Phonons, Condensed Matter Physics 24/25

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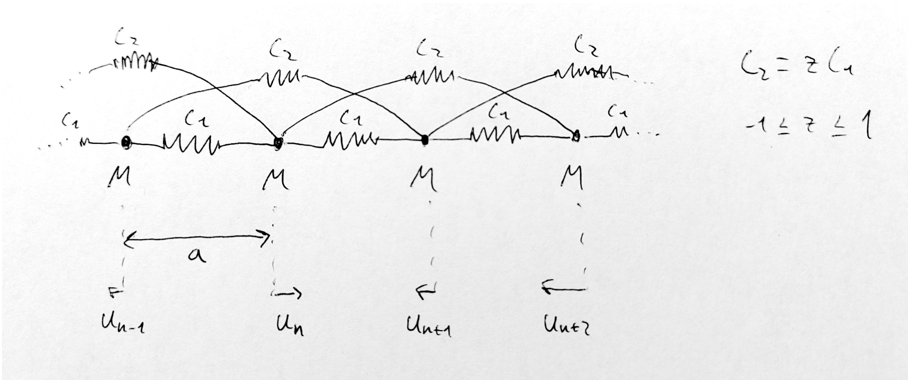
Problem I: One-Dimensional Crystal

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 neighbours, 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

The phonon dispersion relation can be derived using the equations of motion, which come from the potential of the system given by:

$$V_{tot} = V_{eq} + \frac{1}{2}\sum_n C_1(u_n - u_{n+1})^2 + C_2(u_n - u_{n+2})^2$$

giving, through $M\ddot{u}_n = F = -\frac{\partial V_{tot}}{\partial u_n}$, the following equations of motion:

$$\begin{aligned} M\ddot{u}_n &= C_1(u_{n-1} - u_n) + C_1(u_{n+1} - u_n) + C_2(u_{n-2} - u_n) + C_2(u_{n+2} - u_n) = \\ &= C_1(u_{n-1} + u_{n+1} - 2u_n) + C_2(u_{n-2} + u_{n+2} - 2u_n) \end{aligned}$$

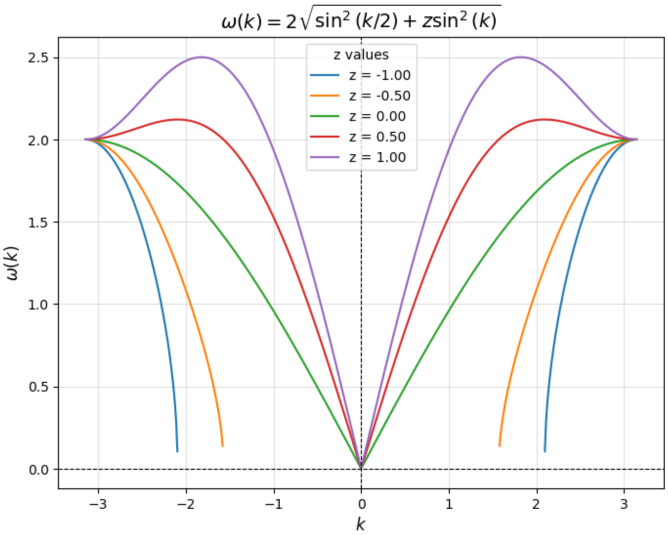
And now, using an ansatz for the collective oscil. modes $u_n = Ae^{i(\omega t + kan)}$, we get:

$$\begin{aligned} -M\omega^2 &= C_1(e^{-ika} + e^{ika} - 2) + C_2(e^{-i2ka} + e^{i2ka} - 2); \\ &= 2C_1\left(\cos(ka) - 1\right) + 2C_2\left(\cos(2ka) - 1\right) = \\ &= -4C_1 \sin^2(ka/2) - 4C_2 \sin^2(ka) = -4C_1\left(\sin^2(ka/2) + z\sin^2(ka)\right) \end{aligned}$$

finally obtaining:

$$\boxed{\omega(k) = 2\sqrt{\frac{C_1}{M}}\sqrt{\sin^2(ka/2) + z\sin^2(ka)}.}$$

Setting $C_1 = M = a = 1$, so we can plot it, we get:



where for $z = 0$, it looks like the studied first neighbour result.

