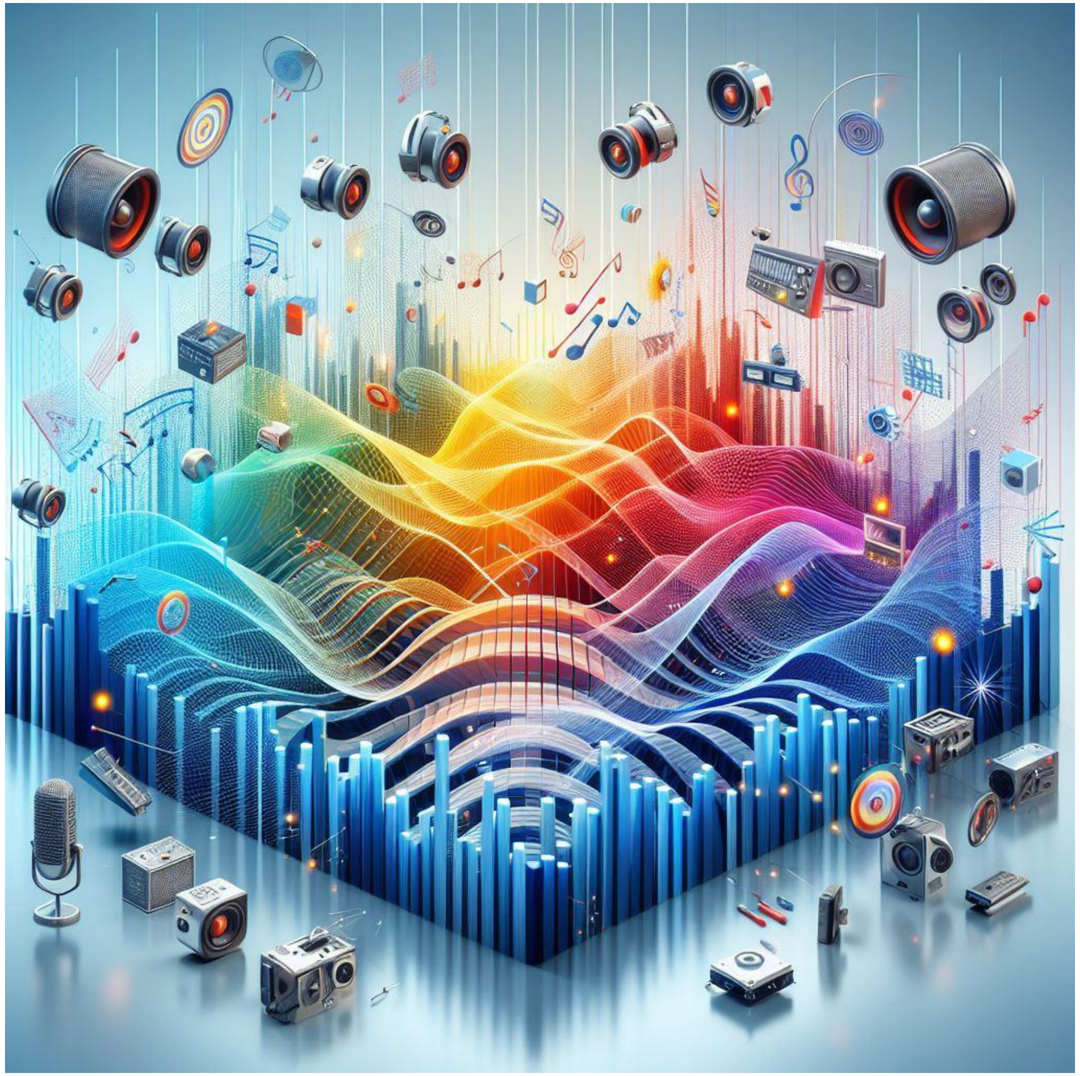
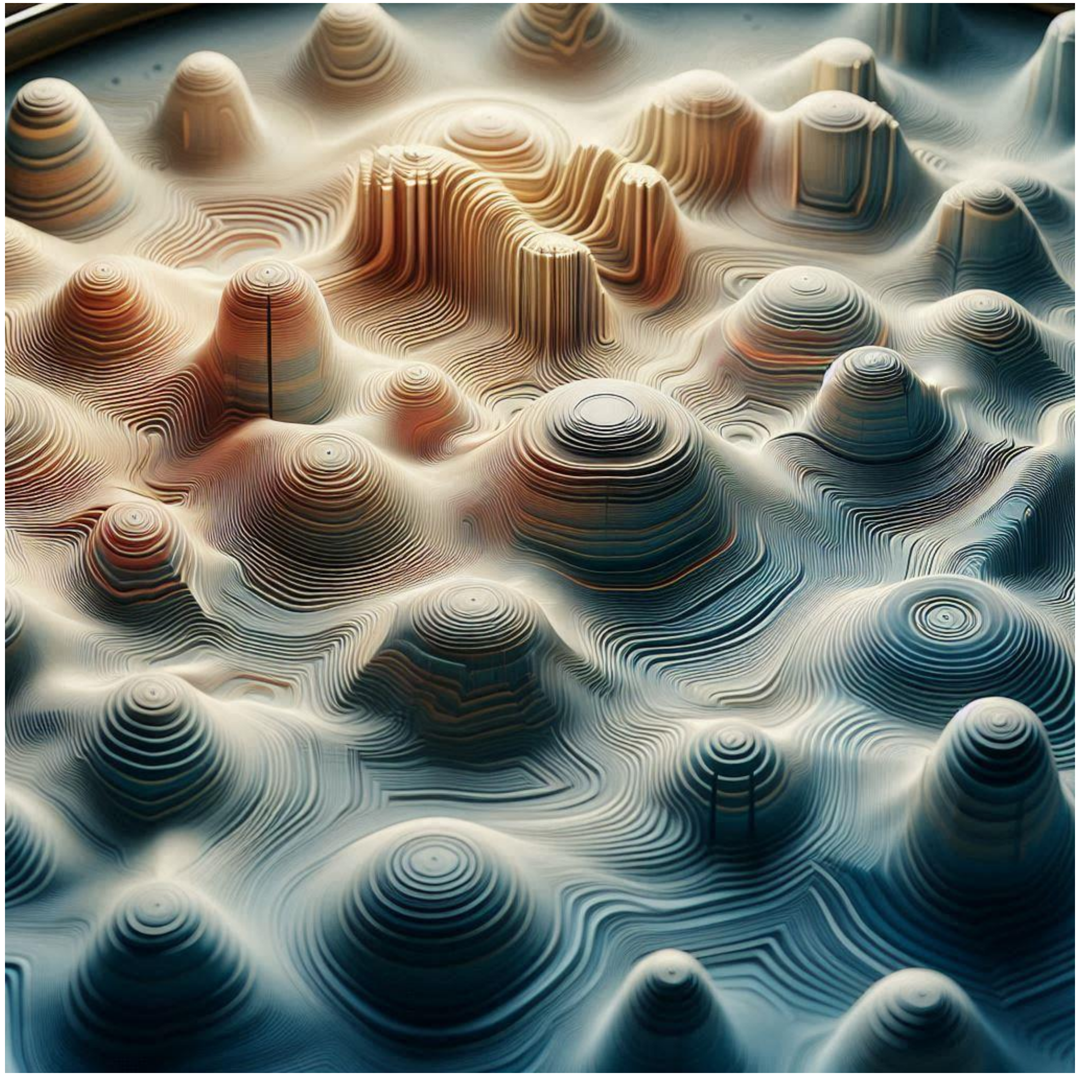
Sound and vibrations: waves and a lattice



