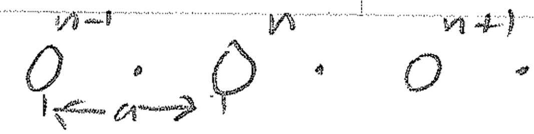
Day 7 Last time



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

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

let $x_n^{Na/Cl} = A_{1/2}\, e^{i\omega t} e^{ikna}$

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

"-ve" case: acoustic branch, supports a sound wave

$\omega(k) = v_s k$ for small ka

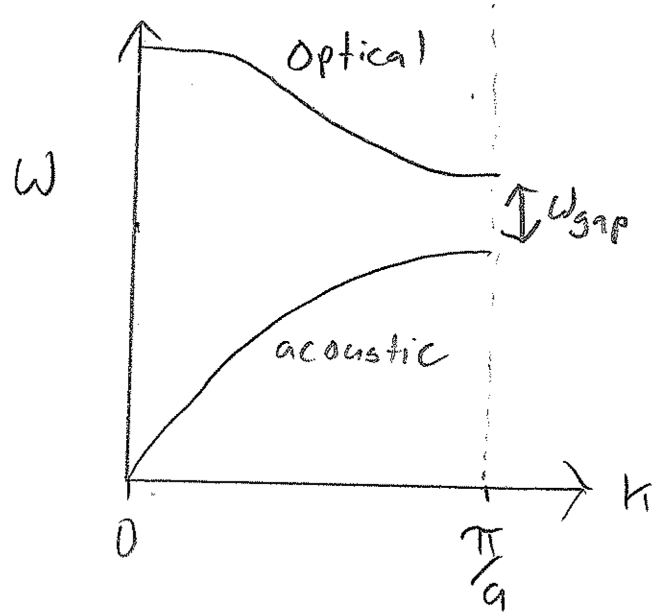
"+ve" case: Optical phonon branch, supports phonons with energy matching that of the photon

Examine the limits:

(1) $\omega(k=0) = 0$ or $\sqrt{\frac{2\alpha}{\mu}}$

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

$\omega_{gap}(k=\pi/a) = \omega_+ - \omega_-$



Phonon Dance Steps — Dance like an atom!

Rules: obey $\omega(k) = \left[\frac{\alpha}{\mu} \pm \alpha\left(\frac{1}{\mu^2} - \frac{4}{Mm}\sin^2\left(\frac{ka}{2}\right)\right)^{1/2} + \frac{g}{\ell}\right]^{1/2}$

you move as: $x_n^{Na}(t) = A_1 e^{ikna} e^{i\omega t}$

$x_n^{Cl}(t) = A_2 e^{ikna} e^{i\omega t}$

① pretend you're all carbon

ⓐ $\lambda = 22a \Rightarrow k_1 = \frac{\pi}{11a}$ show me the normal mode.

ⓑ $k_2 = \frac{2\pi}{11a}$

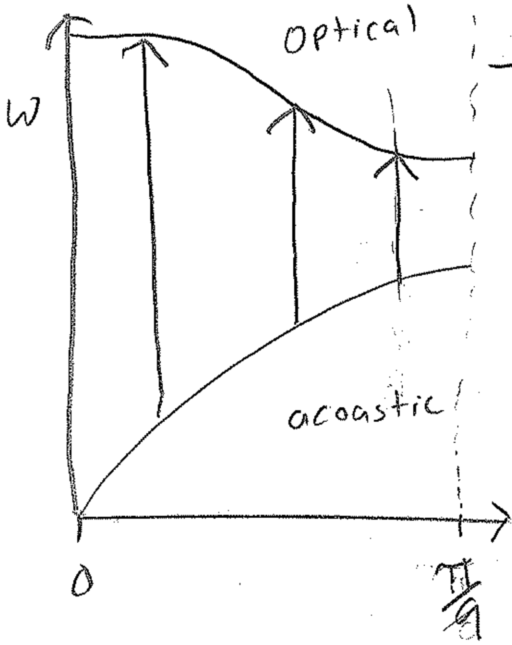
ⓒ $k_{10} = \frac{10\pi}{11a}$

use phet

② Diatomic (approximate infinite chain)

dance call	acoustic	optical
$k \cong 0$	$\omega(k) = v_s k$ Na→ Cl→ Na→ Cl→ Na→ ← ← ← ← ←	$\omega(k) = \sqrt{2\alpha/\mu}$ Na →←Cl Na →←Cl ←→ ←→ Cl^- is slower moves less
$k = \pi/a$	$\omega = \omega_p = 2\sqrt{\alpha/m}$ Cl→ Na ←Cl Na Cl→ Na	Na →Cl← Na Cl Na→Cl←Na
$k = 3\pi/a$		

