Problem I

Consider a one-dimensional crystal, with lattice constant a and monatomic base, formed by atoms of mass M that via the oscillations parallel to the crystal interact harmonically in first and second neighbors, with constants with constants C_1 and $C_2 \equiv zC_1$, respectively, with $-1 \leq z \leq 1$.

1. Determine, based on the parameters M, a, C_1 i z:
   (a) The phonon dispersion relation.
   (b) The speed of sound.
   (c) Check that when $z = 0$ the corresponding results are retrieved in the case with interactions only up to first neighbors.
2. In materials that experience phase transitions or ferroelectricity, the so-called soft phonons are relevant. The aforementioned materials are characterized, among other particularities, by having a Debye temperature much lower than the expected value. Here, we study a material with a Debye temperature that is a quarter of the value that would be expected if only first-neighbor interactions were considered. Use the results from the previous section to determine the value of the constant z of this material.

Problem II

Assuming a two-dimensional crystal, with a square lattice of constant a and basis of two atoms, of masses m and M and located at $(0, 0)$ and at $a(1/2, 1/2)$, respectively. For vibrations perpendicular to the plane, the atoms only interact in first neighbors, harmonically, with a coupling constant C.

1. Write its equations of motion.
2. Show that the dispersion relations of the normal modes of these vibrations can be expressed through the equality:

$$\omega_{\pm}^2(\vec{q}) = 2C\,\frac{m+M}{mM}\left\{1 \pm \sqrt{1 - \frac{4mM}{(m+M)^2}\,(1 - A^2)}\right\}$$

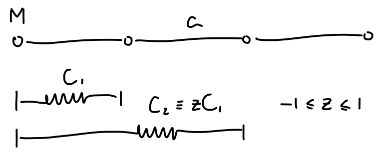
   where

$$|A| = \cos\frac{q_x a}{2}\cos\frac{q_y a}{2}.$$

3. Prove that for $\vec{q} \to 0$ the relation of dispersion of the acoustic branch depends on $|\vec{q}|$ and no of its direction.
4. Determine the speed of sound and check that in this case becomes isotropic.

Problem 1

1.



a) From the harmonic potential U_{ar}, we can reach the equation of motion of the ion:

$$U_{ar} = \frac{1}{2}\left[C_1(u_{n+1}-u_n)^2 + C_1(u_n-u_{n-1})^2 + C_2(u_{n+2}-u_n)^2 + C_2(u_n-u_{n-2})^2\right]$$

$$M\ddot{u}_n = -\frac{\partial U_{ar}}{\partial u_n} = C_1(u_{n+1}+u_{n-1}-2u_n) + C_2(u_{n+2}+u_{n-2}-2u_n)$$

By applying the following ansatz we obtain the phonon dispersion relation:

$$u_n = Ae^{i(kx-\omega t)} \Rightarrow -M\omega^2 = C_1(e^{ika}+e^{-ika}-2) + C_2(e^{ik2a}+e^{-ik2a}-2)$$

$$\Rightarrow -\omega^2 = \frac{2C_1}{M}(\cos(ka) - 1 + z\cos(2ka) - z)$$

b) The speed of sound is obtained by inspecting the form of the dispersion relation when $k \to 0$, which should be like $\omega(k) = |V_s|k$.

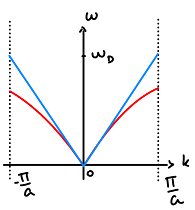
$$k \to 0 \Rightarrow \cos(ka) \approx 1 - \frac{k^2a^2}{2}, \quad \cos(2ka) \approx 1 - 2k^2a^2$$

$$\Rightarrow \omega^2 = \frac{2C_1}{M}\left(+\frac{k^2a^2}{2} + 2z\,k^2a^2\right) = (1+4z)\frac{C_1}{M}k^2a^2$$

$$\Rightarrow \omega = |V_s|k = \sqrt{(1+4z)\frac{C_1}{M}}\cdot ak \Rightarrow V_s = \sqrt{(1+4z)\frac{C_1}{M}}\cdot a$$

c) $z = 0 \Rightarrow \omega^2 = \frac{2C_1}{M}(\cos(ka) - 1)$ and $V_s = \sqrt{\frac{C_1}{M}}\cdot a$, which are the 1st neighbor aproximation results.

