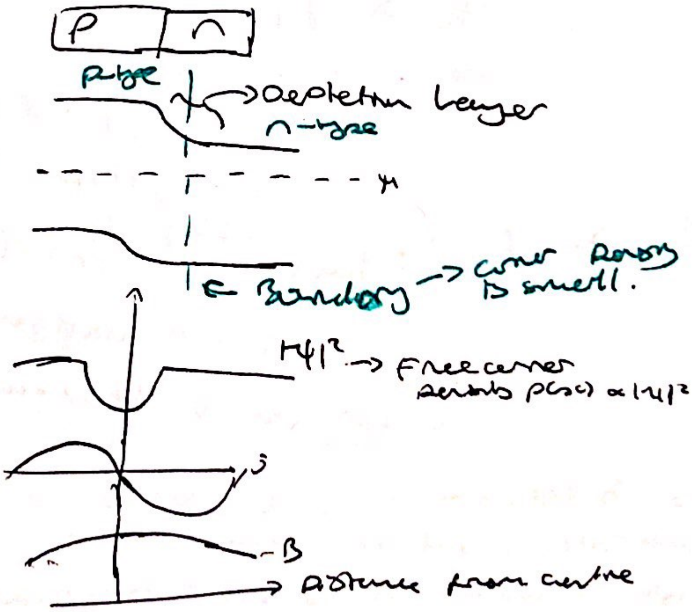
9)





- n-type semiconductors have a greater concentration of "donor" ion impurities, that is, ions which give away free electrons to the conduction band, thus raising the chemical potential.
- P-type semiconductors have a greater concentration of "acceptor" ion impurities, so produce free holes, thus lowering the chemical potential towards the valence band

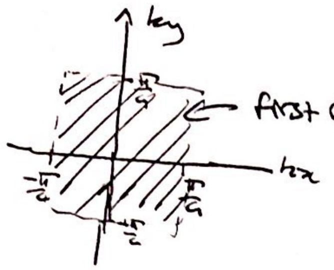
b)



(5)

10) a) as $\underline{G} = h\underline{b}_1 + k\underline{b}_2 + l\underline{b}_3$

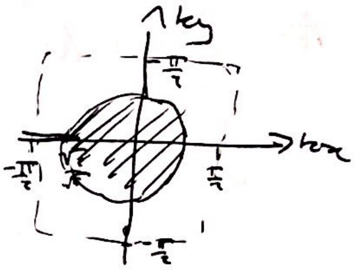
& $\underline{k} = \frac{2\pi}{a}$



b) $\boxed{\pi k_f^2 = \frac{1}{2}\left(\frac{2\pi}{a}\right)^2} \Rightarrow 2D$

$k_f^2 = \frac{1}{2\pi} \cdot \frac{4\pi^2}{a^2} = \frac{2\pi}{a^2}$

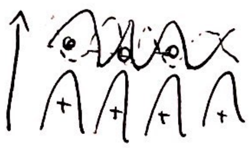
$k_f = \frac{\sqrt{2\pi}}{a} = \frac{\sqrt{2}}{\sqrt{\pi}} \cdot \frac{\pi}{a}$



Shortest distance: $\left(\frac{\pi}{a}\right)$

$\frac{k_f}{r} = \sqrt{\frac{2}{\pi}} \approx 0.80$

c)



the electron potential will change as it interacts with the ion core, as the potential gets stronger, the two interact more. With the surface of the fermi circle bending towards the BZB.

So the Fermi-surface will be more curved outwards as a result. The states within the first BZB will be completely occupied and those in the second BZB will need to be bridged, so the fermi surface will spill into the second BZB.

d) $g(k)\,dk = 2\cancel{\pi}\left(\frac{a}{2\pi}\right)^2 \cdot 2\pi k\,dk = \cancel{\pi}\,\frac{a^2}{\pi^{\cancel{2}}}\,\cancel{\pi} k\,dk = \frac{a^2 k}{\pi}\,dk$

$$g(k)\,dk = g(\varepsilon)\,d\varepsilon$$

$$\frac{a^2 k}{\pi}\frac{dk}{d\varepsilon} = g(\varepsilon)$$

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

$$\frac{d\varepsilon}{dk} = \frac{\hbar^2 k}{m}$$

$$g(\varepsilon) = \frac{a^2 k}{\pi}\cdot\frac{m}{\hbar^2 k} = \frac{m a^2}{\pi\hbar^2}$$

$$E = \int_0^{\varepsilon_f} g(\varepsilon)\,\varepsilon\,d\varepsilon = \frac{m a^2}{\pi\hbar^2}\frac{\varepsilon_f^2}{2} = \frac{m a^2}{\pi\hbar^2}\frac{\varepsilon_f^2}{2}$$

$$N = \int_0^{\varepsilon_f} g(\varepsilon)\,d\varepsilon = \frac{m a^2 \varepsilon_f}{\pi\hbar^2}$$

$$\frac{N}{a^2} = n = \frac{m\varepsilon_f}{\pi\hbar^2}$$

$$\varepsilon_f = \frac{n\pi\hbar^2}{m}$$

e) $N = \int_0^\infty g(\varepsilon) f(\varepsilon)\,d\varepsilon$

$$= \frac{m a^2}{\pi\hbar^2}\int_0^\infty \frac{1}{e^{(\varepsilon-\mu)/kT}+1}\,d\varepsilon$$

$$\cancel{(\varepsilon-\mu/kT) = x} \qquad x = \frac{\varepsilon-\mu}{kT}$$

$$dx = \frac{d\varepsilon}{kT}$$

$$= \frac{m a^2}{\pi\hbar^2}\int_{-\frac{\mu}{kT}}^\infty \frac{kT\,dx}{e^x+1} = \frac{kTma^2}{\pi\hbar^2}\int_{-\frac{\mu}{kT}}^\infty \frac{dx}{e^x+1}$$

$$N = \frac{kTma^2}{\pi\hbar^2}\ln\left(1+e^{-\mu/kT}\right)$$

$$n = \frac{N}{a^2} = \frac{kTm}{\pi\hbar^2}\ln\left(1+e^{-\mu/kT}\right)$$

$$1 = kT\underbrace{\frac{m}{\pi\hbar^2 n}}_{(\varepsilon_f)^{-1}}\ln\left(1+e^{-\mu/kT}\right)$$

$$\frac{\varepsilon_f}{kT} = \ln\left(1+e^{-\mu/kT}\right)$$

$$e^{\varepsilon_f/kT} = 1+e^{-\mu/kT}$$

$$\ln\left(e^{\varepsilon_f/kT}-1\right) = -\mu/kT$$

$$\mu = -kT\ln\left(e^{\varepsilon_f/kT}-1\right)$$