Day 6: Optical vs. acoustic phonons

Last time: acoustic dispersion, $\omega(k) = 2\sqrt{\frac{\alpha}{m}}\,\left|\sin\left(\frac{ka}{2}\right)\right|$

$\simeq v_s k$, for small ka

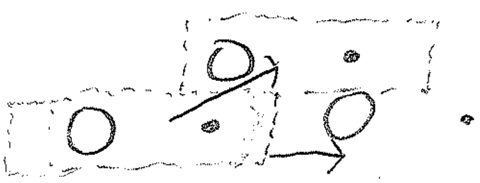
each normal mode (k) supports a phonon.

__phonon__: is a quantized vibrational wavepacket that travels all the way through a perfect crystal with momentum $\hbar k$.

What if the material is diatomic?

"2D - NaCl"

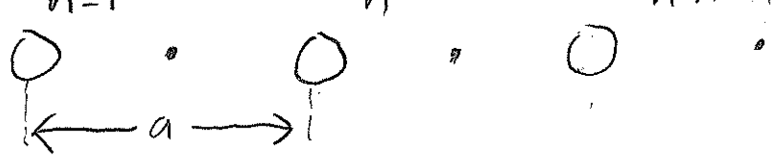
Define a "unit cell" and it translational vector



define 1D translational distance "a"

1D NaCl:

$n-1$ $\quad$ n $\quad$ $n+1$ unit cell



step ① eqn of motion, let $m_{Cl^-} = M$, $m_{Na^+} = m$

n^{th} cell:

i. $M\ddot{x}_n^{Cl} = -\alpha\left(x_n^{Cl} - x_{n-1}^{Na}\right) - \alpha\left(x_n^{Cl} - x_n^{Na}\right)$

ii. $m\ddot{x}_n^{Na} = -\alpha\left(x_n^{Na} - x_n^{Cl}\right) - \alpha\left(x_n^{Na} - x_{n+1}^{Cl}\right)$

Step (2) ansatz #2:

$$\text{let} \quad x_n^{Cl}(t) = C e^{i\omega t} e^{ikna}$$

$$x_n^{Na}(t) = D e^{i\omega t} e^{ikna}$$

plug in i & ii, solve for ω.

i. $$-M\omega^2 C e^{ikna} = -2\alpha C e^{ikna} + \alpha D (e^{ikna} + e^{ik(n-1)a})$$

OR $$-M\omega^2 = -2\alpha + \frac{D}{C}(e^{-ika} + 1)$$

ii. $$-m\omega^2 = -2\alpha + \frac{C}{D}(e^{ika} + 1)$$

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

$$\text{ii} \Rightarrow \frac{D}{C} = \frac{2\alpha e^{ika/2} \cos(ka/2)}{2\alpha - m\omega^2}$$

$$\text{i.} \Rightarrow \frac{D}{C} = \frac{2\alpha - M\omega^2}{2\alpha e^{-ika/2} \cos(ka/2)}$$

set (i) = (ii)

$$(2\alpha - M\omega^2)(2\alpha - m\omega^2) = 4\alpha^2 \cos^2(ka/2)$$

$$= 4\alpha^2 (1 - \sin^2(ka/2))$$

Solve quadratic for ω^2

$$\omega^2(k) = \alpha\left(\frac{M+m}{mM}\right) \pm \alpha\left[\left(\frac{M+m}{Mm}\right)^2 - \frac{4}{mM}\sin^2\frac{ka}{2}\right]^{1/2}$$

"+ve" = optical branch dispersion (excite w/ photons)

"−ve" = acoustic branch dispersion (excite w/ sound)

Examine the limits:

$$\omega(k=0) = 0 \text{ or } \sqrt{\frac{2\alpha}{\mu}}, \quad \mu = \frac{mM}{m+M}$$

$$\omega(k=\pi/a) = \left[\frac{\alpha}{\mu} \pm \alpha\left(\frac{1}{\mu^2} - \frac{4}{Mm}\right)^{1/2}\right]^{1/2}$$