2.



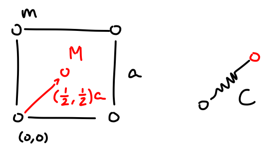
We consider the Debye model, meaning $\omega(k) = |V_s|k$.

Then, the Debye temperature is $\Theta_D = \frac{\hbar}{k_B}\omega_D = \frac{\hbar}{k_B}|V_s|\frac{\pi}{a}$

If $\Theta_D = \frac{1}{4}\Theta_D^{1st\text{-}n}$, with $\Theta_D \propto \omega_D \Rightarrow \omega_D = \frac{\omega_D^{1st\,n}}{4}$

$$\left.\begin{aligned} &\omega_D^{1st.n} = \sqrt{\frac{C_1}{M}}\cdot a\,\frac{\pi}{a} = \sqrt{\frac{C_1}{M}}\cdot\pi \Rightarrow \frac{\omega_D^{1st.n}}{4} = \sqrt{\frac{C_1}{M}}\frac{\pi}{4} \\ &\omega_D = \sqrt{(1+4z)}\sqrt{\frac{C_1}{M}}\pi \end{aligned}\right\} \Rightarrow \frac{1}{4} = \sqrt{1+4z} \Rightarrow z = \frac{1}{4}\left(\frac{1}{16}-1\right) = -0.23 \quad \left(-\frac{15}{64}\right)$$

Problem 2



a,b) For simplicity, we write the equations of motion for the atoms in the (0,0) cell:

$$m\ddot{u}_{00} = C\,(v_{00} + v_{-10} + v_{0-1} + v_{-1-1} - 4u_{00})$$
$$M\ddot{v}_{00} = C\,(u_{00} + u_{10} + u_{01} + u_{11} - 4v_{00})$$

Ansatz $\left\{ \begin{array}{l} u_{\alpha\beta} = A e^{i(\vec{k}\vec{r}_{\alpha\beta})} \\ v_{\alpha\beta} = B e^{i(\vec{k}\vec{r}_{\alpha\beta})} \end{array} \right.$

$$\vec{R}_{10} = a\hat{x} \qquad \vec{R}_{-10} = -a\hat{x}$$
$$\vec{R}_{01} = a\hat{y} \qquad \vec{R}_{0-1} = -a\hat{y}$$
$$\vec{R}_{11} = a(\hat{x}+\hat{y}) \qquad \vec{R}_{-1-1} = -a(\hat{x}+\hat{y})$$

$$\Rightarrow \begin{cases} -\dfrac{mA\omega^2}{C} = B\left(1 + e^{-ik_xa} + e^{-ik_ya} + e^{-i(k_x+k_y)a}\right) - 4A \\ -\dfrac{MB\omega^2}{C} = A\left(1 + e^{ik_xa} + e^{ik_ya} + e^{-i(k_x+k_y)a}\right) - 4B \end{cases}$$

($A\neq 0, B\neq 0$:

$$\begin{vmatrix} m\omega^2 - 4C & C(1+e^{-ik_xa} + e^{-ik_ya} + e^{-i(k_x+k_y)a}) \\ (1+e^{ik_xa} + e^{ik_ya} + e^{i(k_x+k_y)a})C & M\omega^2 - 4C \end{vmatrix} = 0$$

$$\Rightarrow (m\omega^2 - 4C)(M\omega^2 - 4C) - (1+e^{-ik_xa} + e^{-ik_ya} + e^{-i(k_x+k_y)a})C \; C(1+e^{+ik_xa} + e^{+ik_ya} + e^{+i(k_x+k_y)a}) = 0$$

$$\begin{aligned} \Rightarrow mM\omega^4 - 4C(M+m)\omega^2 + 16C^2 &- (1+e^{+ik_xa} + e^{+ik_ya} + e^{+i(k_x+k_y)a})C^2 \\ &- (e^{-ik_xa} + 1 + e^{i(k_y-k_x)a} + e^{ik_ya})C^2 \\ &- (e^{-ik_ya} + e^{i(k_x-k_y)a} + 1 + e^{ik_xa})C^2 \\ &- (e^{-i(k_x+k_y)a} + e^{-ik_ya} + e^{-ik_xa} + 1)C^2 = 0 \end{aligned}$$

$$\Rightarrow mM\omega^4 - 4C(M+m)\omega^2 + 16C^2 - 4C^2\left(\cos(k_xa) + \cos(k_ya) + \frac{\cos[(k_x+k_y)a] + \cos[(k_x-k_y)a]}{2} + 1\right) = 0$$

* $\cos(a\pm b) = \cos(a)\cos(b) \mp \sin(a)\sin(b)$

$$\Rightarrow \frac{\cos[(k_x+k_y)a] + \cos[(k_x-k_y)a]}{2} = \cos(k_xa)\cos(k_ya)$$

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$$\begin{aligned} \cos^2\left(\frac{k_xa}{2}\right)\cos^2\left(\frac{k_ya}{2}\right) &= \frac{\left(e^{i\frac{k_xa}{2}} + e^{-i\frac{k_xa}{2}}\right)^2}{4}\frac{\left(e^{i\frac{k_ya}{2}} + e^{-i\frac{k_ya}{2}}\right)^2}{4} \\ &= \frac{(e^{ik_xa} + e^{-ik_xa} + 2)}{4}\frac{(e^{ik_ya} + e^{-ik_ya} + 2)}{4} \\ &= \frac{\cos(k_xa)+1}{2}\,\frac{\cos(k_ya)+1}{2} \\ &= \frac{1}{4}\left(\cos(k_xa)\cos(k_ya) + \cos(k_xa) + \cos(k_ya) + 1\right) \end{aligned}$$

*
$$\Rightarrow mM\omega^4 - 4C(M+m)\omega^2 + 16C^2 - 4C^2(\cos(k_xa) + \cos(k_ya) + \cos(k_xa)\cos(k_ya) + 1) = 0$$

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$$\Rightarrow mM\omega^4 - 4C(M+m)\omega^2 + 16C^2\left[1 - \cos^2\left(\frac{k_xa}{2}\right)\cos^2\left(\frac{k_ya}{2}\right)\right]$$

$$\Rightarrow \omega^2 = \frac{4C(M+m) \pm \sqrt{(4C(M+m))^2 - 4mM\,16C^2(1-A^2)}}{2mM} = \frac{2C(m+M)}{mM}\left(1 \pm \sqrt{1 - \frac{4mM}{(m+M)^2}(1-A^2)}\right), \quad |A| \equiv \cos\left(\frac{k_xa}{2}\right)\cos\left(\frac{k_ya}{2}\right)$$

c) $\vec{k} \to 0 \Rightarrow \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) \to \left(1-\frac{(k_x a)^2}{2^3}\right)\left(1-\frac{(k_y a)^2}{2^3}\right) \approx 1 - \frac{k_y^2 a^2}{8} - \frac{k_x^2 a^2}{8} + \frac{k_x^2 k_y^2 a^4}{8} = 1 - \frac{a^2}{8}k^2 = |A|$

By ignoring the higher order term $\sim k_x^2 k_y^2$, we get a dispersion relation that depends only on $k^2 \equiv k_x^2 + k_y^2$:

$$\Rightarrow \omega^2 = \frac{2C(M+m)}{mM}\left[1 \pm \sqrt{1 - \frac{4mM}{(m+M)^2}\left(1-\left(1-\frac{a^2}{8}k^2\right)^2\right)}\right] = \frac{2C(M+m)}{mM}\left[1 \pm \sqrt{1 - \frac{4mM}{(m+M)^2}\left(\frac{a^2}{4}k^2 - \frac{a^4}{8^2}k^4\right)}\right]$$

d) The speed of sound is determined by the form of the acoustic branch when $k \to 0$:

$$\omega_-^2 \approx \frac{2C(M+m)}{mM}\left[1 - \sqrt{1 - \frac{mM}{(m+M)^2}a^2k^2}\right] \underset{\sqrt{1-x}\,\approx\, 1-\frac{x}{2}}{\approx} \frac{2C(M+m)}{mM}\left(1 - \left(1 - \frac{mM}{(m+M)^2}\frac{a^2k^2}{2}\right)\right) = \frac{C}{m+M}a^2k^2$$

$$\Rightarrow \omega_- = \sqrt{\frac{C}{m+M}}\,a k \quad \Rightarrow V_{so} = \sqrt{\frac{C}{m+M}}\,a$$