On to phonons! 1) Bosons (not really particles, so no Pauli exclusion)
2) $\mu = 0$ (thermal phonons can be created/destroyed by random energy fluctuations, unlike eg electrons
No extra potential energy involved w/ bringing them into the system)

recall

Suppose temp, T. how many phonons in that state? Answer: $N_{ave} = \frac{1}{e^{\hbar\omega/\tau} - 1}$

Kittel symbol: $\tau = kT$ Thermal units $\beta = \frac{1}{kT}$

On (time) average, what's the (total) energy of all the phonons in that state?

$$E_{ave} = \left(N_{ave} + \frac{1}{2}\right)\hbar\omega$$

Since we're interested in $C = \frac{\partial U}{\partial T}$, ← symbol for internal energy ($\frac{\partial E}{\partial T}$)
disregard factor of $+\frac{1}{2}$
Kittel doesn't even write it.

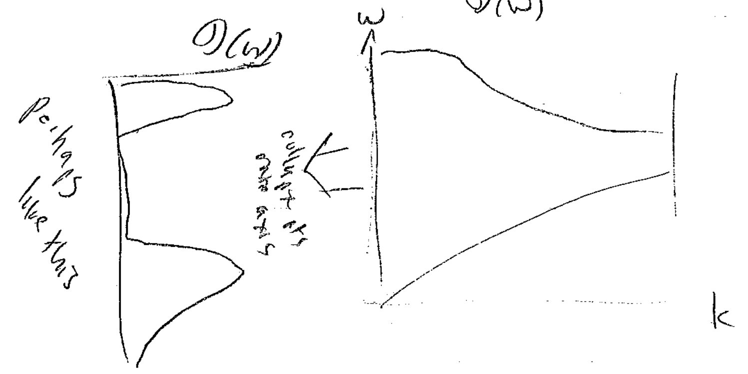
U_{tot} = U for that pt, plus U for every other pt.

Could sum over k

... but in practice summing over ω is better
(due in part from $\hbar\omega$ term in energy)

Caveats: 1). but not over all ω's! Not any ω's in band gap, etc.
2) Need to weight some ω's more heavily than others.

Solution: "Density of States" → like histogram, tells us weighting of ω's
$D(\omega)$



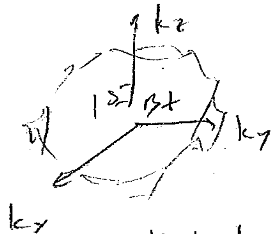
Other items in our plan:

— Pts are discrete, ~~so~~ but separation is tiny,

so make it into a function not a histogram and do integral, not summation

— extending to 3D will be tricky

$$\sum_{k_x}\sum_{k_y}\sum_{k_z} \to \iiint f\, dk_x\, dk_y\, dk_z \to \text{single integral over } \omega.$$



(3 · #atoms = # pts)
↓
2 transv
1 long

horrible limits of integration

Goal: total energy = $\frac{\text{energy}}{\text{phonon}}$ × # phonons for each pt in k-space → added up for all k

w/weighting: $U = \int_0^\infty \hbar\omega \, D(\omega) \frac{1}{e^{\hbar\omega/kT}-1} \, d\omega$

Then $C = \frac{dU}{dT}$

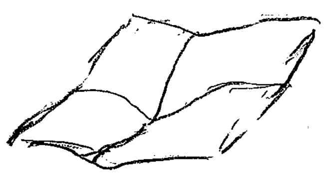
Density of states will depend on two items

- spacing between pts on k axis (note these are equally spaced)
- slope of dispersion curve.

↳ where dispersion curve is flat,
density of states will be large!

HW problem

Do a numerical histogram for the 2D situation on previous HW

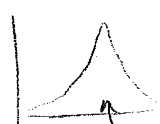


Divide into grid

Determine ω for each grid pt

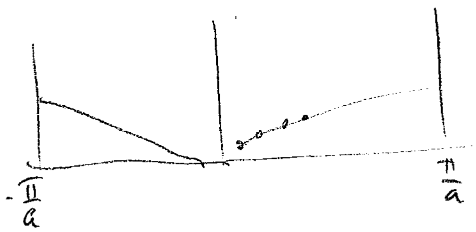
Sort all ω's by value

Plot histogram of results



Can do it numerically, but how to get eqn for $D(\omega)$?

What is spacing between pts ?



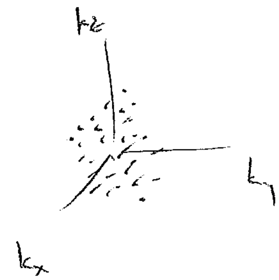
if 1D : have N pts between $-\frac{\pi}{a}$ and $\frac{\pi}{a}$, equally spaced

lattice pts, not # atoms

$$\text{Spacing} = \frac{2\pi}{a}\frac{1}{N} = \frac{\text{amount of k-space}}{\text{pt.}}$$

$Na = L$! total length of chain

if 3D



spacing in each direction is $\frac{2\pi}{L}$

$$\frac{\text{amount of k-space volume}}{\text{pt}} = \left(\frac{2\pi}{L}\right)^3$$

$$\frac{\#\text{ pts}}{\text{unit "volume" in k-space}} = \frac{1}{\left(\frac{2\pi}{L}\right)^3}$$

Summation to integral in k space :

$$U = \iiint \hbar\omega \cdot \frac{1}{\left(\frac{2\pi}{L}\right)^3} \, dk_x \, dk_y \, dk_z$$

↳ density of states in 3D k-space

Spherical approximation : $\iiint dk_x dk_y dk_z \longrightarrow \int 4\pi k^2 \, dk$

convert to integral in W ... what goes inside dw integral?

$$D(w)\,dw = \frac{1}{\left(\frac{2\pi}{L}\right)^3} \cdot 4\pi k^2 dk$$

$$\boxed{D(w) = \frac{1}{\left(\frac{2\pi}{L}\right)^3} \cdot 4\pi k^2 \cdot \frac{1}{\frac{dw}{dk}}}$$

spacing between pts

slope, notice when slope $\to 0$, $D(w) \to \infty$

Notes about 2D and 1D case - HW problem

$D(w)\,dw = \frac{1}{\left(\frac{2\pi}{L}\right)^2}\, 2\pi k^2\, dk$ 2D

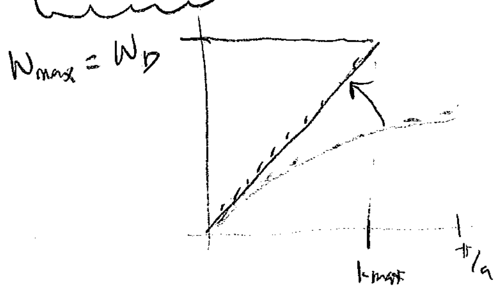
$D(w)\,dw = \frac{1}{2\pi/L} \cdot 2\,dk$ 1D

Can calculate if exact shape of $W(k)$ is known. (There's a 1D HW problem like that)

However...

Still very much used is the "Debye Model", a linear approximation

Handout



Linear, with slope = velocity

$$W = vk$$

Then $\frac{dw}{dk} = v$

and $k^2 = \left(\frac{W}{v}\right)^2$

$$D(w) = \frac{\text{Volume}}{8\pi^3} \times 4\pi\left(\frac{W}{v}\right)^2 \cdot \frac{1}{v}$$

That's easy ... trade off is you need to find W_D.

Force # pts to be = # lattice pts

$$N = \int_0^{\omega_D} D(\omega)\, d\omega$$

just count up all pts in histogram

$$N = \int_0^{\omega_D} \frac{V}{8\pi^3}\, 4\pi \frac{\omega^2}{v^2} \frac{1}{v}\, d\omega$$

$$\frac{N}{V} = \frac{1}{2} \frac{1}{\pi^2} \cdot \frac{1}{v^3} \cdot \frac{1}{3}\omega_D^3$$

$$\omega_D = \left(\frac{N}{V} \cdot 6\pi^2 v^3\right)^{1/3}$$

Plan: complete Debye model calculation

$$U = \int_0^{\omega_D} \hbar\omega \cdot D(\omega) \frac{1}{e^{\hbar\omega/kT} - 1}\, d\omega$$

as just found, $D(\omega) = \frac{V}{8\pi^3} 4\pi \left(\frac{\omega}{v}\right)^2 \frac{1}{v}$

Do integral $d\omega$

then take $\frac{\partial U}{\partial T}$ to get C

Debye Model for 3D - summary by Dr. Colton - Class Handout

(a) Density of states $D(\omega) = \frac{1}{(2\pi/L)^3} \cdot 4\pi k^2 \cdot \frac{1}{v}$

$$= \frac{V}{8\pi^3} \cdot 4\pi \left(\frac{\omega}{v}\right)^2 \cdot \frac{1}{v}$$

$$\boxed{D(\omega) = \frac{V}{2\pi^2 v^3} \omega^2}$$

(b) cutoff frequency

$$N = \int_0^{\omega_D} D(\omega)\, d\omega$$

$$= \int_0^{\omega_D} \frac{V}{2\pi^2 v^3} \omega^2 d\omega$$

$$= \frac{V}{2\pi^2 v^3} \frac{1}{3} \omega_D^3$$

$$\boxed{\omega_D = \left(6\pi^2 v^3 \frac{N}{V}\right)^{1/3}}$$

(c) energy

$$U = \underbrace{3}_{\#\text{ of acoustic branches}} \times \int_0^{\omega_D} D(\omega) f(\omega) \hbar\omega\, d\omega$$

$$= 3 \cdot \int_0^{\omega_D} \left(\frac{V}{2\pi^2 v^3} \omega^2\right)\left(\frac{1}{e^{\hbar\omega/kT} - 1}\right) \hbar\omega\, d\omega$$

let $x = \frac{\hbar\omega}{kT} \rightarrow \omega = \frac{kT}{\hbar} x$

$\left(x_D = \frac{\hbar\omega_D}{kT}\right)$ $\quad d\omega = \frac{kT}{\hbar} dx$

$$= 3 \int_0^{x_D} \left[\frac{V}{2\pi^2 v^3}\left(\frac{kT}{\hbar} x\right)^2\right]\left(\frac{1}{e^x - 1}\right) \hbar \left(\frac{kT}{\hbar} x\right)\left(\frac{kT}{\hbar} dx\right)$$

$$\boxed{U = \frac{3V}{2\pi^2 v^3} \frac{k^4 T^4}{\hbar^3} \int_0^{x_D} \frac{x^3}{e^x - 1} dx}$$

(d) low T: $x_D \rightarrow \infty$

$$U = \frac{3V}{2\pi^2 v^3} \frac{k^4 T^4}{\hbar^3} \underbrace{\int_0^{\infty} \frac{x^3}{e^x - 1} dx}_{\frac{\pi^4}{15}}$$

(via Mathematica)

3D cont

(d) low T, cont.

$$U = \frac{\pi^2}{10}\frac{V}{v^3}\frac{k^4}{\hbar^3}T^4$$

$$C_v = \frac{\partial U}{\partial T} = \frac{\pi^2}{10}\frac{V}{v^3}\frac{k^4}{\hbar^3}(4T^3)$$

$$\boxed{C_v = \frac{2\pi^2}{5v^3}\frac{k^4}{\hbar^3}T^3 V}$$

(can put in terms of N and $\Theta_D = \frac{\hbar\omega_D}{k}$, if desired)

(e) high T: x = small $\rightarrow e^x - 1 \simeq (1+x) - 1 = x$

$$U = \frac{3}{2}\frac{V}{\pi^2 v^3}\frac{k^4T^4}{\hbar^3}\underbrace{\int_0^{x_D}\frac{x^3}{x}dx}_{\frac{1}{3}x_D^3}$$

$$= \frac{1}{3}\frac{\hbar^3\omega_D^3}{k^3T^3}$$

$$= \frac{1}{3}\frac{\hbar^3}{k^3T^3}\left(6\pi^2 v^3\frac{N}{V}\right)$$

$$U = \frac{3}{2}\frac{\cancel{V}}{\pi^2 v^3}\frac{k^4T^4}{\hbar^3}\cdot\left[\frac{1}{3}\frac{\hbar^3}{k^3T^3}6\pi^2v^3\frac{N}{\cancel{V}}\right]$$

$$U = 3kTN$$

$$C_v = \frac{dU}{dT} = \boxed{3kN}$$

This matches the Dulong-Petit law!
(and the equipartition theorem, given 6 degrees of freedom)