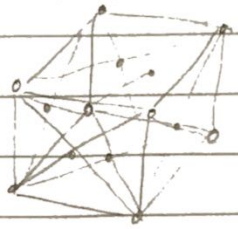
QUESTION 1

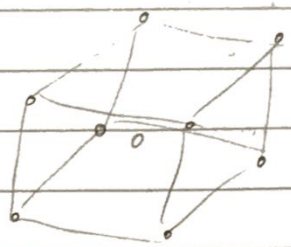
PHYS A WEEK 1 ~~EASTER~~
SOFIA VASIEVA
FOR WILL BARKER

primitive cubic:

face-centred cubic:



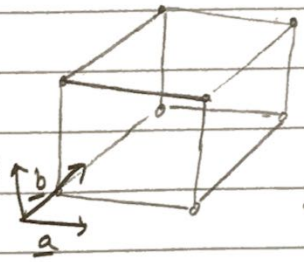
body centred cubic



← sketches

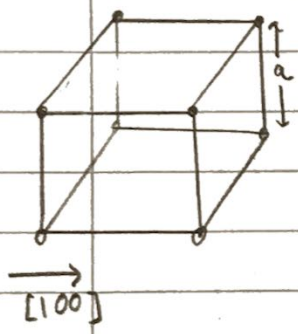
more detailed sketches now:

** assuming that this is the setup we use (?):



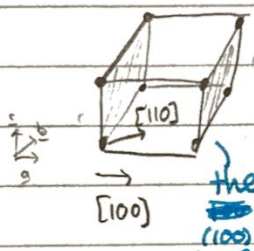
assuming I'm right in thinking $\underline{a} = (100)$, $\underline{b} = (010)$, $\underline{c} = (001)$.

primitive cubic:



Q: by putting these dots in, have I correctly "sketched the atomic positions within the (100), (110) and (111) faces"?)

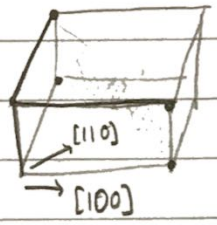
(100) atoms



there's 2 possible (100) planes here, did I need to do both?

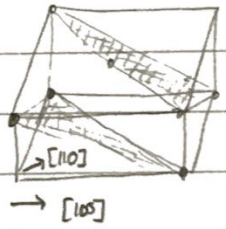
separation of atoms: $a, \sqrt{2}a$

(110) atoms



separation of atoms: a, $a\sqrt{2}$

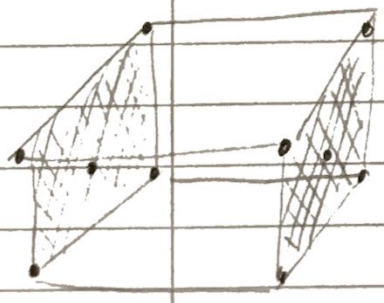
(111) atoms



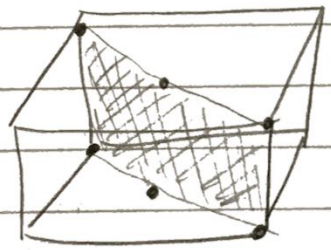
separation of atoms: $a\sqrt{2}$

face-centred cubic:

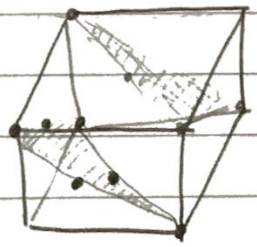
(100) atoms



(110) atoms

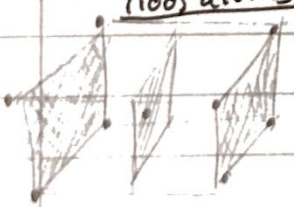


(111) atoms

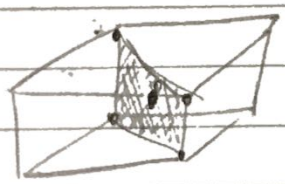


body centred cubic

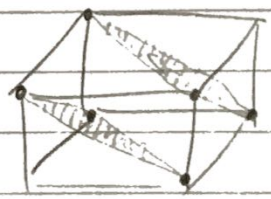
(100) atoms



(110) atoms



(111) atoms



QUESTION 2

* please do tell me if any of the following is wrong/incomplete.

