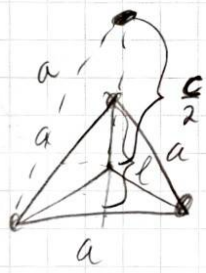
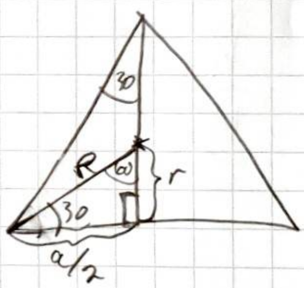
Task 1

a) Each point on the boundary contain $\frac{1}{6}$ atoms, the two bottom and top center points contain half an atom each,
And there are three whole atoms in the domain

$$\Rightarrow \frac{1}{6} \cdot 12 + 3 + \frac{1}{2} \cdot 2 = \underline{\underline{6 \text{ atoms}}}$$

b) There is a distance 'a' between all atoms.





$$\frac{a}{2} \cdot \frac{1}{R} = \cos 30$$

$$\Rightarrow R = \frac{a}{2\cos 30} = \frac{a}{\sqrt{3}}$$

$$\Rightarrow R^2 + \left(\frac{c}{2}\right)^2 = a^2$$

$$\Rightarrow c^2 = 4(a^2 - R^2)$$

$$= 4\left(a^2 - \frac{a^2}{3}\right)$$

$$\Rightarrow c^2 = 4 \cdot \frac{2}{3} a^2 \Rightarrow \underline{\underline{c = 1{,}633a}}$$

c) Show that Volume of atoms to Volume of unit cell ratio is 74%:

Gotta assume the atoms take $\frac{a}{2}$ length of space ($r = \frac{a}{2}$)

$$\Rightarrow V_a = \frac{4}{3}\pi \left(\frac{a}{2}\right)^3 \cdot \underbrace{6}_{\text{atoms}}$$

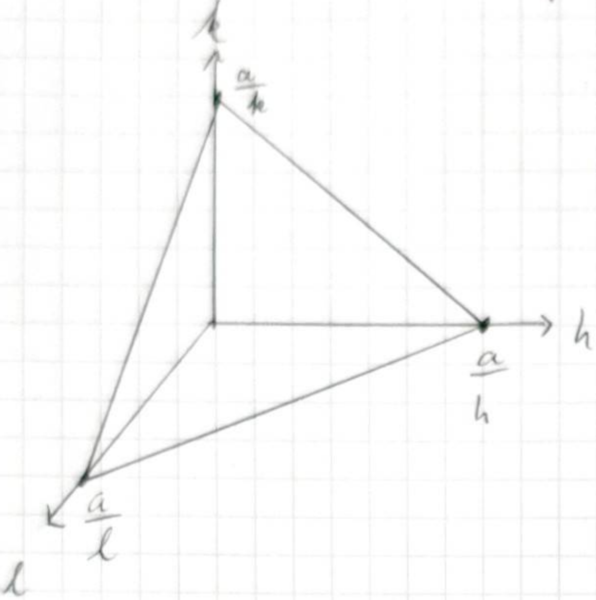
$$V_S = \frac{1}{2} 3\sqrt{3}\, a^2 \cdot h \quad , \quad h = 1{,}633a$$

$$\Rightarrow \frac{V_a}{V_S} = \frac{8\pi \frac{a^3}{8}}{\frac{1}{2} 3\sqrt{3} \cdot 1{,}633a^3} = \frac{2\pi a^3}{3\sqrt{3} \cdot 1{,}633\, a^3}$$

$$= \frac{2\pi}{3 \cdot \sqrt{3} \cdot 1{,}633} = 0{,}74 = \underline{\underline{74\%}}$$

Task 2

Show that $d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$



This plane can be parameterized to

$$h_x + l_y + k_z = a$$

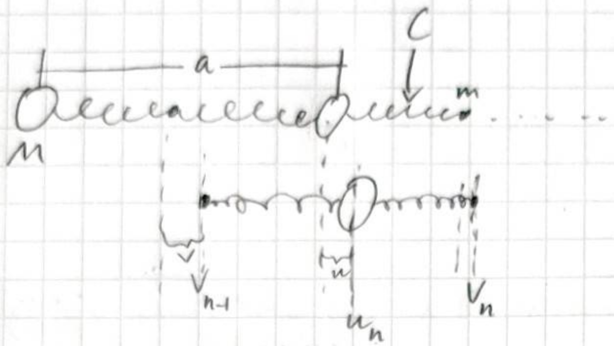
The next plane would be of the form

$$h_x + l_y + k_z = 2a$$

And we know the formula for distance between two planes of this form is

$$d = \frac{|a-2a|}{\sqrt{h^2+l^2+k^2}}$$

Task 3



a) $M \frac{\partial^2 u_n}{\partial t^2} = F^u_{n,n-1} + F^u_{n,n+1}$

$m \frac{\partial^2 v_n}{\partial t^2} = F^v_{n,n-1} + F^v_{n,n+1}$

$$M \frac{\partial^2 u_n}{\partial t^2} = -C(u_n - v_{n-1}) - C(u_n - v_n) = C(v_{n-1} + v_n - 2u_n)$$

$$m \frac{\partial^2 v_n}{\partial t^2} = -C(v_n - u_n) - C(v_n - u_{n+1}) = C(u_{n+1} + u_n - 2v_n)$$

Assume the solution has the form

$u_n = u e^{i(nka - \omega t)}$, $v_n = v e^{i(nka - \omega t)}$

$$-M\omega^2 u_n = C(v_{n-1} + v_n - 2u_n) \quad ①$$

$$-m\omega^2 v_n = C(u_{n+1} + u_n - 2v_n) \quad ②$$

①:

$$-M\omega^2 u = C\left(\frac{v e^{-ika} \cancel{e^{inka}} e^{-i\omega t} + v \cancel{e^{inka}} e^{-i\omega t} - 2u \cancel{e^{inka}} e^{-i\omega t}}{\cancel{e^{inka}} e^{-i\omega t}}\right)$$

$$= Cv\left(1+e^{-ika}\right) - 2Cu$$

Same procedure goes for ②

$$\Rightarrow \quad -m\omega^2 v = Cu\left(e^{ika}+1\right) - 2Cv$$

$$\Rightarrow \left.\begin{aligned} u(2C - M\omega^2) - Cv(1+e^{-ika}) &= 0 \\ v(2C - m\omega^2) - Cu(1+e^{ika}) &= 0 \end{aligned}\right\} ③$$

The homogenous set of linear eq. ③ have a non-trivial solution when the determinant of the matrix of coefficiants is 0.

$$\Rightarrow \begin{vmatrix} 2C - M\omega^2 & -C(1+e^{-ika}) \\ -C(1+e^{ika}) & 2C - m\omega^2 \end{vmatrix} = 0$$

$$\Rightarrow (2c - M\omega^2)(2c - m\omega^2) - c^2(1+e^{ika})(1+e^{-ika}) = 0$$

$$\Rightarrow 4c^2 - 2c(M\omega^2 + m\omega^2) + Mm\omega^4 - c^2(1+1+e^{ika}+e^{-ika}) = 0$$

$$\frac{e^{ika}+e^{-ika}}{2} = \cos(ka)$$

$$\Rightarrow 4c^2 - 2c\omega^2(M+m) + Mm\omega^4 - 2c^2(1+\cos(ka)) = 0$$

$$\Rightarrow Mm\omega^4 - 2c\omega^2(M+m) + 2c^2(1-\cos(ka)) = 0$$

Replacing ω^2 by x gives

$$Mm\,x^2 - 2c\,x(M+m) + 2c^2(1-\cos(ka)) = 0$$

$$\Rightarrow \omega^2 = \frac{\cancel{2}c(M+m) \pm \left(\cancel{4}c^2(M+m)^2 - \cancel{4}Mm\,2c^2(1-\cos(ka))\right)^{1/2}}{\cancel{2}Mm}$$

$$\Rightarrow \omega^2 = \frac{c(M+m)}{Mm} \pm \left(c^2\frac{(M+m)^2}{(Mm)^2} - \frac{2c^2}{Mm}(1-\cos(ka))\right)^{1/2}$$

This gives 4 possibilities for ω:

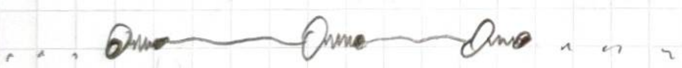
$$\omega = \left(\frac{C(M+m)}{Mm} \overset{\text{optical}}{\underset{\text{acoustic}}{\pm}} \left(C^2 \frac{(M+m)^2}{(Mm)^2} - \frac{2C^2}{Mm}\left(1-\cos(ka)\right) \right)^{1/2} \right)^{1/2}$$

Comment; We don't include the negative frequencies from $\omega = \pm\sqrt{x}$

b)

Optical branch:

Have higher frequencies that occur when the two different types of atoms oscillate out of phase



Acoustic branch:

They oscillate in phase with lower frequencies.

Task 4) Real space k-space

The area of the k-space unit cell is

$$S_u = \frac{1}{2} 3\sqrt{3} \left(\frac{2\pi}{L}\right)^2$$

So the Number of modes of a circle of radius k is

$$N = \frac{\pi k^2}{S_u}$$

And the density of states is

$$D(\omega) = \frac{dN}{d\omega} \frac{1}{v_g}$$

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

$$\frac{dN}{d\omega} = \frac{2\pi\omega}{S_u v_g^2} = \frac{4\pi \omega L^2}{4\pi^2 3\sqrt{3}\, v_g^2}$$

$$\Rightarrow D(\omega) = \begin{cases} \dfrac{\omega S}{3\sqrt{3}v_g^3} & , \omega \leq \omega_D \\ 0 & , \omega > \omega_D \end{cases}$$

S - surface of entire crystal

Max allowed states is theorized to be 2N in 2D crystal.