Thermal vibrations in materials



$\longrightarrow$ $n_{k,\text{optical}} > n_{k,\text{acoastic}} \Rightarrow$ pop inversion

"a phaser"

Classically, each normal mode store an energy, $k_B T$.

$$U_{tot} = \underset{\text{dim}}{3}\ n\ k_B T$$

n → # of normal modes excited

k_B → Boltzmann constant

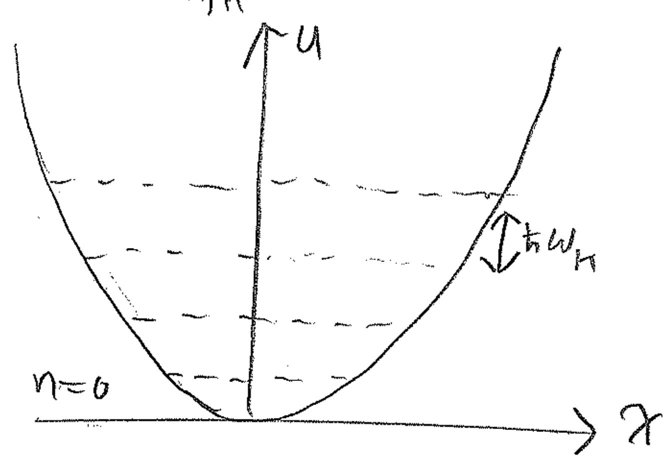
In QM, the normal mode energy (E) gets quantized.

and if $E_{mode} > k_B T$, we say the mode is frozen out, not populated.

In a spring-mass system, $U(x) = \frac{1}{2}\alpha x^2$, so the energy ($E_{mode}$) are: $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}\alpha x^2 \psi = E\psi$

in capstone you'll solve this to find: $E_n = \hbar\sqrt{\alpha/m}\,(n+\frac{1}{2})$

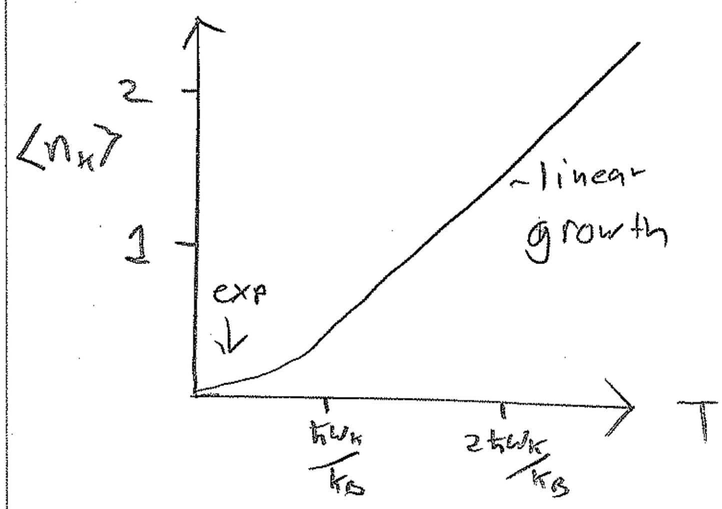
OR $E_{n,k} = \hbar\omega_k(n_k + \frac{1}{2})$, n_k is the # of phonons occupying mode k.



n_k must be an integer, but the populations changes w/time.

Let's define an average occupancy $\langle n_k \rangle$, given by Bose-Einstein statistics:

$$\langle n_k \rangle = \frac{1}{e^{\hbar\omega_k/k_B T} - 1}$$



When $T < \frac{\hbar\omega_k}{k_B}$ phonon population is exponentially suppressed or frozen out.

The total energy in the system is now:

$$U(T) = \sum_{\text{all } k} 3\hbar\omega_k \left(\langle n_k \rangle + \tfrac{1}{2}\right)$$

Compare vs. $U = 3n k_B T$ (classical mech)

A materials <u>heat capacity</u> is defined as:

$$C \equiv \frac{dU}{dT}$$

$$= \sum_k 3\hbar\omega_k \frac{d\langle n_k \rangle}{dT}$$