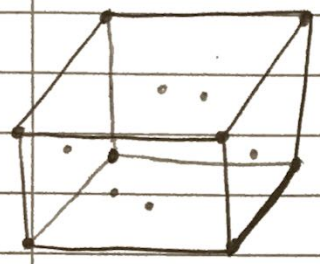
(a) A reciprocal lattice is an infinite set of uniformly separated points in "1D wavevector space" or "K-space"

$$f(x) = \sum_{h=-\infty}^{\infty} C_h e^{iK_h x} \qquad \text{where } K_n = \frac{2\pi h}{a}$$

They are useful because then, any periodic function can be transformed into a set of uniformly spaced points.

A reciprocal lattice is associated with a "real" (?) lattice via a Fourier transform.

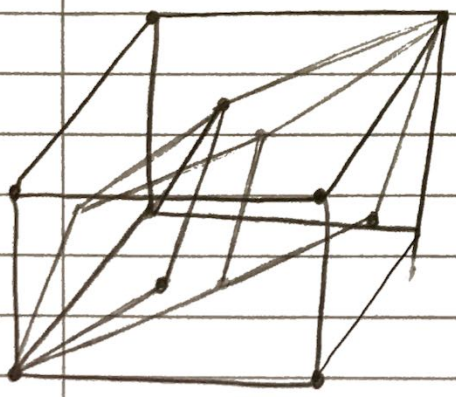
(b)



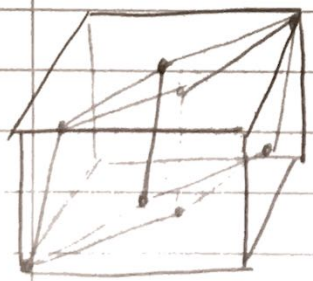
- 8 corner points, each corner point associated w/ 8 cubes ⇒ 1 corner point per cube.
- 6 face points, each face point associated w 2 cubes ⇒ $\frac{6}{2} = 3$ face points per cube.

⇒ there are $1+3 = 4$ lattice points in the standard, non-primitive unit cell.

Volume of the primitive fcc unit cell



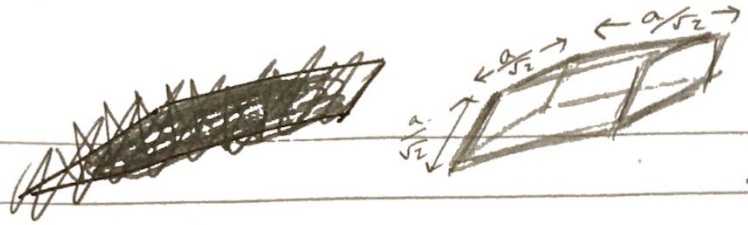
- since there are 3 face points & one corner point per cube, I assume this means the primitive cell should be made up of 3 face points & 1 corner point (?).
  ↳ (well, apparently not (after looking at the lecture notes))



it's a parallelipiped!
but it seems like all the sides are $\frac{\sqrt{2}}{2}a$

* sorry but I don't think the cell volume is "clearly" $V = \frac{1}{4}a^3$ ... ∴

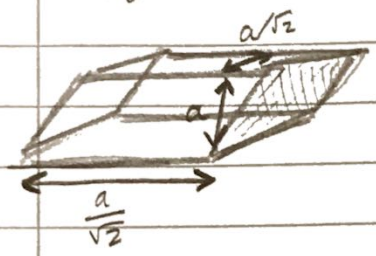
How do I get the volume??? I am so baffled.



"clearly" the volume is $\frac{a^3}{4}$

... CLEARLY???

... nothing is clear in this life.



I SEE NOW.

IT IS MORE CLEAR NOW.

$$V = a \cdot \frac{a}{\sqrt{2}} \cdot \frac{a}{\sqrt{2}} = \frac{a^3}{4} \Rightarrow V = \frac{a^3}{4}$$

(c) Reciprocal lattice is given by the FT.

3D reciprocal lattice: $f(x,y,z) = \sum_{h,k,l=-\infty}^{\infty} C_{hkl}\, e^{i(K_h x + K_k y + K_l z)}$

$$f(\underline{r}) = \sum_{h,k,l=-\infty}^{\infty} C_{hkl}\, e^{i(\underline{K}_{hkl} \cdot \underline{r})}$$

Apparently the reciprocal lattice vectors are given by:

$$\underline{A} = 2\pi \frac{\underline{b} \times \underline{c}}{\underline{a} \cdot \underline{b} \times \underline{c}} \qquad \underline{B} = 2\pi \frac{\underline{c} \times \underline{a}}{\underline{a} \cdot \underline{b} \times \underline{c}} \qquad \underline{C} = 2\pi \frac{\underline{a} \times \underline{b}}{\underline{a} \cdot \underline{b} \times \underline{c}}$$

