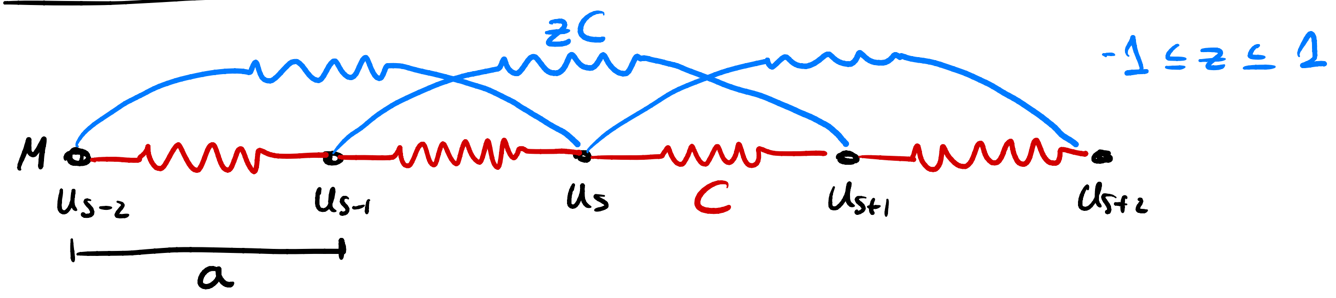
Problem 1



1a

We first need to set up the equations of motion:

$$M\frac{d^2u_s}{dt^2} = -C(u_s - u_{s-1}) + C(u_{s+1} - u_s)$$

$$-zC(u_s - u_{s-2}) + zC(u_{s+2} - u_s)$$

$$= -C\left[(2u_s - u_{s-1} - u_{s+1}) + z(2u_s - u_{s-2} - u_{s+2})\right]$$

Since we are looking for collective oscillation modes, we propose a solution of the form

$$u_s = Ae^{i(\omega t - kx)} = Ae^{i(\omega t - ksa)}$$

And implementing this into the E.o.m

$$-M\omega^2 \cancel{A}\cancel{e^{i\omega t}}\cancel{e^{-iksa}} = -\cancel{A}\cancel{e^{i\omega t}}\cancel{e^{-iksa}}\,C \times$$

$$\left[2 - e^{ika} - e^{-ika} + 2z - ze^{i2ka} - ze^{-i2ka}\right]$$

$$\Rightarrow M\omega^2 = 2C\left[1 - \cos(ka) + z\left(1 - \cos(2ka)\right)\right]$$

$$\omega = 2\sqrt{\frac{C}{M}}\sqrt{\sin^2\left(\frac{ka}{2}\right) + z\sin^2(ka)}$$

1b-c| We can get the speed of sound in the limit $k \to 0$

$$\omega \simeq 2\sqrt{\frac{C}{M}}\sqrt{\left(\frac{ka}{2}\right)^2 + z(ka)^2}$$

$$= \sqrt{\frac{C}{M}}\, a\sqrt{1+4z}\,|k| = V_s |k|$$

$$\Rightarrow V_s = \sqrt{\frac{C}{M}}\, a\sqrt{1+4z}$$

Which obviously recovers the regular case with only first neighbour interactions when $z=0$

The two signs of z show the following behaviours

- $z>0 \Rightarrow$ The material is more bounded together and so collective oscillations travel faster $\Rightarrow V_s \uparrow\uparrow$
- $z<0 \Rightarrow$ We have dampening that, if $z<-1/4$ eliminate totally the collective oscillation and phonons do not propagate

2|

In the Debye model we have a cutoff frequency that limits the amount of modes available. This cutoff is related to the Debye temperature through:

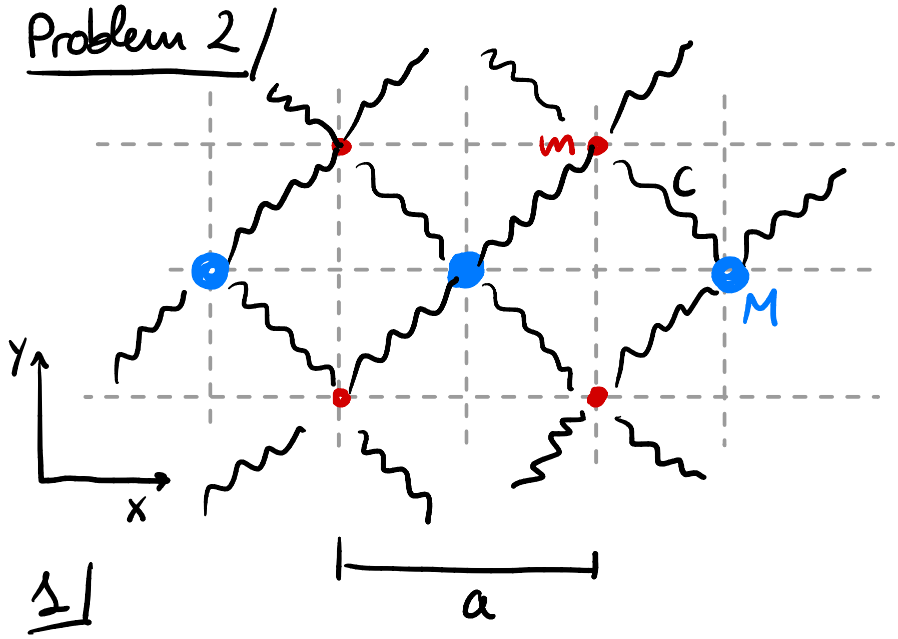
$$T_D = \frac{\hbar \omega_D}{K_B}$$

On the other hand, we know that, regardless of the dimensionality of the system, $\omega_D \propto V_s$. If we then have a $T_D(z) = \frac{1}{4} T_D(z=0)$, this will mean

$$\frac{V_S(z)}{V_S(0)} = \frac{1}{4} = \sqrt{1+4z} \Rightarrow z = \frac{\frac{1}{16} - 1}{4} = -\frac{15}{64}$$

$$\boxed{z = -\frac{15}{64}}$$

Problem 2 /



1 /

We will denote by $u_{(x,y)}$ and $V_{(x,y)}$ the displacement from the plane of the red (m) and blue (M) atom, respectively.

Assuming that the oscillations are small enough, we can leverage $\lim_{x \to 0} \tan(x) \simeq x$ and take that the "spring" elongations are proportionally related to the absolute values of the atoms perpendicular displacements

With this in mind, the E.o.M for the two types of atoms read:

$$M \frac{d^2 v_{xy}}{dt^2} = -C\left(4V_{xy} - u_{x+\frac{a}{2},y+\frac{a}{2}} - u_{x+\frac{a}{2},y-\frac{a}{2}} - u_{x-\frac{a}{2},y+\frac{a}{2}} - u_{x-\frac{a}{2},y-\frac{a}{2}}\right)$$

$$m \frac{d^2 u_{xy}}{dt^2} = -C\left(4u_{x,y} - V_{x+\frac{a}{2},y+\frac{a}{2}} - V_{x+\frac{a}{2},y-\frac{a}{2}} - V_{x-\frac{a}{2},y-\frac{a}{2}} - V_{x-\frac{a}{2},y+\frac{a}{2}}\right)$$

Or by using the reference frame of a unit cell

$$\begin{cases} M\dfrac{d^2 v_{00}}{dt^2} = -C\left(4v_{00} - u_{\frac{a}{2}\frac{a}{2}} - u_{\frac{a}{2}-\frac{a}{2}} - u_{-\frac{a}{2}\frac{a}{2}} - u_{-\frac{a}{2}-\frac{a}{2}}\right) \\ m\dfrac{d^2 u_{00}}{dt^2} = -C\left(4u_{00} - v_{\frac{a}{2}\frac{a}{2}} - v_{\frac{a}{2}-\frac{a}{2}} - v_{\frac{a}{2}\frac{a}{2}} - v_{\frac{a}{2}-\frac{a}{2}}\right) \end{cases}$$

2)

A usual, we are looking for collective oscillatory phenomena and so we propose solutions of the form:

$$\begin{cases} u_{xy} = Ae^{i(\vec{k}\cdot\vec{r}-\omega t)} = Ae^{i(k_x x + k_y y - \omega t)} \\ v_{xy} = Be^{i(\vec{k}\cdot\vec{r}-\omega t)} = Be^{i(k_x x + k_y y - \omega t)} \end{cases}$$

If we plug these ansatz into the EoM:

$$-M\omega^2 A \cancel{e^{-i\omega t}} = -4AC\cancel{e^{-i\omega t}} - BC \times$$

$$\times\left[e^{i\frac{a}{2}(k_x+k_y)\cancel{-i\omega t}} + e^{i\frac{a}{2}(k_x-k_y)\cancel{-i\omega t}} + e^{i\frac{a}{2}(-k_x+k_y)\cancel{-i\omega t}} + e^{-i\frac{a}{2}(k_x+k_y)\cancel{-i\omega t}}\right]$$

$$\Rightarrow -M\omega^2 A = -4AC - 2BC\left(\cos\left(\frac{a}{2}(k_x+k_y)\right) + \cos\left(\frac{a}{2}(k_x-k_y)\right)\right)$$

$$= -4AC - 4BC\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)$$

$$-m\omega^2 B\cancel{e^{-i\omega t}} = -4BC\cancel{e^{-i\omega t}} - AC \times$$

$$\times\left[e^{i\frac{a}{2}(k_x+k_y)\cancel{-i\omega t}} + e^{i\frac{a}{2}(k_x-k_y)\cancel{-i\omega t}} + e^{i\frac{a}{2}(-k_x+k_y)\cancel{-i\omega t}} + e^{-i\frac{a}{2}(k_x+k_y)\cancel{-i\omega t}}\right]$$

$$\Rightarrow -m\omega^2 B = -4BC - 4AC\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)$$

$$\Rightarrow \begin{cases} -A(4C - M\omega^2) - 4BC\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) = 0 \\ -4AC\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) - B(4C - m\omega^2) = 0 \end{cases}$$

We can think about this pair of equations as a system of linear equations for (A,B) $\Rightarrow$ We have to enforce a null determinant for the coefficient matrix

$$\begin{vmatrix} -(4C - M\omega^2) & -4C\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) \\ -4C\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) & -(4C - m\omega^2) \end{vmatrix} = 0$$

$$\Rightarrow mM\left(\frac{4C}{M} - \omega^2\right)\left(\frac{4C}{m} - \omega^2\right) - 16C^2\cos^2\left(\frac{k_x a}{2}\right)\cos^2\left(\frac{k_y a}{2}\right) = 0$$

$$16C^2 - 4mC\omega^2 - 4MC\omega^2 + mM\omega^4 - 16C^2\cos\left(\frac{k_x a}{2}\right)\cos^2\left(\frac{k_y a}{2}\right) = 0$$

$$mM\omega^4 - 4C(m+M)\omega^2 + C^2\left(16 - 16\overbrace{\cos\left(\frac{k_x a}{2}\right)\cos^2\left(\frac{k_y a}{2}\right)}^{=\alpha^2}\right) = 0$$

$$\Rightarrow \omega_\pm^2 = \frac{4C(m+M) \pm \sqrt{16C^2(m+M^2) - 64mMC^2(1-\alpha^2)}}{2mM}$$

$$= 2C\,\frac{m+M}{mM}\left\{1 \pm \sqrt{1-4\frac{mM}{(m+M)^2}(1-\alpha^2)}\right\} \quad \checkmark$$

3)

To study the case $\vec{k}\to 0$ we just have to study α's behaviour

$$\alpha = \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) \underset{|\vec{k}|\to 0}{\simeq} \left(1-\frac{k_x^2 a^2}{8}\right)\left(1-\frac{k_y^2 a^2}{8}\right)$$

$$= 1 - \frac{k_x^2 a^2}{8} - \frac{k_y^2 a^2}{8} + \mathcal{O}(k^4) \simeq 1 - \frac{a^2|\vec{k}|^2}{8}$$

And since there aren't more dependencies on $\vec{k}$ in $\omega_\pm$ it is obvious that $\omega_\pm$ also does not depend on the diretion of $\vec{k}$ but just in its modulus

4)

$$\vec{V}_s = \lim_{k\to 0} \vec{\nabla}_{\vec{k}}\, \omega_-(\vec{k})$$

We will work with $\omega_\pm$ already in the $\vec{k}\to 0$ case used in the previous section

$$\alpha \simeq 1 - \frac{a^2k^2}{8} \Rightarrow 1-\alpha^2 = 1 - \left(1 - \frac{a^2k^2}{4} + \mathcal{O}(k^4)\right)$$

$$\Rightarrow \omega_-^2(\vec{q}) = 2C\,\frac{m+M}{mM}\left\{1 - \sqrt{1 - \frac{mMa^2k^2}{(m+M)^2}}\right\}$$

We can use that for $k\to 0 \Rightarrow \sqrt{1-x} \simeq 1 - \frac{x}{2}$

$$\omega_+^2(\vec{q}) \simeq \cancel{2}C\,\frac{\cancel{m+M}}{\cancel{mM}}\left\{\cancel{1} - \cancel{1} + \frac{\cancel{m}Ma^2k^2}{\cancel{2}(m+M)^{\cancel{2}}}\right\} = \frac{Ca^2}{2(m+M)}|k|^2$$

$$\Rightarrow \vec{V}_s = \sqrt{\frac{Ca^2}{(m+M)}}\frac{1}{|k|^2}(k_x\hat{a}_x + k_y\hat{a}_y) \to |\vec{V}_s| = \sqrt{\frac{Ca^2}{m+M}} \Rightarrow \text{Isotropic!}$$