$$\Rightarrow 2N = \frac{S}{3\sqrt{3}\,v_g^3} \int_0^{\omega_D} \omega \, d\omega$$

$$= \frac{S\omega_D^2}{2 \cdot 3\sqrt{3}\,v_g^3}$$

$$\Rightarrow \omega_D^2 = \frac{4 \cdot 3\sqrt{3}\,v_g^3 \cdot 2N}{S}$$

$$\Rightarrow \omega_D = \left(8 \cdot 3\sqrt{3}\,v_g^3\right)^{1/2} \cdot \rho_S^{\frac{1}{2}}$$

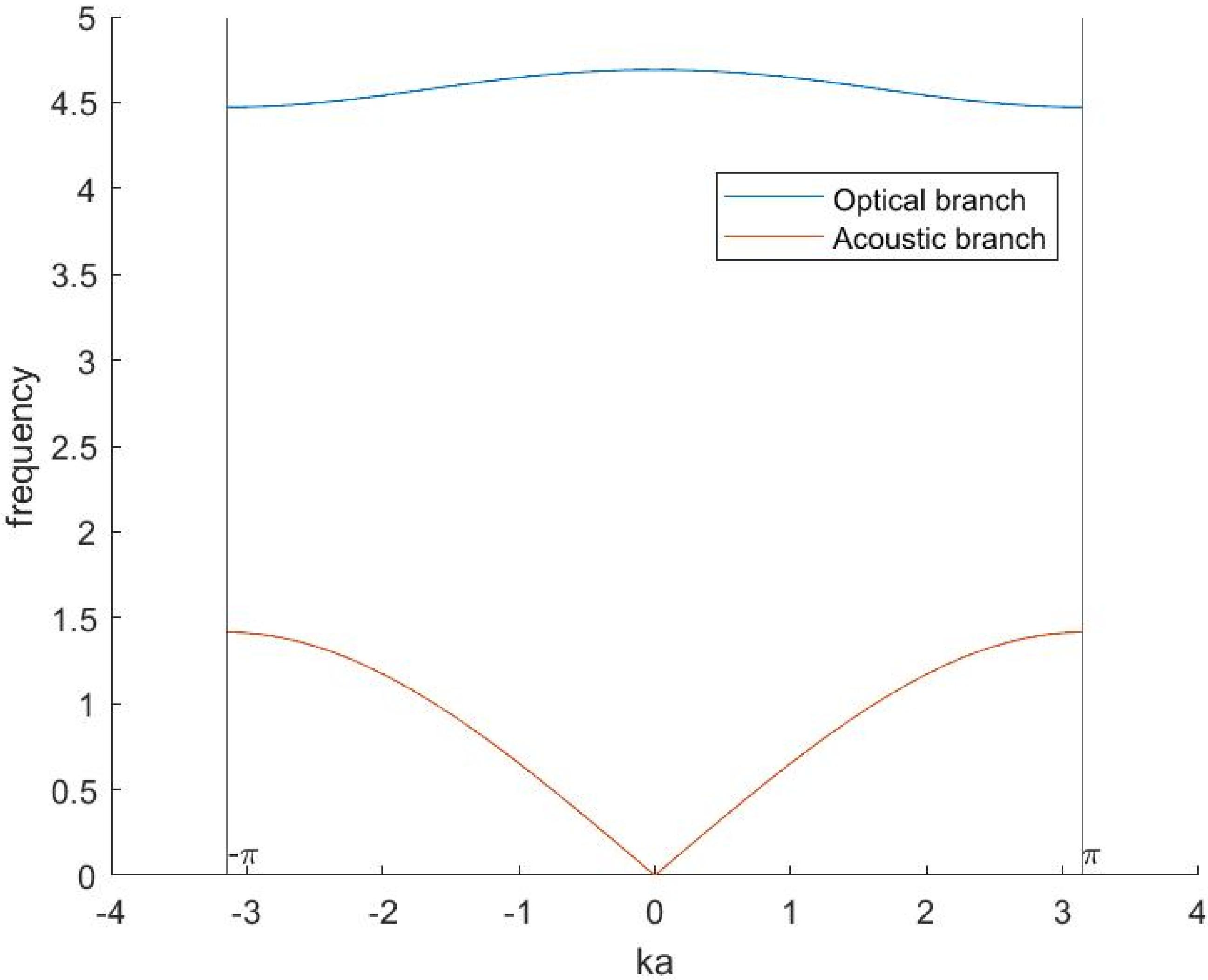
ρ is the number of atoms per area, and would be the same as the number of atoms per unit cell.

$$\Rightarrow \rho_S = \frac{3\,\text{atoms}}{\frac{1}{2}\,3\sqrt{3}\,a^2} = \frac{2}{\sqrt{3}\,a^2}$$

So the Debye frequency is therefore

$$\omega_D = \left(8 \cdot 3\sqrt{3} \cdot (10^3)^3\right)^{1/2} \cdot \left(\frac{2}{\sqrt{3} \cdot 3 \cdot 10^{-10}}\right)^{1/2}$$

$$= \underline{\underline{1{,}265 \cdot 10^{10}\, s^{-1}}}$$



Optical branch
Acoustic branch
frequency
ka
-π
π
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
-4
-3
-2
-1
0
1
2
3
4