Q: how do I derive these? It feels like they were pulled from thin air.

applying these formulae to get the reciprocal lattice.

$$\underline{a} = \frac{a}{2}\begin{pmatrix}1\\0\\1\end{pmatrix} \qquad \underline{b} = \frac{a}{2}\begin{pmatrix}1\\1\\0\end{pmatrix} \qquad \underline{c} = \frac{a}{2}\begin{pmatrix}0\\1\\1\end{pmatrix}$$

$$\underline{b} \times \underline{c} = \frac{a^2}{4}\begin{vmatrix} \underline{i} & \underline{j} & \underline{k} \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{vmatrix} = \frac{a^2}{4}\left(\underline{i} - \underline{j} + \underline{k}\right) = \frac{a^2}{4}\begin{pmatrix}1\\-1\\1\end{pmatrix}$$

$$\underline{c} \times \underline{a} = \frac{a^2}{4}\begin{vmatrix} \underline{i} & \underline{j} & \underline{k} \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \frac{a^2}{4}\left(-\underline{i} + \underline{j} - \underline{k}\right) = \frac{a^2}{4}\begin{pmatrix}-1\\1\\-1\end{pmatrix}$$

$$\underline{a} \times \underline{b} = \frac{a^2}{4}\begin{vmatrix} \underline{i} & \underline{j} & \underline{k} \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{vmatrix} = \frac{a^2}{4}\left(\underline{i} - \underline{j} - \underline{k}\right) = \frac{a^2}{4}\begin{pmatrix}1\\-1\\-1\end{pmatrix}$$

$$\Rightarrow \underline{a} \cdot (\underline{b} \times \underline{c}) = \frac{a^2}{4} \cdot \frac{a}{2}\begin{pmatrix}-1\\-1\\1\end{pmatrix} \cdot \begin{pmatrix}1\\1\\0\end{pmatrix} = \frac{a^3}{8}(-1-1) = -2\left(\frac{a^3}{8}\right) = -\frac{a^3}{4}$$

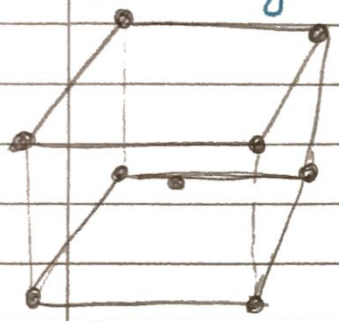
$$\Rightarrow \underline{A} = 2\pi\left(\frac{a^2}{4}\right)\begin{pmatrix}-1\\-1\\1\end{pmatrix}\left(-\frac{4}{a^3}\right) = -\frac{2\pi}{a}\begin{pmatrix}-1\\-1\\1\end{pmatrix} = \frac{2\pi}{a}\begin{pmatrix}1\\1\\-1\end{pmatrix}$$

$$\underline{B} = 2\pi\left(\frac{a^2}{4}\right)\begin{pmatrix}-1\\1\\-1\end{pmatrix}\left(-\frac{4}{a^3}\right) = -\frac{2\pi}{a}\begin{pmatrix}-1\\1\\-1\end{pmatrix} = \frac{2\pi}{a}\begin{pmatrix}1\\-1\\1\end{pmatrix}$$

$$\underline{C} = 2\pi\left(\frac{a^2}{4}\right)\begin{pmatrix}-1\\-1\\1\end{pmatrix}\left(-\frac{4}{a^3}\right) = \frac{2\pi}{a}\begin{pmatrix}1\\1\\-1\end{pmatrix}$$

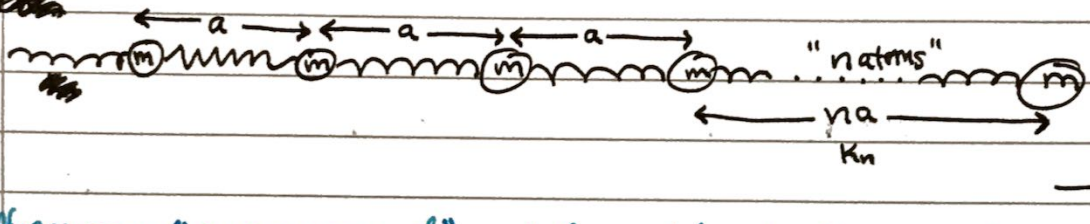
Now, we need to show that these reciprocal lattice vectors are in fact those of bcc. Q: How do I know what the bcc vectors are?