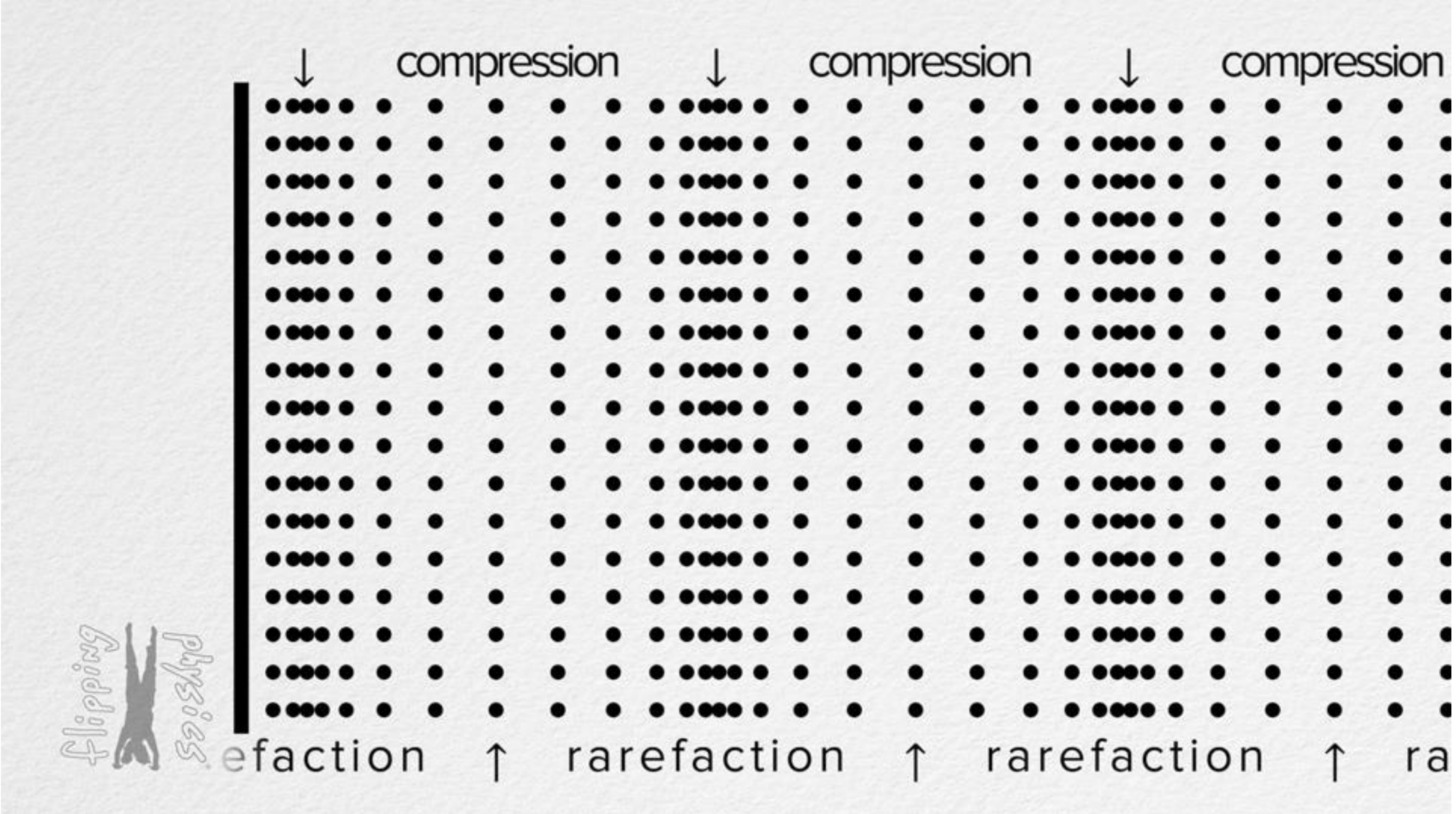
2024 DALL-E 3, prompt = “sound waves”

Simon,
Ch 9



2025 MS Copilot, prompt = “vibrations on a drumhead”

What is sound?



Sound in gas is propagated as compression/rarefaction of density – only one polarization.

Longitudinal sound – displacement parallel to propagation $\mathbf{k}$

Speed of sound

Speed of sound related to “stiffness” and restoring forces.

Start with a continuum model.

should be partial derivative

For ***longitudinal*** sound, $c_s = \sqrt{\frac{K_s}{\rho}}$ $K_s \equiv -V \frac{dP}{dV}\bigg|_s = \rho \frac{dP}{d\rho}\bigg|_s$ (isentropic/adiabatic) bulk modulus

(adiabatic/isentropic b/c it’s assumed that sound is (a) gentle, and (b) faster than diffusion of energy as heat)

solids faster, much less compressible

$$c_s = \sqrt{\frac{dP}{d\rho}}$$ (dropping subscript)

5km sec steel
330m/sec is
like gas

- Question: based on this, should sound be faster or slower in liquids and solids vs. gases?

- **Faster** in liquids and solids – those phases are *much less compressible* than gases!

how stiff is the matter.

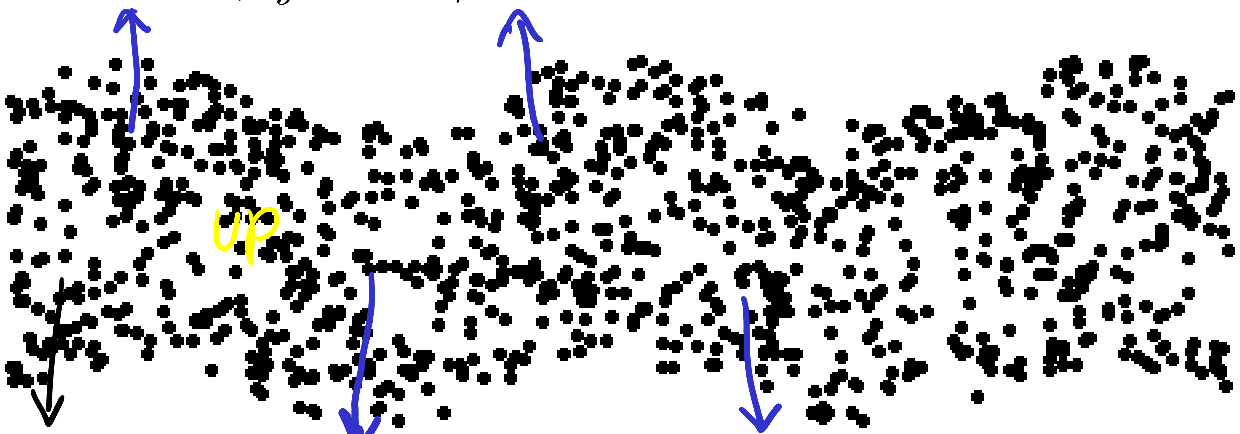
Speed of sound

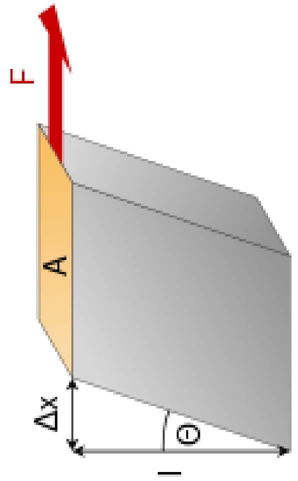
For ***transverse*** sound, displacement transverse to propagation $\mathbf{k}$

$$c_{s,t} = \sqrt{\frac{G}{\rho}} \qquad G = \frac{\tau_{xy}}{\gamma_{xy}} = \frac{F/A}{\Delta x/l}$$

