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Chapter 5! "Phonons II, Thermal Properties"

(Two lectures ago?) ~~Last lecture~~:

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$(n+\frac{1}{2})\hbar\omega$ = energy for all phonons (n) with frequency ω.

How many phonons is that?

Answer: $n_{ave} = \dfrac{1}{e^{\hbar\omega/kT}-1}$

$k = k_B = 1.38\ 10^{-23}\ J/K$ Not wavevector!

Kittel: sometimes $\tau = kT$

Where does that come from?

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Two major results of Physics 360: What's likelihood of a given energy state E being occupied?

$\boxed{\text{Bose Einstein Distribution} \quad n_{ave} = \dfrac{1}{e^{(E-\mu)/kT}-1}}$

for particles w/o Pauli exclusion (photons, phonons, etc) "Bosons"

Side note: $n_{ave} \to \infty$ as $T \to 0$ "Bose Einstein Condensation"

or at least weighty (μ changes w/ Temp too)

$\boxed{\text{Fermi-Dirac Distribution} \quad n_{ave} = \dfrac{1}{e^{(E-\mu)/kT}+1}}$

for particles w/ Pauli exclusion (electrons, protons, neutrons, etc) "Fermions"

μ = "Chemical Potential", needed if you have a fixed # of particles $\Delta E = \mu \Delta N$ I think.

For photons/phonons: $\mu = 0$ because you can add/take away particles with no problem.

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Boltzmann distribution

$\boxed{n_{ave} = N_{tot} \dfrac{e^{-E/kT}}{\sum_{\text{all BFs}}}}$ ← or really $(E-\mu)/kT$

if $E \gg \mu$, all three are the same

(eg. low concentration of electrons, as we'll see in next chapter)

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Back to phonons ...   Goal: how much energy stored in phonon modes

or really... heat capacity, $\frac{dU}{dT}$

compare $Q = mc\Delta T$

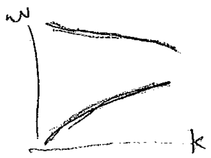
in general, we've got a whole set of phonon modes which are occupied to varying degrees

$$U_{tot} = \sum_n \left(n_{ave} + \tfrac{1}{2}\right)\hbar\omega_n$$

$$= \sum_n \left(\frac{1}{e^{\hbar\omega_n/kT}-1} + \frac{1}{2}\right)\hbar\omega_n$$

D may drop the 1/2 here (Kittel never includes)

Problem 1: What do we sum over? All possible ω's



Are these discrete? No if crystal is infinite, but yes if crystal is finite.

Do this earlier, in lecture 15 (before quantum SHO)

Consider —ww-o-ww-o-ww-o—

Before: $m\frac{d^2u_s}{dt^2} = C\left[(u_{s+1}-u_s)-(u_s-u_{s-1})\right]$

We assumed an infinite wave, but really we have N coupled equations.

The right way:

$$-m\omega^2\begin{pmatrix} \vdots \\ \vdots \end{pmatrix} = \begin{pmatrix} \text{mostly diagonal} \end{pmatrix}\begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix}$$

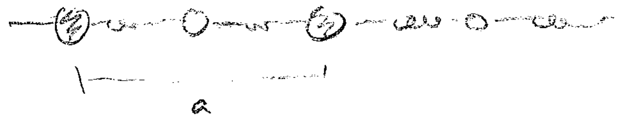
top & bottom rows from bdry conds.

Result: N eigenvalues!

N discrete frequencies.

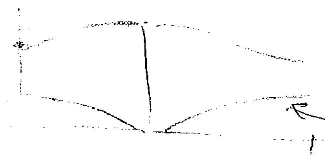
Possible HW problem: Compare to infinite 1D result

Consider diatomic lattice



$2N$ = # atoms

N = # unit cells

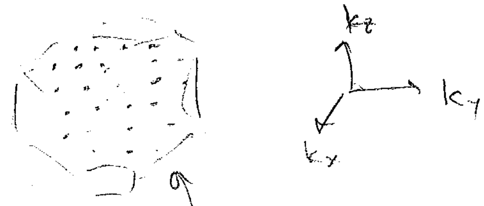


still N discrete frequencies.

Consider 3D lattice. Any guesses?

$\rightarrow$ get N^3 discrete pts = $\boxed{\text{total \# atoms}}$

× 3, actually, because of 2 transv + 1 longitud.



1st BZ shape

request model?

Note: also mention polarizations?

Later!

Macroscopic: N is huge, of course

$\rightarrow$ spacing between $\vec{k}$ values is tiny

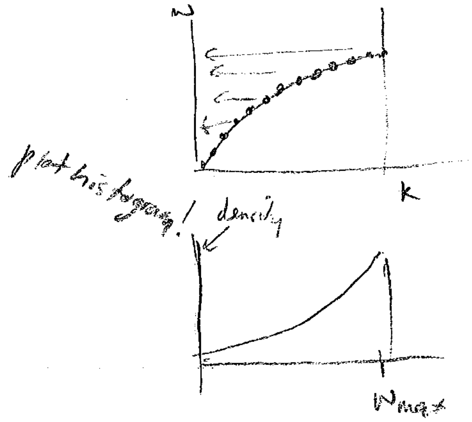
Problem 1: how do we convert sum into an integral?