*Q: I don't really understand some of your diagrams because they seem to have too many circles!



(d) since ~~FT "backwards" supp~~ inverse FT supposedly gives what we started out with, the reciprocal lattice of a bcc lattice is an fcc lattice.

QUESTION 3 (a) account of propagation of atomic vibrations along a monatomic chain of atoms:



*Q: when they say "give an account", what exactly do they want me to say?

- Assume there are N atoms with cyclic BCs, and so there are N normal modes (one per degree of freedom)
- Suppose each of the atoms is displaced by a distance u_n.
- Now, consider the n^{th} atom & apply Hooke's law ~~to it~~ & N2 to it: (& setting +ve direction as is in the direction of increasing n)

$$m\ddot{u}_n = \alpha(u_{n+1} - u_n) - \alpha(u_n - u_{n-1}) = \alpha(u_{n+1} + u_{n-1} - 2u_n)$$

↑ the next atom along exerts force αx on atom n, where α = constant & x = separation between atoms

↑ the $(n-1)^{th}$ atom exerts the same magnitude of force, but backwards.

- All the atoms are equivalent (same mass), so that EOM applies to them all. Hence, there is lots of symmetry going on:
  - all the atoms have the same amplitude. let u_0 = amplitude of oscillation.
  - all the atoms have the same frequency of oscillation, ω.

- there can only be a constant phase shift, δ, between one atom and the next: $u_{n+1} = u_n e^{i\delta}$ $u_{n-1} = u_n e^{-i\delta}$ Q: I don't really understand this point

- We wish to find normal mode solutions

⇒ assume the position coordinate of each atom has the form $u_n = u_0 e^{-i\omega t}$

⇒ substituting this into the equation of motion:

DERIVATIVES: $u_n = u_0 e^{-i\omega t}$ ⇒ $\dot{u}_n = -i\omega u_0 e^{-i\omega t}$ ⇒ $\ddot{u}_n = -\omega^2 u_0 e^{-i\omega t} = -\omega^2 u_n$

And using the phase difference assumption from above:

$u_{n+1} = u_n e^{i\delta} = e^{i\delta} u_0 e^{-i\omega t}$

$u_{n-1} = u_n e^{-i\delta} = e^{-i\delta} u_0 e^{-i\omega t}$

⇒ substituting everything into the EOM gives:

$-m\omega^2 u_0 e^{-i\omega t} = \alpha\left(e^{i\delta} u_0 e^{-i\omega t} + e^{-i\delta} u_0 e^{-i\omega t} - 2u_0 e^{-i\omega t}\right)$

$= \alpha\left(e^{i\delta} + e^{-i\delta} - 2\right) u_0 e^{-i\omega t}$

$= \alpha\left(2\cos\delta - 2\right) u_0 e^{-i\omega t}$

$\cos 2\theta = 1 - 2\sin^2\theta$

$\sin^2\theta = \frac{1-\cos 2\theta}{2}$

⇒ $m\omega^2 = \alpha(2 - 2\cos\delta) = 2\alpha(1-\cos\delta) = 2\alpha\left(2\sin^2\left(\frac{\delta}{2}\right)\right) = 4\alpha\sin^2\left(\frac{\delta}{2}\right)$

⇒ $\boxed{m\omega^2 = 4\alpha\sin^2\left(\frac{\delta}{2}\right)}$ where δ is a "constant"

↑ .... is that right?

⇒ Therefore, the frequency of oscillation is $\boxed{\omega(\delta) = \sqrt{\frac{4\alpha}{m}}\left|\sin\left(\frac{\delta}{2}\right)\right|}$

where δ = the phase difference between adjacent atoms in the oscillation.

*Q: again, how much of an "account" do they want? Should I start talking about the dispersion relationship?

- Meaning of "wavevector" q: the quantity qa gives the phase shift in the wave between subsequent unit cells. $q = \frac{2\pi}{\lambda}$

Q: is that always true? →

Showing that phonons in a 1D chain with nearest AND next-nearest harmonic interactions have frequencies given by $\omega^2 = \frac{4}{m}\left(K_1 \sin^2\left(\frac{qa}{2}\right) + K_2 \sin^2(qa)\right)$

To do this, we must "extend" the EOM that we wrote earlier, because the earlier one only ~~consid~~ took nearest-neighbour interactions into account.