(b) The speed of sound

To compute the speed of sound, we go to the limit of small k ($\sin^2(x) \approx x^2 - O[x]^4$), where the dispersion becomes linear:

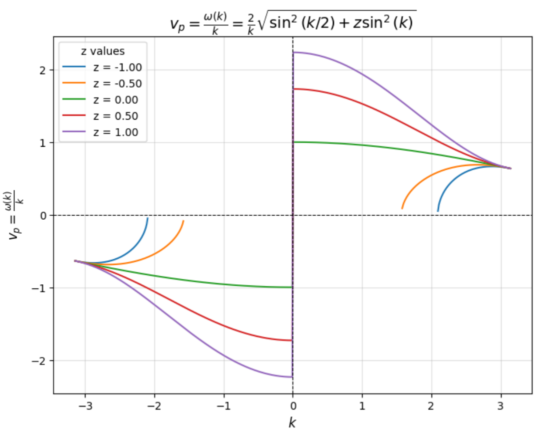
$$\lim_{k \longrightarrow 0} \omega(k) \approx 2\sqrt{\frac{C_1}{M}}\sqrt{(ka/2)^2 - O[k]^4 + z(ka)^2 - zO[k]^4} \approx \sqrt{\frac{C_1}{M}(1+4z)}\; ka = v_s k$$

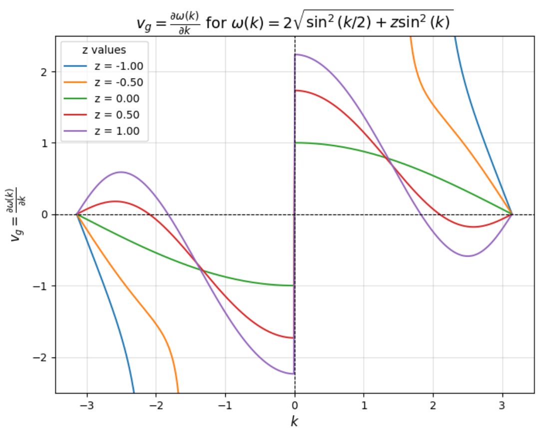
leaving the speed of sound to be: $\boxed{v_s = a\sqrt{\frac{C_1}{M}(1+4z)}.}$

This result, matches the behaviour of the plot above, close to $k = 0$, where:

- for $z \geq 0$, z makes the plot more or less steep since it's inside v_s.
- but for $z < 0$, the plot doesn't go to 0 since v_s becomes imaginary.

Finally, if we plot the phase velocity (v_p) and group velocity (v_g) of our wave:





We see that close to $k = 0$, both graphs converge into the same values, as it should be, since:

$$v_p = \frac{\omega(k)}{k} \xrightarrow[k\to 0]{} v_s \quad \text{and} \quad v_g = \frac{\partial\omega(k)}{\partial k} \xrightarrow[k\to 0]{} v_s \quad \text{then} \quad \lim_{k\to 0} v_p = v_g$$

And we can check that it matches the computed $v_{s_{C_1=M=a=1}} = \sqrt{1+4z}$, for:

- $z = 0 \ \rightarrow \ v_s = \sqrt{1+0} = 1$ (graph green line)
- $z = 0.5 \ \rightarrow \ v_s = \sqrt{1+2} \approx 1.732$ (graph red line)
- $z = 1 \ \rightarrow \ v_s = \sqrt{1+4} \approx 2.236$ (graph purple line)

matching the convergence ($k \to 0$) observed on the graph, in each case.

(c) Check that when $z = 0$ the corresponding results are retrieved in the case with interactions only up to first neighbors:

In the first plot, we can already kind of see that the obtained dispersion relation, looks like the one of first neighbours. But let's compute it explicitly now, setting $z = 0$:

$$\omega(k)_{z=0} = 2\sqrt{\frac{C_1}{M}}\sqrt{\sin^2(ka/2) + 0\sin^2(ka)} = \boxed{2\sqrt{\frac{C_1}{M}}\,|\sin(ka/2)|}$$

which is the same result from class. And the speed of sound, then:

$$v_{s_{z=0}} = a\sqrt{\frac{C_1}{M}(1+0\ 4)} = \boxed{a\sqrt{\frac{C_1}{M}}}$$

which again, is the one obtained in class.

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.

Since we can express the Debye temperature T_D, like:

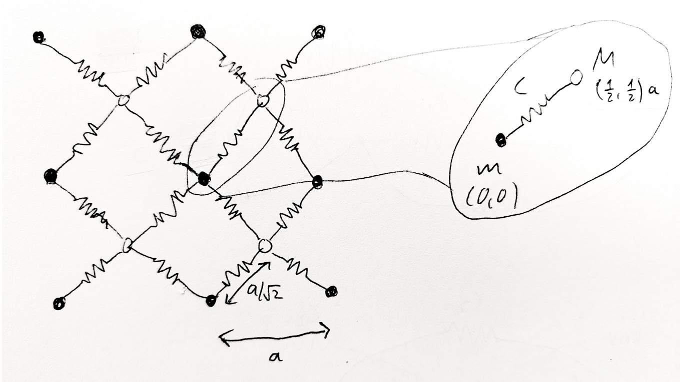
$$T_D = \frac{h\omega_D}{k_b} = \frac{hv_s(6\pi^2 N)^{1/3}}{Lk_b} = A\ v_s = A'\sqrt{1+4z}$$

Where A and A' are just constants. Then in a material with a T_D that is a quarter of the expected value with only first-neighbor interactions, we get:

$$\frac{1}{4} = \frac{T_D}{T_{D_{z=0}}} = \frac{A'\sqrt{1+4z}}{A'\sqrt{1+0\ 4}} = \sqrt{1+4z} \ \rightarrow \ \boxed{z = \left(\frac{1}{4^2} - 1\right)/4 = -\frac{15}{64} \approx -0.234}.$$

Problem II: Two-Dimensional Crystal

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 neighbours, harmonically, with a coupling constant C.



1. Write its equations of motion

Assuming that the oscillations are small enough, so only the parallel movement with respect to the string will matter for each interaction (for small x, $\tan(x) \approx \sin(x) \approx x$).

If use u for the black particles, and v for the white ones, the E.o.M. can be written as:

$$m\ddot{u}_{i,j} = C \sum_{a,b\in -\frac{1}{2},\frac{1}{2}} v_{(i+a,j+b)} - u_{i,j} = C\left(v_{(i+\frac{1}{2},j+\frac{1}{2})} + v_{(i+\frac{1}{2},j-\frac{1}{2})} + v_{(i-\frac{1}{2},j+\frac{1}{2})} + v_{(i-\frac{1}{2},j-\frac{1}{2})} - 4u_{i,j}\right)$$

$$M\ddot{v}_{i,j} = C \sum_{a,b\in -\frac{1}{2},\frac{1}{2}} u_{(i+a,j+b)} - v_{i,j} = C\left(u_{(i+\frac{1}{2},j+\frac{1}{2})} + u_{(i+\frac{1}{2},j-\frac{1}{2})} + u_{(i-\frac{1}{2},j+\frac{1}{2})} + u_{(i-\frac{1}{2},j-\frac{1}{2})} - 4v_{i,j}\right)$$

where $i,j \in \mathbb{N}$ for u, and $i,j \in \mathbb{N}+\frac{1}{2}$ for v, expanding the two separate sets of points, inside the surface. Notice that all the indices relations between u and v, are always with a $\frac{1}{2}n$ of difference, which jumps from one set of points to the other.

2. Show that the dispersion relations of the normal modes of these vibrations can be expressed through the equality:

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

where

$$|A| = \cos\left(\frac{q_x a}{2}\right)\cos\left(\frac{q_y a}{2}\right).$$

As in the previous exercise, we are again interested in the collective oscillations (normal) modes, so we will start with an ansatz of the form:

$$u_{x,y} = Ae^{i(\vec{k}\vec{r}+\omega t)} = Ae^{i(k_x x + k_y y + \omega t)}$$

$$v_{x',y'} = Be^{i(\vec{k}\vec{r'}+\omega t)} = Be^{i(k_x x' + k_y y' + \omega t)}$$

which together with the E.o.M, give:

$$-m\omega^2 A = C\left(Be^{i\frac{a}{2}(k_x+k_y)} + Be^{i\frac{a}{2}(k_x-k_y)} + Be^{i\frac{a}{2}(-k_x+k_y)} + Be^{i\frac{a}{2}(-k_x-k_y)} - 4A\right)$$
$$-M\omega^2 B = C\left(Ae^{i\frac{a}{2}(k_x+k_y)} + Ae^{i\frac{a}{2}(k_x-k_y)} + Ae^{i\frac{a}{2}(-k_x+k_y)} + Ae^{i\frac{a}{2}(-k_x-k_y)} - 4B\right)$$

that can be written like:

$$m\omega^2 = C\left(4 - \frac{B}{A}\left(e^{i\frac{a}{2}k_x} + e^{-i\frac{a}{2}k_x}\right)\left(e^{i\frac{a}{2}k_y} + e^{-i\frac{a}{2}k_y}\right)\right) = 4C\left(1 - \frac{B}{A}\cos\!\left(\frac{k_x a}{2}\right)\cos\!\left(\frac{k_y a}{2}\right)\right)$$
$$M\omega^2 = C\left(4 - \frac{A}{B}\left(e^{i\frac{a}{2}k_x} + e^{-i\frac{a}{2}k_x}\right)\left(e^{i\frac{a}{2}k_y} + e^{-i\frac{a}{2}k_y}\right)\right) = 4C\left(1 - \frac{A}{B}\cos\!\left(\frac{k_x a}{2}\right)\cos\!\left(\frac{k_y a}{2}\right)\right)$$

where it's obvious that our ω solution only depends on the ratio A/B, so let's express our equation a bit simpler, using the proposed variable $|Q| = \cos\!\left(\frac{k_x a}{2}\right)\cos\!\left(\frac{k_y a}{2}\right)$ and $R = A/B$:

$$m\omega^2 = 4C\left(1 - \frac{|Q|}{R}\right) \;\rightarrow\; R(m\omega^2 - 4C) + 4C|Q| = 0$$
$$M\omega^2 = 4C\left(1 - |Q|R\right) \;\rightarrow\; (M\omega^2 - 4C) + 4C|Q|R = 0$$

and now solving the 2nd equation for R, and plugin it in the 1st one, gives:

$$0 = (m\omega^2 - 4C)(M\omega^2 - 4C) - 16C^2|Q|^2 = \underbrace{mM}_{a}\omega^4 \underbrace{-4C(m+M)}_{b}\omega^2 \underbrace{+16C^2(1-|Q|^2)}_{c}$$

which only involves square and forth powers of ω, therefore can be solved with the quadratic equation for ω^2, giving:

$$\omega^2 = \frac{-b \pm \sqrt{b^2 - 4ac}}{a} = \frac{4C(m+M) \pm \sqrt{16C^2(m+M)^2 - 4mM16C^2(1-|Q|^2)}}{2mM}$$

which finally, after extracting some common factors, gives the desired result:

$$\boxed{\omega^2(\vec{k}) = 2C\frac{m+M}{mM}\left(1 \pm \sqrt{1 + \frac{4mM}{(m+M)^2}(1-|Q|^2)}\right)}$$

with also the given variable, which we called $|Q|$ instead:

$$\boxed{|Q(\vec{k})| = \cos\!\left(\frac{k_x a}{2}\right)\cos\!\left(\frac{k_y a}{2}\right)}$$

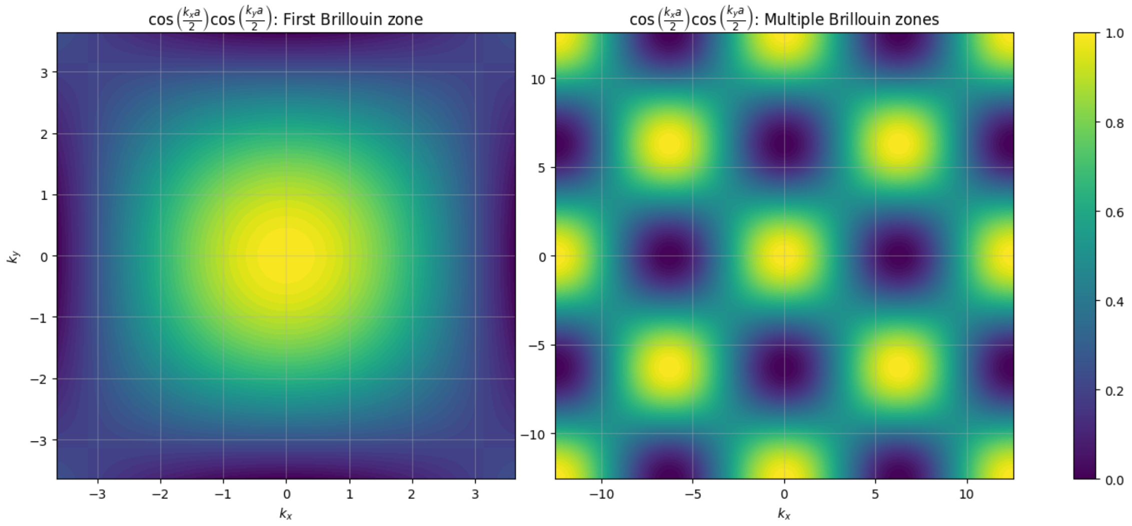
3. Prove that for $\vec{q} \to 0$ the relation of dispersion of the acoustic branch depends on $|\vec{q}|$ and no of its direction.

Since $\omega(\vec{k})$ only depends on $\vec{k}$ through $|Q(\vec{k})|$, we can just study this last part, with the Taylor series of the cosines ($\cos(x) = 1 - \frac{x^2}{2} + O[x]^4$):

$$|Q(\vec{k})| = \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) \xrightarrow[\vec{k}\to 0]{} \left(1 - \frac{k_x^2 a^2}{8} + O[k_x]^4\right)\left(1 - \frac{k_y^2 a^2}{8} + O[k_y]^4\right) =$$
$$= 1 - \frac{k_x^2 a^2}{8} - \frac{k_y^2 a^2}{8} + \frac{k_x^2 k_y^2 a^4}{64} + \ldots \boxed{\approx 1 - \frac{a^2}{8}|\vec{k}|^2 + O[\vec{k}]^4}$$

where we see, that it only depends on the absolute value of $|\vec{k}|$ in the lowest term.

To see it even more clear, we can plot $|Q(\vec{k})|$, getting:



where in the left plot we can see that as we get close to $\vec{k} = 0$, the graph becomes isotropic, as proven above. One last cool thing we can see from the right plot, is the periodicity in the 2D space of $\vec{k}$, seeing the multiple Brillouin zones in action.

4. Determine the speed of sound and check that in this case becomes isotropic.

To compute the speed of sound (v_s) we will propagate the approximate result from $|Q(\vec{k})|$ and keep doing Taylor expansions, until we get into a linear expression for $\omega(\vec{k})$:

$$|Q(\vec{k})|^2 = \left(1 - \frac{a^2}{8}|\vec{k}|^2\right)^2 = 1 - \frac{a^2}{4}|\vec{k}|^2 + O[|\vec{k}|]^4$$

and inserting it into our dispersion relation, gives us:

$$\omega^2(\vec{k}) = 2C\frac{m+M}{mM}\left(1 \pm \sqrt{1 - \frac{4mM}{(m+M)^2}\frac{a^2}{4}|\vec{k}|^2}\right) = 2C\frac{m+M}{mM}\left(1 \pm 1 \mp \frac{mMa^2}{2(m+M)^2}|\vec{k}|^2\right)$$

where we used $\sqrt{1-x} \approx 1 - \frac{x}{2}$ for small x's. And here we already see that the $\omega(\vec{k})$ that we need to focus on (the acoustic), will be the one with no constant component, meaning that will converge to 0 when $\vec{k} \to 0$. So focusing on the acoustic, we get:

$$\omega_{\text{ac}}^2(\vec{k}) = 2C\frac{m+M}{mM}\left(\frac{mMa^2}{2(m+M)^2}|\vec{k}|^2\right) = \frac{Ca^2}{m+M}|\vec{k}|^2 = v_s^2|\vec{k}|^2$$

finally getting:

$$\boxed{v_s = \sqrt{\frac{C}{m+M}}a}$$

where is obviously isotropic since everything it depends on is already isotropic for $\vec{k} \to 0$, which is where the computation of the speed of sound, has to be made by definition!