Problem 2: how to make it an integral over ω, (not a triple integral over k_x, k_y, k_z)

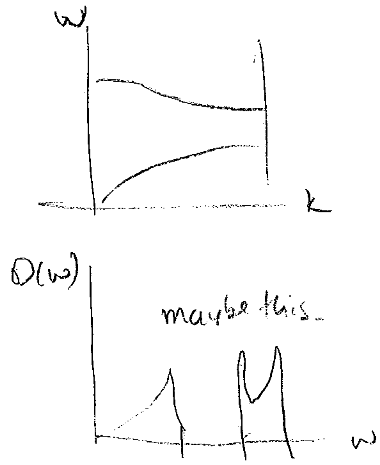
Solution: "Density of states"

What is "density of states"?

1D simplest case



1D diatomic lattice

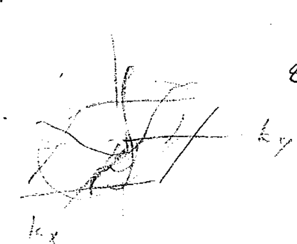


1D feature: singularity whenever $w(k)$ is horizontal

3D: sometimes singularities, sometimes jumps, sometimes kinks.

2D square lattice done for homework

discuss this in detail! Prob 5.2?



look up shape ☆

histogram: $D(w)$

☆

computer plot for HW? ☆

Histogram $D(w)$ needed because when we integrate over w instead of k, we need to more heavily weight the contributions from regions that have more states at that w!

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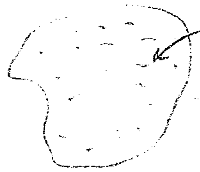
Side note: "periodic bndy conditions" another way to justify discrete pts.

General way to find $D(\omega)$

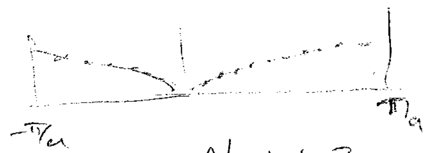


1 point every $\left(\frac{2\pi}{L}\right)^3$

region of k-space with points inside

density pts $= \frac{1}{(2\pi)^3/V} = \frac{V}{(2\pi)^3}$

1D



N pts in $\frac{2\pi}{a}$

1 pt in $\frac{2\pi}{Na}$

$\boxed{1 \text{ pt in } \frac{2\pi}{L}}$ ★ very important!

density of pts $= \frac{1}{2\pi/L}$

For a given ω

Assume spherical symmetry.

$$\int d^3k \longrightarrow \int 4\pi k^2 dk \times \underbrace{\text{density of pts}}_{V/(2\pi)^3}$$

skip until next time

Approx: if linear dispersion

$v = \omega/k \rightarrow k = \frac{\omega}{v}$

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

Summary: $D(\omega)d\omega = 4\pi k^2 dk \left(\frac{L}{2\pi}\right)^3$

$D(\nu)d\nu = \left(\frac{L}{2\pi}\right)^3 4\pi k^2 dk$

$$\underbrace{\int 4\pi \left(\frac{\omega}{v}\right)^2 \left(\frac{d\omega}{v}\right) \frac{Vol}{(2\pi)^3}}_{D(\omega)\,d\omega}$$

So $\boxed{D(\omega) = \frac{Vol}{(2\pi)^3} 4\pi \left(\frac{\omega}{v}\right)^2 \frac{1}{v}}$

GRE / Qual Exam

2D: $\int d^2k \longrightarrow \int 2\pi k\, dk \times \frac{Area}{(2\pi)^2} = \int 2\pi \left(\frac{\omega}{v}\right) \frac{d\omega}{v} \frac{A}{(2\pi)^2}$

$\boxed{D(\omega) = \frac{A}{(2\pi)^2} \cdot 2\pi \left(\frac{\omega}{v}\right) \frac{1}{v}}$

1D $\int dk \longrightarrow \int 2\, dk \times \frac{L}{(2\pi)} = \int 2 \left(\frac{d\omega}{v}\right) \frac{L}{2\pi}$

$\boxed{D(\omega) = \frac{L}{2\pi} \cdot 2 \cdot \frac{1}{v}}$

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If not linear dispersion, then eg

$$1D: \quad D(\omega) = \frac{L}{2\pi} \cdot 2 \cdot \frac{1}{(d\omega/dk)}$$

$$3D: \quad D(\omega) = \frac{Vol}{(2\pi)^3} \times (4\pi k^2) \times \frac{1}{d\omega/dk}$$

or if not even spherical approximation

$$\frac{Vol}{(2\pi)^3} \times \int_{\text{surface constant } \omega} \frac{dA}{|\nabla_k \omega|}$$

$\nabla_k \omega$ is $\frac{\partial\omega}{\partial k_x} + \frac{\partial\omega}{\partial k_y} + \frac{\partial\omega}{\partial k_z}$

pg 118, we won't ever use

Back to main problem

from before $U_{tot} = \sum_{\text{all pts}} (n_{ave} + \frac{1}{2}) \hbar\omega_n = \sum \left(\frac{1}{e^{\hbar\omega_n/kT} - 1} + \frac{1}{2} \right) \hbar\omega_n$

drop $\frac{1}{2}$ (Kittel never includes) since we'll be taking derivative

Translate to integral

$$U = \int D(\omega)\, d\omega \cdot \underbrace{\frac{1}{e^{\hbar\omega/kT} - 1}}_{\text{prob. of mode}} \times \underbrace{\hbar\omega}_{\text{energy of mode}}$$

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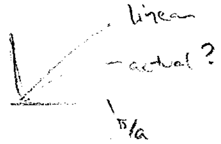
Linear Dispersion now

Another problem!
Limits of integration = ?

Debye model

use $\omega = vk$ approximation
(only acoustic branch, 1 atom/unit cell)



we know that $\int D(\omega)\, d\omega = N$ (# atoms),

so cut off integral early to force that to be true