Q: but what if I wanted to take ALL the interactions into account, i.e. not just nearest & next nearest neighbours, but all the way to n_{∞} & $n_{-\infty}$? How would I write the EOM / solution for that?

EOM (considering only nearest & next-nearest):

$$m\ddot{u}_n = K_1(u_{n+1} - u_n) - K_1(u_n - u_{n-1}) + K_2(u_{n+2} - u_n) - K_2(u_n - u_{n-2})$$
$$= K_1(u_{n+1} + u_{n-1} - 2u_n) + K_2(u_{n+2} + u_{n-2} - 2u_n)$$

Where: K_1 = force constant between neighbouring atoms.
K_2 = force constant between next-door-but-one atoms.

Q: is there a way to write K_2 in terms of K_1, without making any inaccurate assumptions?

Now, as before, to find normal modes we assume solutions of the form: $u_n = u_0 e^{-i\omega t}$ and phase difference relations between the atoms as follows:

$$u_{n+1} = u_n e^{i\delta}\ ;\ u_{n+2} = u_n e^{2i\delta}\ ;\ u_{n-1} = u_n e^{-i\delta}\ ;\ u_{n-2} = u_n e^{-2i\delta}$$

- substituting everything into the EOM:

$$-m\omega^2 u_n = K_1(u_n e^{i\delta} + u_n e^{-i\delta} - 2u_n) + K_2(u_n e^{2i\delta} + u_n e^{-2i\delta} - 2u_n)$$

$$\Rightarrow -m\omega^2 = K_1(e^{i\delta} + e^{-i\delta} - 2) + K_2(e^{2i\delta} + e^{-2i\delta} - 2)$$

$$\Rightarrow \omega^2 = \frac{1}{m}\left[K_1(-2\cos(\delta) + 2) + K_2(-2\cos(2\delta) + 2)\right]$$

$$= \frac{2}{m}\left[K_1(-\cos\delta + 1) + K_2(-\cos(2\delta) + 1)\right]$$

$$= \frac{2}{m}\left(2K_1 \sin^2\left(\frac{\delta}{2}\right) + 2K_2 \sin^2(\delta)\right)$$

$$= \frac{4}{m}\left(K_1 \sin^2\left(\frac{\delta}{2}\right) + K_2 \sin^2(\delta)\right)$$

But $\cos 2\theta = 1 - 2\sin^2\theta$
$\Rightarrow 1 - \cos 2\theta = 2\sin^2\theta$
$\Rightarrow 1 - \cos\delta = 2\sin^2\left(\frac{\delta}{2}\right)$
$1 - \cos(2\delta) = 2\sin^2(\delta)$

But $\delta = qa$ ← By definition, right?

$$\Rightarrow \boxed{\omega^2 = \frac{4}{m}\left(K_1 \sin^2\left(\frac{qa}{2}\right) + K_2 \sin^2(qa)\right)}$$ as required! :)

Longitudinal waves in lead

- maximum phonon frequency corresponds to smallest possible wavelength.

- $\lambda = 2a$ is the shortest possible wavelength because $q = \frac{\pi}{a}$ is the largest unique wavevector and $\Rightarrow \lambda_{min} = \frac{2\pi}{q_{max}} = \frac{2\pi a}{\pi} = 2a$.

- $q = \frac{\pi}{a}$ is the largest unique q because $\delta = qa$ and the maximum unique phase shift, δ, between two atoms is π

$\Rightarrow \pi = q_{max} a \Rightarrow q_{max} = \frac{\pi}{a}$

Q: Hang on, does this all only apply when we assume only nearest-neighbour interactions are having an effect.

Q: I thought 2π would be the maximum unique phase shift. Why is $q_{max} = \frac{2\pi}{a}$ not the maximum unique wavevector?

Lead

- assuming that we use this eq. to approximate lead behaviour:

$$\omega^2 = \frac{4}{m}\left(K_1 \sin^2\left(\frac{qa}{2}\right) + K_2 \sin^2(qa)\right) = \frac{4}{m}\left(K_1 \sin^2\left(\frac{\delta}{2}\right) + K_2 \sin^2\delta\right)$$

$$\Rightarrow \omega^2_{max} = \frac{4}{m}\left(K_1 \sin^2(0.4\pi) + K_2 \sin^2(0.8\pi)\right)$$