(isentropic/adiabatic) *shear* modulus

sideways force





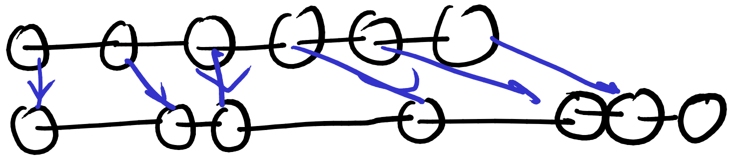
- Transverse sound only in solids! (liquids, gases have no shear modulus)
- Two independent transverse polarizations possible
- Transverse sound generally slower than longitudinal sound

https://www.acs.psu.edu/drussell/demos/waves/wavemotion.html

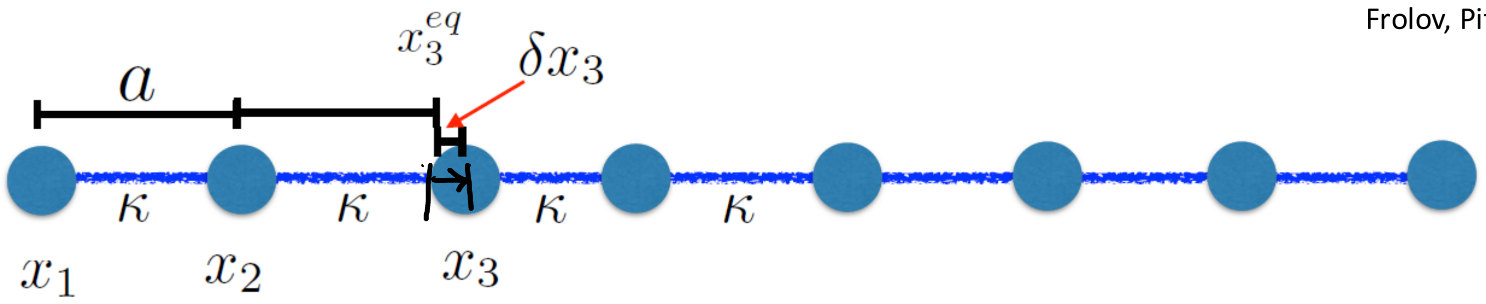
Atomistic picture chapter 09

Consider a chain of atoms, lattice constant a

Equilibrium position of nth atom $x_n^{eq} = na$



Frolov, Pitt

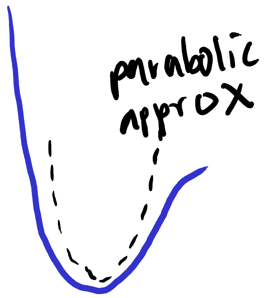


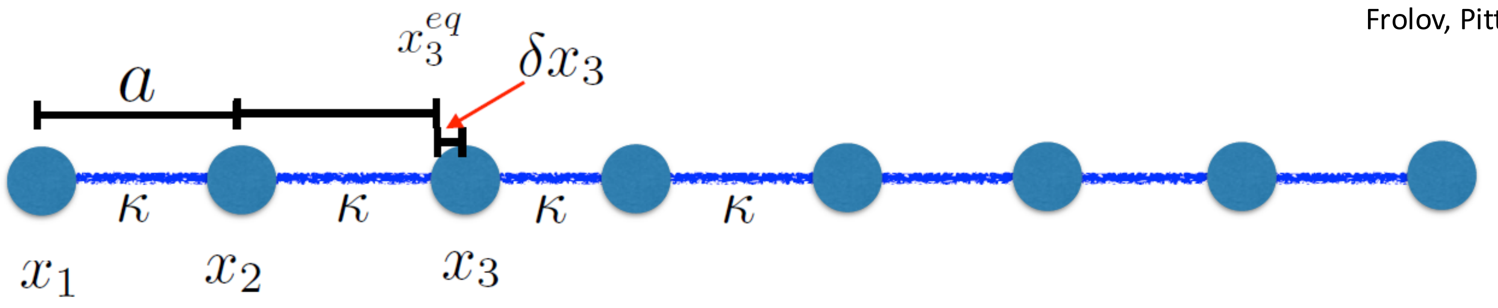
Displacement from equilibrium: $\delta x_n = x_n - x_n^{eq}$

Only going to worry about longitudinal sound for now.

Atomistic picture

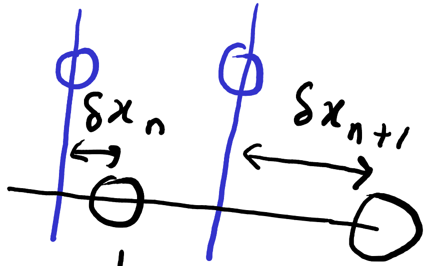
Frolov, Pitt





$$\delta x_n = x_n - x_n^{eq}$$

Assume a harmonic potential (springs!) between atoms, equilibrium spring length a



Potential energy proportional to square of deformation of each spring

$i \sim i+1$

$$V_{tot} = \sum_i \frac{1}{2}\kappa(\underbrace{x_{i+1} - x_i - a}_{\text{distortion per spring at } (i,\, i+1)})^2$$

$\Delta_{tot} = \Delta_1 - \Delta_0$

Force on *n*th atom: $F_n = \kappa(\delta x_{n+1} - \delta x_n) - \kappa(\delta x_n - \delta x_{n-1}) = \kappa(\delta x_{n+1} + \delta x_{n-1} - 2\delta x_n)$

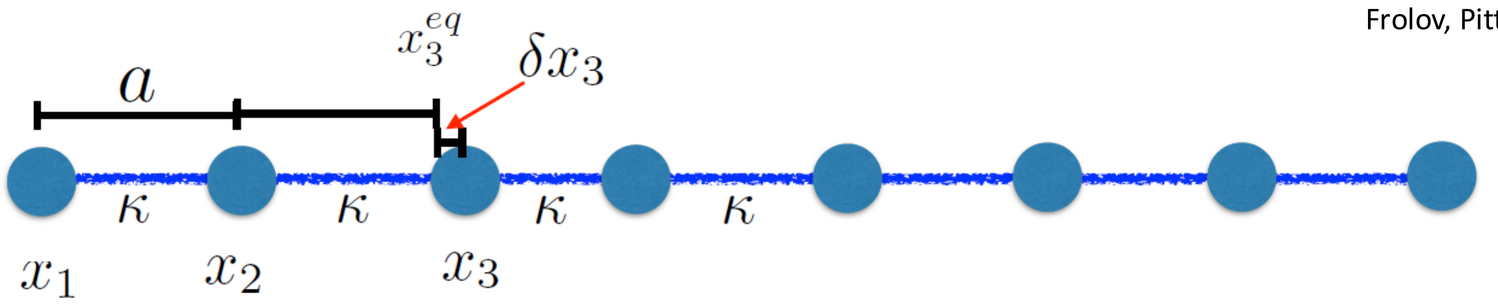
Equations of motion: $$m\frac{d^2(\delta x_n)}{dt^2} = \kappa(\delta x_{n+1} + \delta x_{n-1} - 2\delta x_n)$$

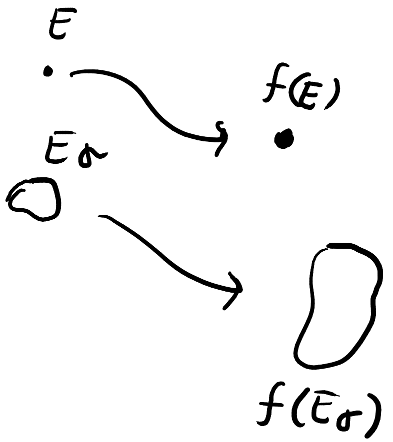
if you wanted, you could solve for lagrangian

Atomistic picture

instead of working with E, we can define that to be a set $E_\sigma \subset \mathbb{R}$ where $E+\xi \in E_\sigma$ where E_σ is a neighborhood of E.

Frolov, Pitt





$$V_{tot} = \sum_i \frac{1}{2}\kappa(x_{i+1} - x_i - a)^2$$

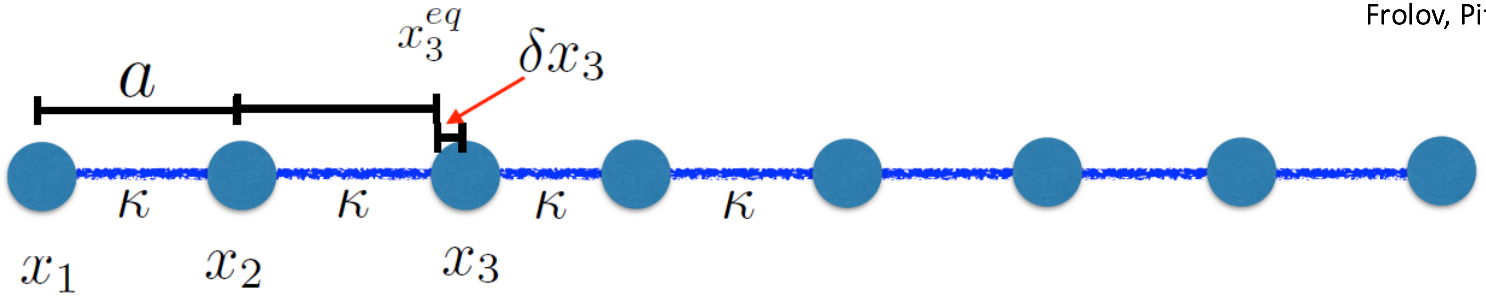
To get a ball-park estimate for the spring constant, recall that covalent chemical bond energies are on the order of 2 eV.

→ Displacing an atom by a full atomic diameter of around 0.3 nm should cost that much

$$\kappa \approx 7 \text{ N/m}$$

Atomistic picture

Frolov, Pitt



$$m\frac{d^2(\delta x_n)}{dt^2} = \kappa(\delta x_{n+1} + \delta x_{n-1} - 2\delta x_n)$$

“Normal mode” problem = all particles move at same frequency

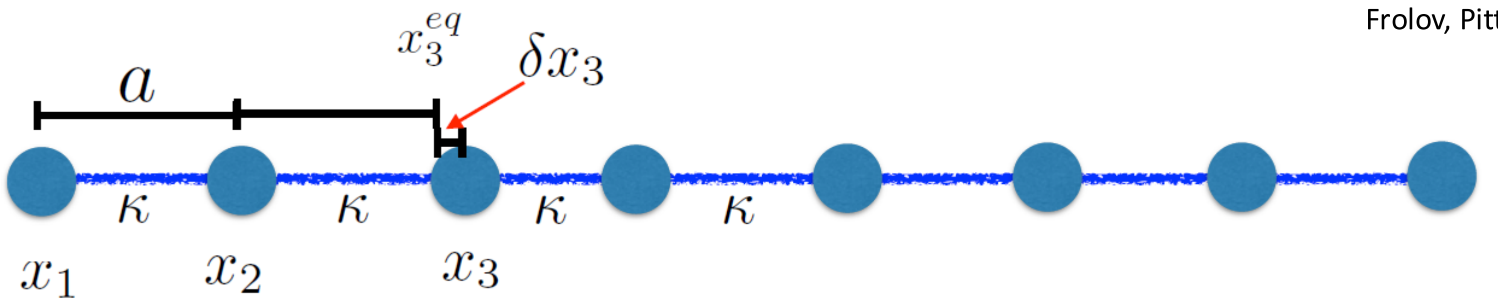
Trial solution: $\delta x_n = Ae^{i\omega t - ikna}$

solve for $x_n(t)$ and be able to predict what happens.

Displacements are the real parts of this wave. Can specify $\omega > 0, \quad k > 0$ or $k < 0$

Atomistic picture

Frolov, Pitt



$$m\frac{d^2(\delta x_n)}{dt^2} = \kappa(\delta x_{n+1} + \delta x_{n-1} - 2\delta x_n) \qquad \delta x_n = Ae^{i\omega t - ikna}$$

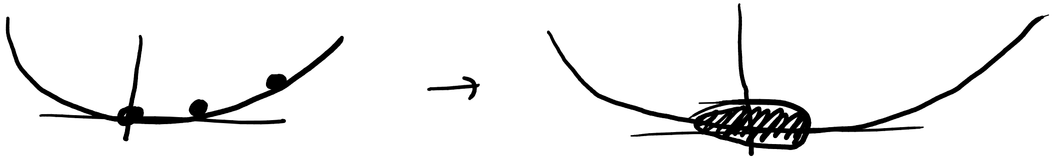
Plugging in the ansatz solution, what we get is

$$-m\omega^2 Ae^{i\omega t-ikna} = \kappa Ae^{i\omega t}\left[e^{-ika(n+1)} + e^{-ika(n-1)} - 2e^{-ikna}\right]$$

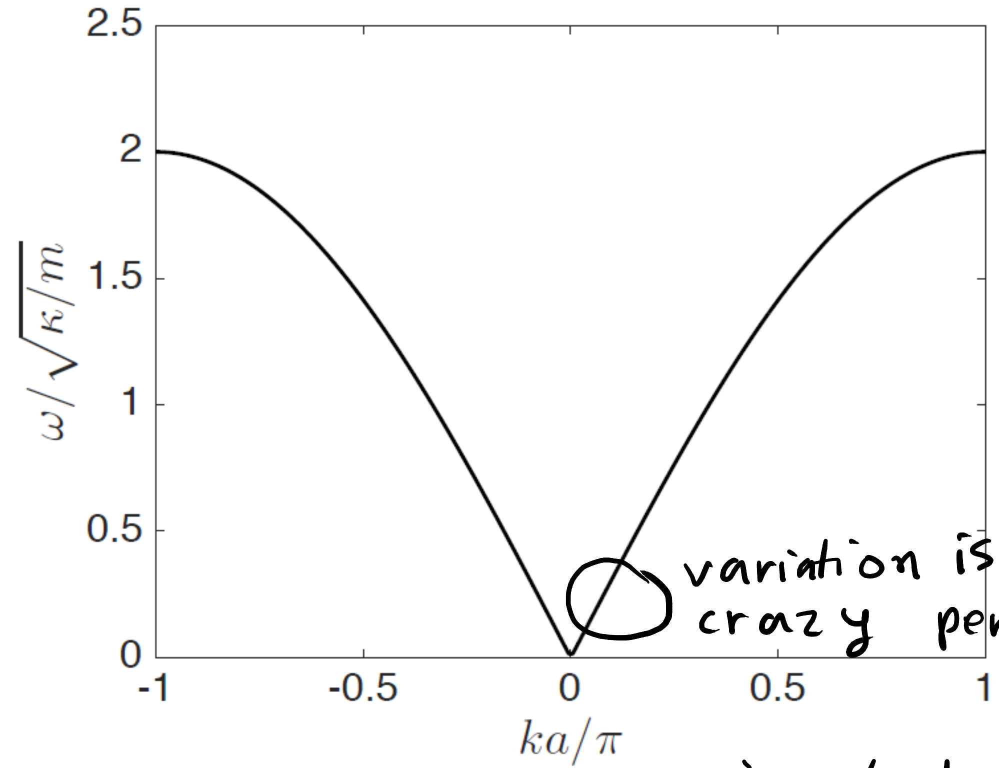
$$\omega^2 = \frac{4\kappa}{m}\sin^2(ka/2) \qquad \omega = 2\sqrt{\frac{\kappa}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

$$\sin\left(\frac{ka}{2}\right)^2 = \left(\frac{e^{+i\frac{ka}{2}} - e^{-i\frac{ka}{2}}}{2}\right)^2$$

1D mono-atomic chain



$$\omega = 2\sqrt{\frac{\kappa}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$



variation is not that crazy per atom

'atoms would be moving but your eye will not be picking up propagation" standing wave

For small k $\qquad \lambda = 2\pi/k \gg a$

Looks like longitudinal sound as we expect.

$$\omega \approx 2\sqrt{\frac{\kappa}{m}}\left|\frac{ka}{2}\right|$$

$$c_s = \frac{\omega}{k} = a\sqrt{\frac{\kappa}{m}}$$

(phase velocity near $k = 0$)

Group velocity: intuition for group velocity. –

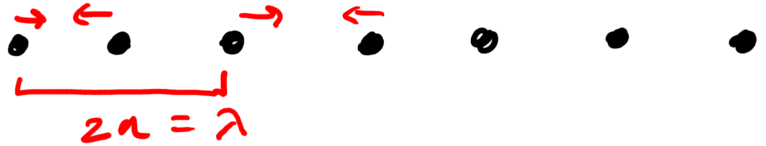
$$v_g = \frac{d\omega}{dk}$$

Group velocity = 0 at $k = \pm\frac{\pi}{a}$ ***standing wave***

Frolov, Pitt

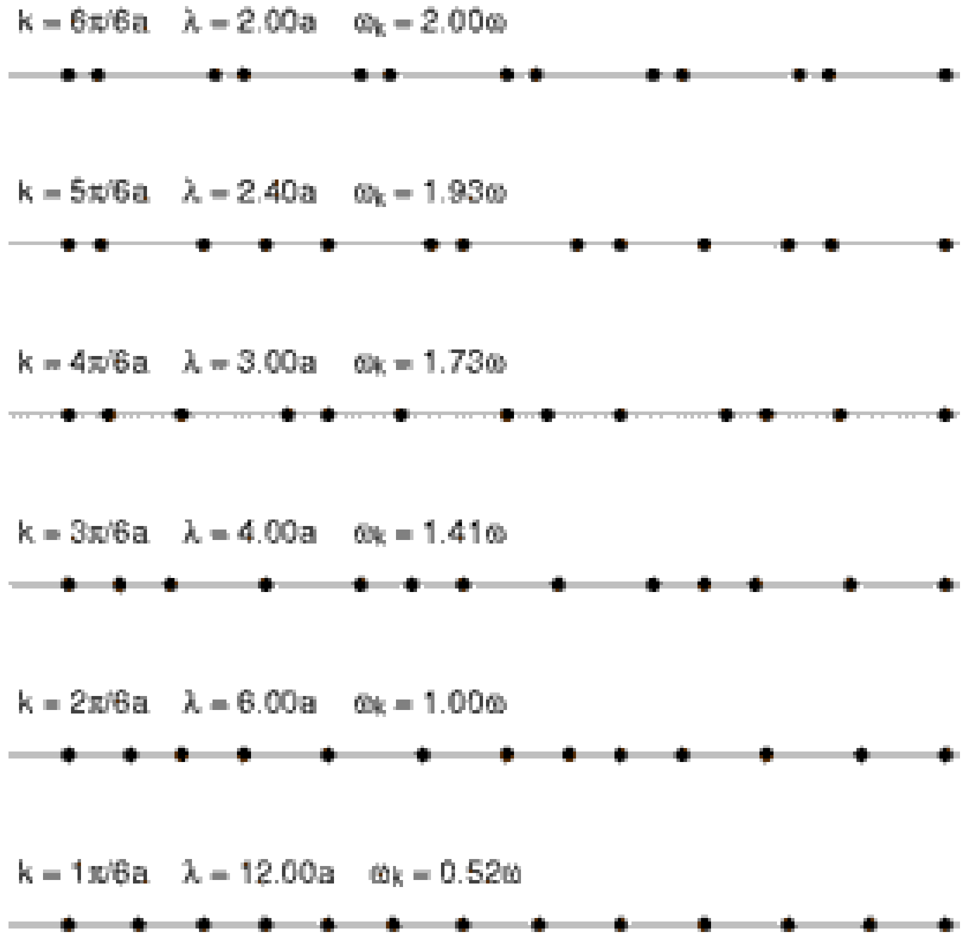
1D mono-atomic chain

$\lambda = 2a$



$$\omega = 2\sqrt{\frac{\kappa}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

Group velocity = 0 at $k = \pm\frac{\pi}{a}$ ***standing wave***



Two questions come to mind:

- What happens at large *k*?
- What values of *k* can we have?

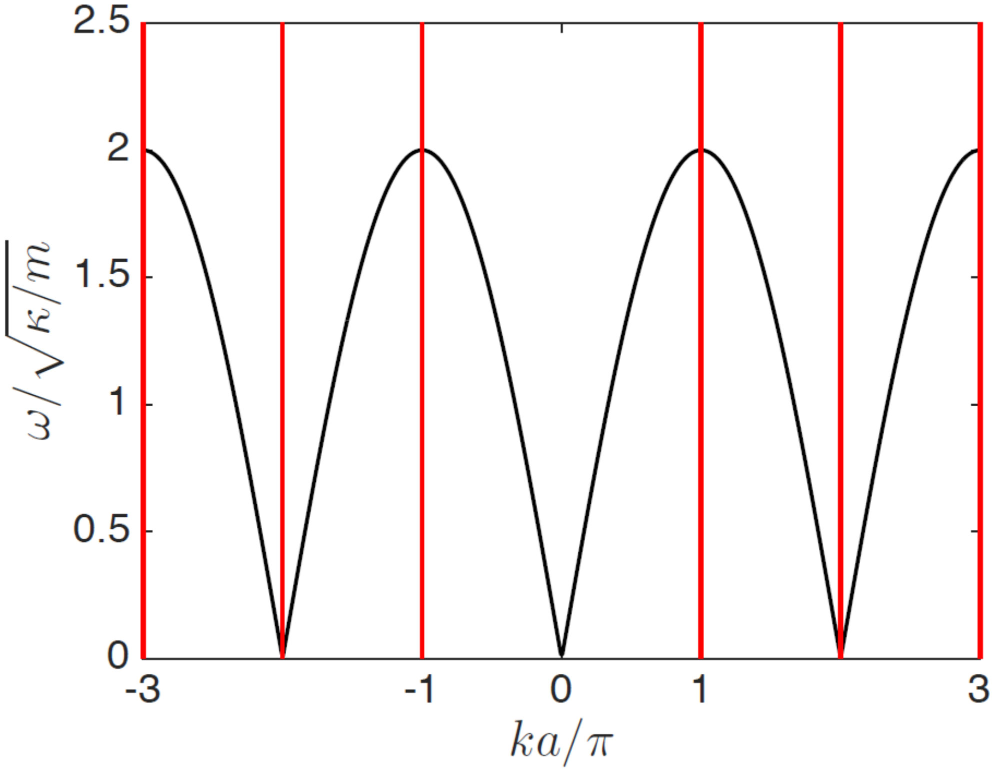
QUANTUM!

k doesn't look bounded

https://en.wikipedia.org/wiki/Phonon

1D mono-atomic chain: *k*-space

$$\omega = 2\sqrt{\frac{\kappa}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$



The dispersion relation is periodic in *k*:

$$k \rightarrow k + (2\pi/a)$$

$2\pi/a$

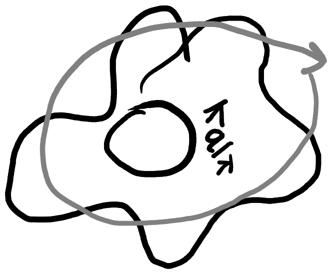
k

Law of Reciprocal Space:

A system with periodicity *a* in real space has (wavelike solutions) that are periodic in ***reciprocal space*** (*k*) with periodicity 2π/*a*.

Indeed, shifting *k* by any integer multiple of 2π/*a* gets back to the original wave!

$$\delta x_n = Ae^{i\omega t - ikna}$$



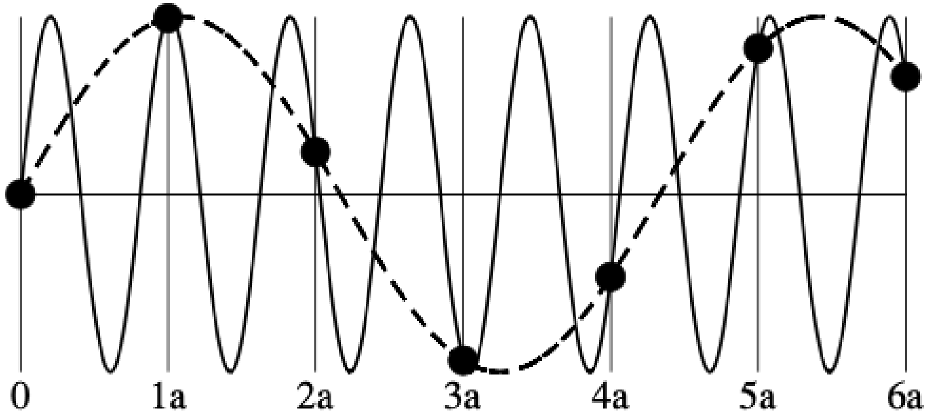
dispertion relation repeats itself.

1D mono-atomic chain: k-space

$$\omega = 2\sqrt{\frac{\kappa}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

The dispersion relation is periodic in *k*:

$$k \to k + (2\pi/a)$$



A system with periodicity *a* in real space has (wavelike solutions) that are periodic in ***reciprocal space*** (*k*) with periodicity $2\pi/a$.

Indeed, shifting *k* by any integer multiple of $2\pi/a$ gets back to the original wave!

$$\delta x_n = Ae^{i\omega t - ikna}$$

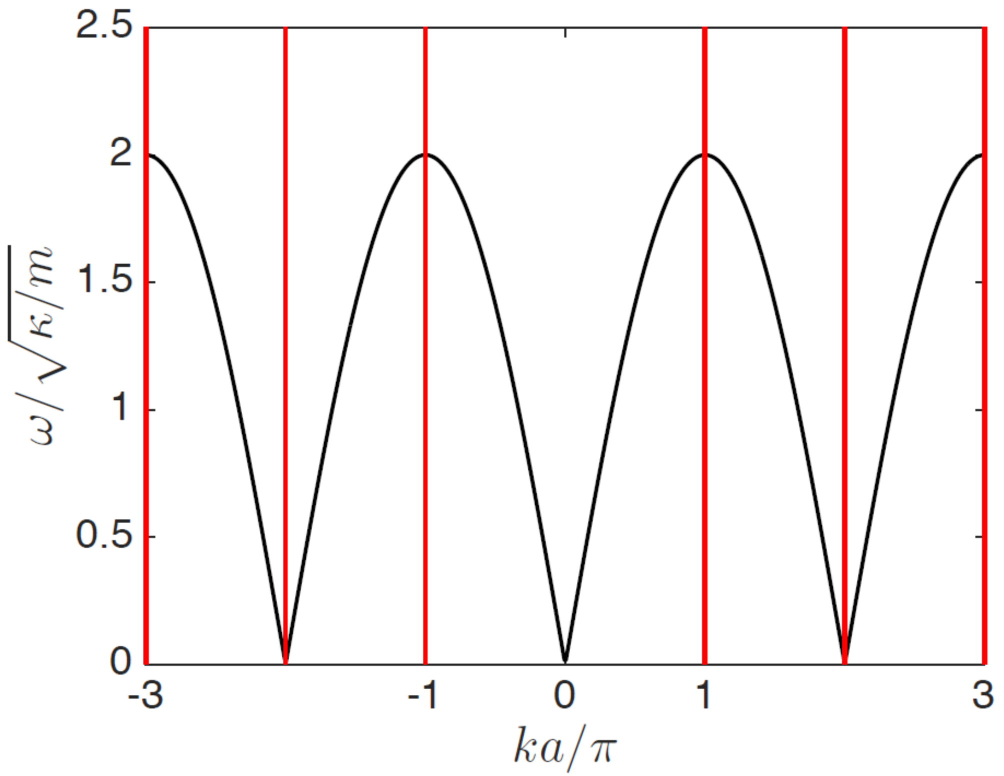
Wavevector $k \to k + (2\pi/a)$ "aliasing"

solutions repeat if you keep making k is bigger

Can get all possible wavelike solutions by limiting our choice of $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$

1D mono-atomic chain: *k*-space

$$\omega = 2\sqrt{\frac{\kappa}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$



The dispersion relation is periodic in *k*:

$$k \to k + (2\pi/a)$$

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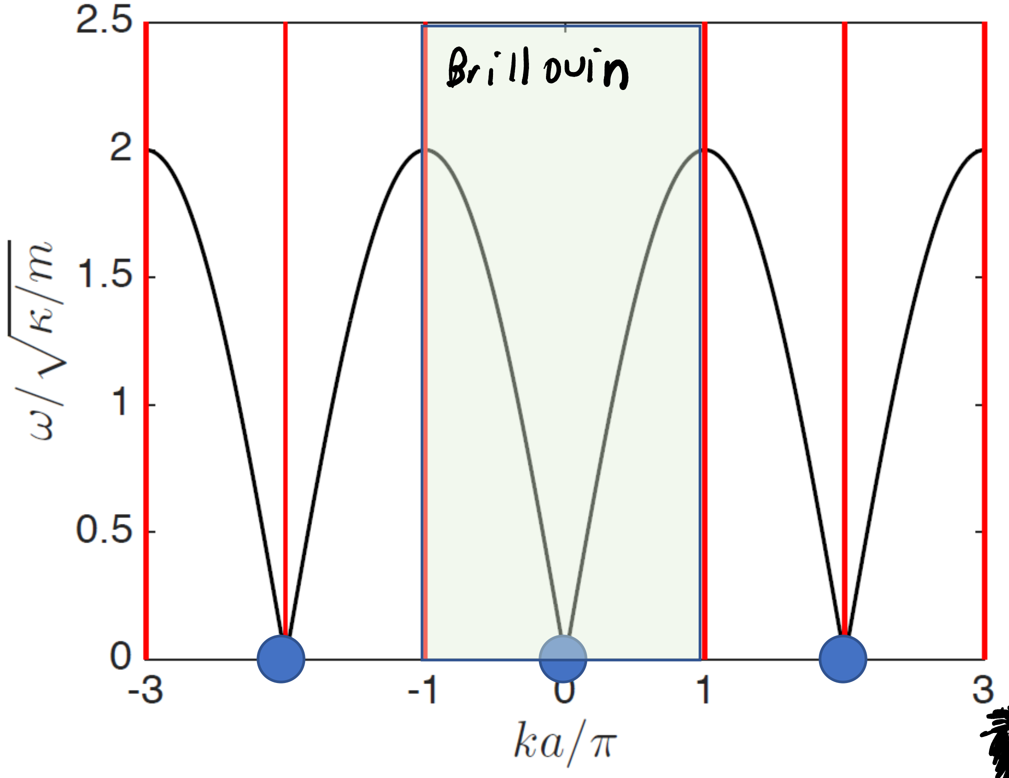
Indeed, shifting *k* by any integer multiple of 2π/*a* gets back to the original wave!

$$\delta x_n = Ae^{i\omega t - ikna}$$

Can get all possible wavelike solutions by limiting our choice of $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$

1D mono-atomic chain: *k*-space and Brillouin zone

$$\omega = 2\sqrt{\frac{\kappa}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$



infinitely big, no distinction:

A system with periodicity *a* in real space has (wavelike solutions) that are periodic in ***reciprocal space*** (*k*) with periodicity 2π/*a*.

Real space lattice:

$$x_n = \ldots \quad -2a \quad -a \quad 0 \quad a \quad 2a \quad \ldots$$

k points that are equivalent to *k*=0 form the ***reciprocal lattice*** in *k*-space:

$$G_n = \ldots \quad -2\left(\frac{2\pi}{a}\right) \quad -\left(\frac{2\pi}{a}\right) \quad 0 \quad \left(\frac{2\pi}{a}\right) \quad 2\left(\frac{2\pi}{a}\right) \quad \ldots$$

Region immediately around *k* = 0 that contains all wave modes = "***first Brillouin zone***"

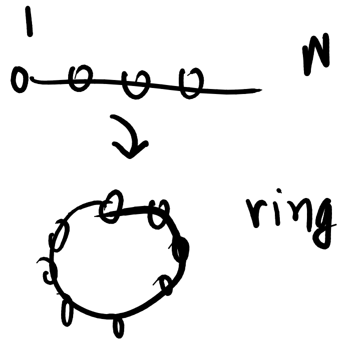
1D mono-atomic chain: allowed k values

ask, what k values are we allowed to have?

Can't pick any arbitrary k.

We know from mechanics that, for N coupled oscillators, there should be N normal modes.

Easiest approach: pick periodic boundary conditions, connecting atom N to atom 1



ring that

$$e^{i\omega t - ikna} = e^{i\omega t - ik(N+n)a}$$

$$e^{ikNa} = 1 \quad \rightarrow kNa = 2\pi p \qquad p = 0, 1, 2, 3, \ldots \text{ upto } N-1$$

capped the chain at N

$$k = \frac{2\pi p}{Na} = \frac{2\pi p}{L}$$

length of whole system

$\boxed{\text{Allowed modes in } k \text{ spaced by } \frac{2\pi}{L} \text{ in } k \text{ space}}$

How many modes are in that first Brillouin zone?

$-\pi/a \rightarrow \pi/a$ (size)

$$= \frac{2\pi/a}{2\pi/L} = \frac{2\pi/a}{2\pi/Na} = N$$

how many dense

Quantizing: Phonons

N normal modes, each with a harmonic response at frequency ω

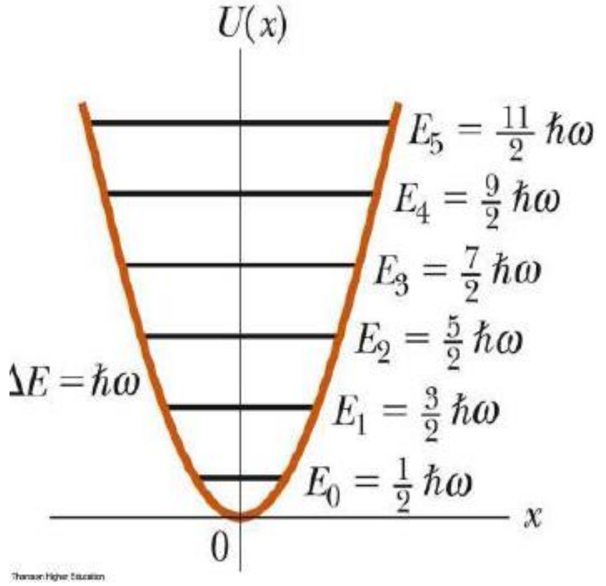
We know how to think about *quantum* harmonic oscillators

$n \in \mathbb{Z}^+$

with ω, I can stick any vibrational quanta.

$$\epsilon_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

"occupation number"



- Think of each mode $\omega(k)$ as a distinct harmonic oscillator
- An excitation of such an oscillator = a ***phonon***, a discrete quantum of a particular vibrational mode
- Analogous to photons for electromagnetic radiation
- Can sum occupation numbers of all the allowed modes to get total number of phonons
- In principle, occupation number is can run $0 \to \infty$ → phonons are ***bosons***

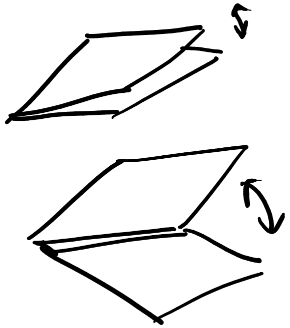
oscillator excitation is ⟨phonon⟩

optical phonon → lattice, same spring if lattice two different kinds

acoustic solution + sol related to each atom dependent solution

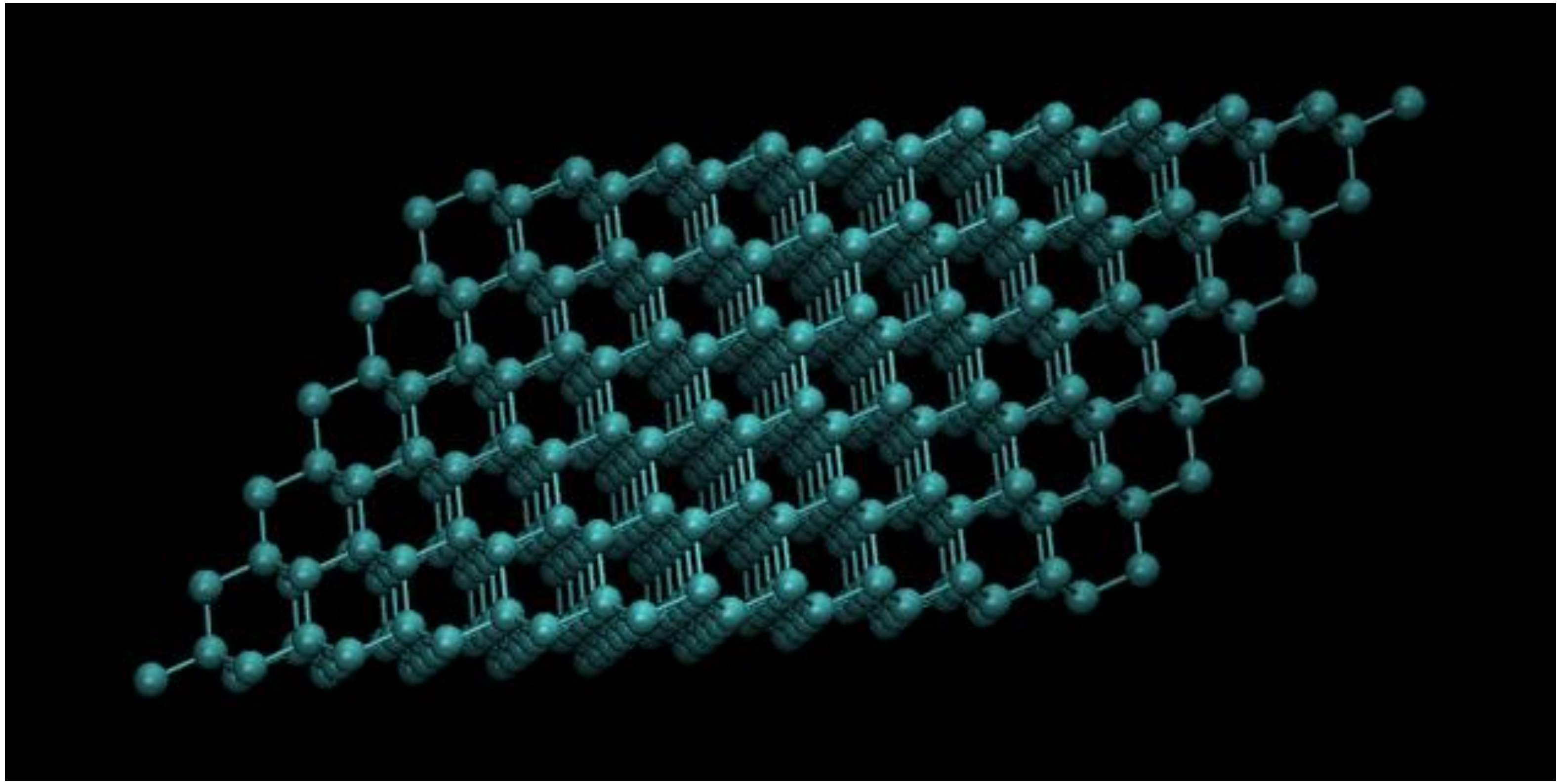
they can be optically seen.

Phonons



CDMS

transition edge detectors



More phonons in a given mode (higher occupancy) = larger displacements

pump up mode, pattern same high amplitude

Phonons are *quasiparticles* – act like particles in many ways

kinda follow statistics of bosons but they can be created or destroyed.

Phonons

Suppose system is in thermal contact with some reservoir at temperature *T*

System is free to exchange energy with the reservoir – different phonon modes have probabilities of being excited. Can think about average occupation number of each mode.

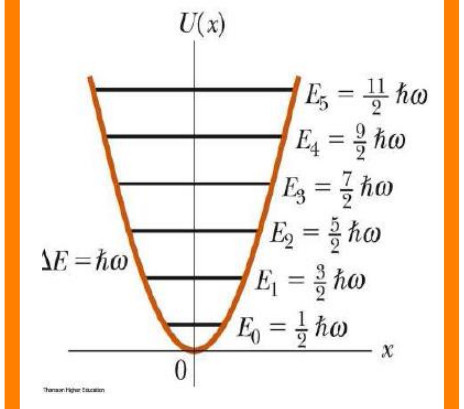
Average occupation number of mode is given by Bose-Einstein distribution (no chemical potential here, because phonons are not conserved particles):

$$n_B(\omega, T) = \frac{1}{e^{\hbar\omega/k_{\mathrm{B}}T} - 1}$$

Derivation based on statistical mechanics….

Quantum harmonic oscillator – example stat mech derivation

Suppose system is in thermal contact with some reservoir at temperature T



Energy of state with occupancy n is $\epsilon_n = (n + \frac{1}{2})\hbar\omega$

Partition function: $Z = \sum_{n=0}^{\infty} \exp(-\epsilon_n / k_{\mathrm{B}}T) = \sum_{n=0}^{\infty} \exp(-(n+1/2)\hbar\omega/k_{\mathrm{B}}T)$

$$= \exp(-\beta\hbar\omega/2) \sum_{n=0}^{\infty} \exp(-n\beta\hbar\omega) \quad \beta \equiv \frac{1}{k_{\mathrm{B}}T}$$

Average value of n is $= \frac{1}{Z} \exp(-\beta\hbar\omega/2) \sum_{n=0}^{\infty} n \exp(-n\beta\hbar\omega) = \frac{\sum_{n=0}^{\infty} n \exp(-n\beta\hbar\omega)}{\sum_{n=0}^{\infty} \exp(-n\beta\hbar\omega)}$

trick

$$= -\frac{1}{\hbar\omega}\frac{\partial}{\partial\beta} \ln \sum_{n=0}^{\infty} \exp(-n\beta\hbar\omega)$$

Bose Distribution for phonon

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \rightarrow \sum_{n=0}^{\infty} \exp(-n\beta\hbar\omega) = \frac{1}{1-\exp(-\beta\hbar\omega)}$$

$$n_B(\omega, T) = \frac{1}{e^{\hbar\omega/k_{\mathrm{B}}T} - 1}$$

Phonons

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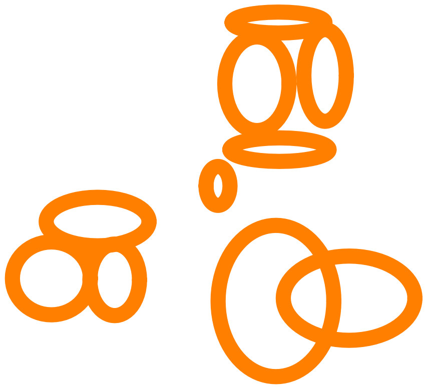
$$n_B(\omega, T) = \frac{1}{e^{\hbar\omega/k_{\mathrm{B}}T} - 1}$$

how many of the mode are occupied

So, total energy contained in the vibrations at temperature T

$$\beta \equiv \frac{1}{k_{\mathrm{B}}T}$$



$$E_{tot} = \sum_k \hbar\omega(k) \left(n_B(\beta\hbar\omega(k)) + \frac{1}{2} \right)$$

Phonons

For large systems, *k* points become very close together.

$$\sum_k \to \int_{-\pi/a}^{\pi/a} dk/(2\pi/L) = \frac{Na}{2\pi}\int_{-\pi/a}^{\pi/a} dk$$

Just like the mode counting argument for the Fermi gas, though no factor of 2 for spin

For real lattices, define dispersion relations in appropriate dimensionality, $\omega(\mathbf{k})$

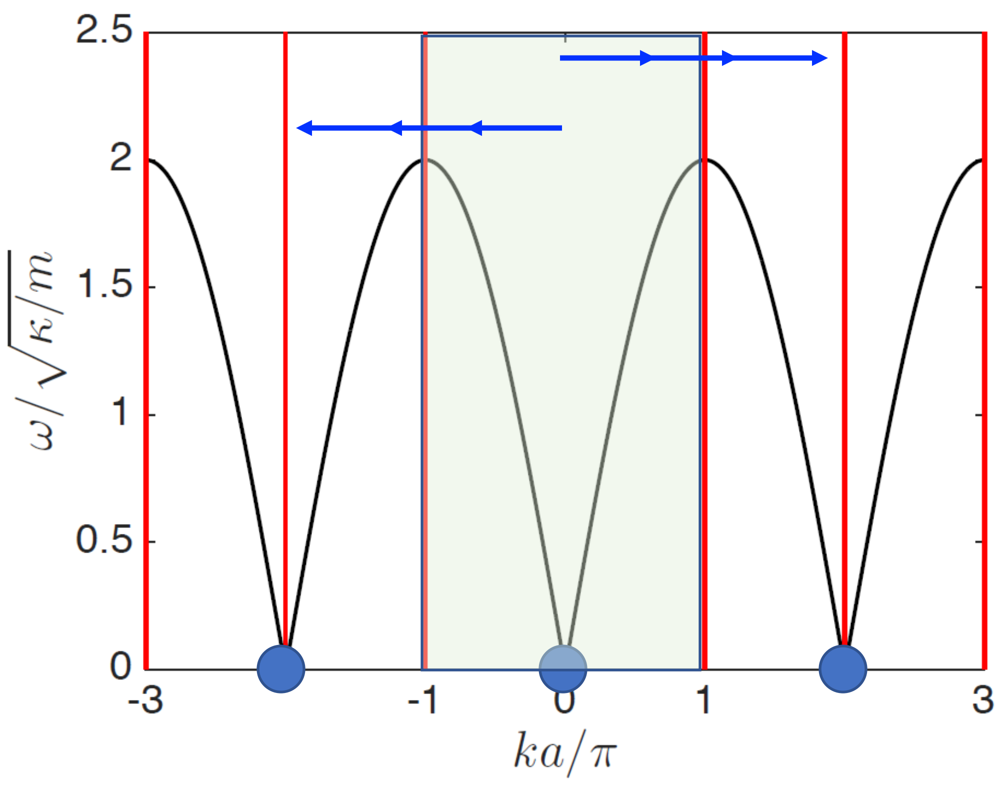
Then can think about densities of states for phonons in *k*-space, $g_p(\mathbf{k})$

And can convert to densities of states for phonons in frequency, $g_p(\omega)$

Phonons and crystal momentum

To make a random ass assumption

Very tempting to think about phonons with wavevector k carrying momentum $\hbar k$



$$G_m = \frac{2\pi m}{a}$$

However, we know that a mode at k is the same as a mode at any $k + G_m$

Crystal momentum = $\hbar k$ "not real-real momentum"

Defined in the first Brillouin zone

Scattering processes involving phonons conserve crystal momentum (momentum up to a reciprocal wavevector)

Ex from book: 3 phonons with momentum $(2/3)\pi/a$ can collide and become 3 phonons with momentum $-(2/3)\pi/a$ because initial and final momenta are equivalent

the whole lattice has kind of recoiled

Summary

- Sound comes from elastic response to deformation of material
- Only longitudinal sound in gases and liquids, long + 2x transv sound in solids
- In 1D, N identical masses + springs = N normal modes
- Wave-like solutions, can get all N allowed solutions with k values btw +/- π/a ("first Brillouin zone"), modes spaced by $\Delta k = 2\pi/Na = 2\pi/L$
- Dispersion is periodic in k, with zero group velocity at k = +/- π/a and equivalent *reciprocal lattice points*
- Quantize each harmonic mode = phonons
- In thermal equilibrium, occupation of each mode given by Bose distribution
- Crystal momentum

Next time:

Diatomic chains, more about phonons

Next time:

Diatomic chains, more about phonons

Next time:

Diatomic chains, more about phonons

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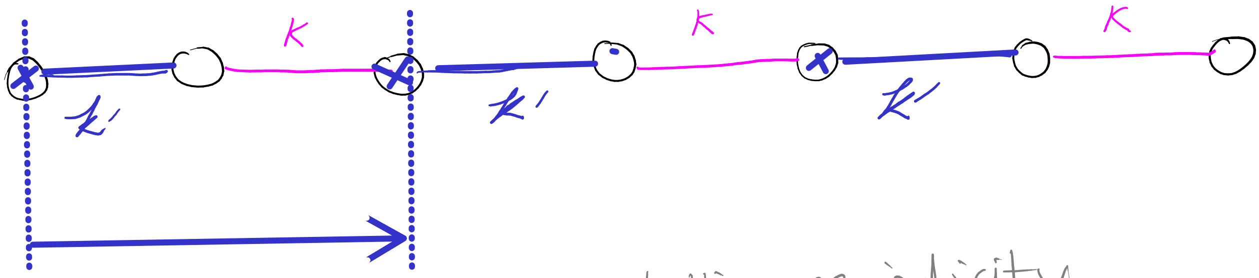
Next time:

Diatomic chains, more about phonons

Related to next class



characteristic spacing, lattice periodicity

acoustic mode / optical mode :