Oh! Differentiation! ☺

$$\frac{\partial \omega}{\partial \delta} = \frac{4}{m}\left(2K_1 \sin\left(\frac{\delta}{2}\right)\cos\left(\frac{\delta}{2}\right)\cdot\frac{1}{2} + 2K_2 \sin\delta\cos\delta\right)$$

$$= \frac{4}{m}\left(K_1 \sin\left(\frac{\delta}{2}\right)\cos\left(\frac{\delta}{2}\right) + 2K_2 \sin\delta\cos\delta\right)$$

$$= \frac{4}{m}\left(\frac{K_1}{2}\sin\delta + K_2 \sin(2\delta)\right)$$

substituting $\delta = 0.8\pi$ when $\frac{\partial \omega}{\partial \delta} = 0$

$$\Rightarrow 0 = \frac{4}{m}\left(\frac{K_1}{2}\sin(0.8\pi) + K_2 \sin(1.6\pi)\right)$$

$$\Rightarrow \frac{K_1}{2}\sin(0.8\pi) = -K_2 \sin(1.6\pi)$$

$$\Rightarrow \frac{K_1}{K_2} = -2\frac{\sin(1.6\pi)}{\sin(0.8\pi)} = -4\frac{\sin(0.8\pi)\cos(0.8\pi)}{\sin(0.8\pi)} = -4\cos(0.8\pi)$$

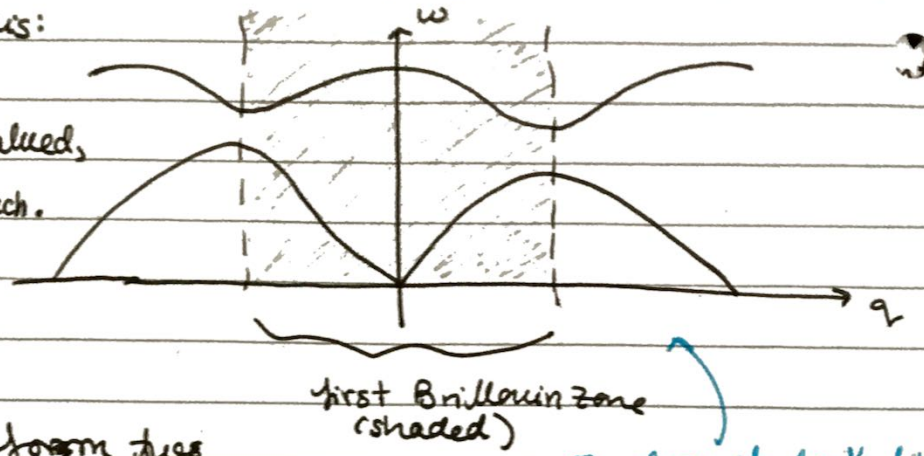
$$= 3.236\ldots$$

$$\Rightarrow \boxed{\frac{K_1}{K_2} \approx 3.24}$$

correct answer! Hooray! ☺

QUESTION 4 optical & acoustic branches of a phonon spectrum (qualitatively)

- If we plot the dispersion relationship graph $\omega(q)$ against q, then the graph looks like this:



- Since ω is not single-valued, we have two "outputs", as such.

- The two solutions for ω form two "branches" in the dispersion relationship.

* Q: does it look like this only for a 1D diatomic lattice? How would $\omega(q)$ be similar / different for other situations?

- The lower branch is the acoustic mode/acoustic branch and corresponds to sound waves in the long-wavelength limit, where $\omega \to 0$ as $q \to 0$

- The upper branch is the optical mode/optical branch, where $\omega \to$ finite value as $q \to 0$.

The optical branch:

- interacts strongly w/ EM radiation (of appropriate ω) in polar crystals.
- experiences strong optical absorption (photons created & annihilated)

↳ hence the name "optical".

Representing relative motion of atoms in each mode & region:

I will use transverse waves to represent the motion more easily - is that (always) OK?

Q: (all the arrows in the illustration below are the same length - is this correct?)

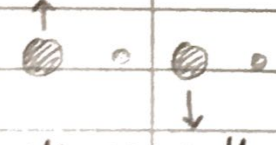
ACOUSTIC MODES

= particle w/ mass m_1

= particle w/ mass m_2

- edge of 1st Brillouin zone:

$\omega \approx \sqrt{\frac{2\kappa}{m_1}}$ ← are these the correct way around?

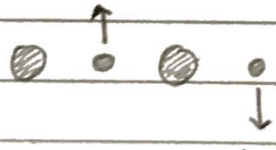


- middle of 1st Brillouin zone:

OPTICAL MODES

- edge of 1st Brillouin zone:

$\omega \approx \sqrt{\frac{2\alpha}{m_2}}$



- middle of 1st Brillouin zone: