Chapter 5: "Phasons II, Thermal Properties"

Energy for all phonons with frequency \( \omega \):

\[(n+\frac{1}{2})h\omega = \text{energy} \]

How many phonons are there?

Answer:

\[ N_{\text{Phasons}} = \frac{1}{e^{(E-\mu)/kT} - 1} \]

\[ k = k_B = 1.38 \times 10^{-23} \text{ J/K} \]

Kittel: sometimes \( \gamma = kT \)

Where does that come from?

Two major results of Ficks: 350: What's Heisenberg; a good energy state being occupied?

**Bose-Einstein Distribution**

\[ N_{\text{Bose}} = \frac{1}{e^{-\frac{E-\mu}{kT}} - 1} \]

for particles \( \rightarrow \) no Pauli exclusion (photons, phonons, etc.)

**Fermi-Dirac Distribution**

\[ N_{\text{Fermi}} = \frac{1}{e^{-\frac{E-\mu}{kT}} + 1} \]

for particles \( \rightarrow \) Pauli exclusion (electrons, protons, neutrons, etc.)

\( \mu \) = "Chemical Potential".

(357-358 "Bose-Einstein Condensation"

\( \gamma \) = \mu

\( \text{needs if you have a fixed def of particles E > \mu and} \)

\( \gamma \) = \mu

For photons/phonons \( \gamma = 0 \) because you can add/lose particles with no problem.

**Boltzmann Distribution**

\[ N_{\text{Boltzmann}} = N_0 e^{-\frac{E-\mu}{kT}} \]

\( E \gg \mu \), all three are the same.

(e.g., low concentration of electrons)

(As we'll see in next chapter).
Back to phonons... 

Goal: how much energy stored in phonon modes 
or really... heat capacity, $C_v$

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

$$U_{tot} = \sum_n \left( \frac{1}{E_n} - \frac{1}{2} \right) k_v n_n$$

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

Are these discrete? No: crystal is infinite, but $w_n$: if crystal is finite.

Consider $w_1-w_2-w_3-...$ 

Before: $m \frac{d^2 U_i}{dt^2} = c \left[ (U_{i+1} - U_i) - (U_{i-1} - U_i) \right]$ 

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

the right way:

$$\mathbf{w}^{2} \mathbf{u} = \left( \begin{array}{c} \mathbf{M} \\ \mathbf{D} \end{array} \right) \mathbf{u}$$

top is bottom rows from body waves.

Result: $N$ eigenvalues! 

$N$ discrete frequencies.
Consider discrete lattice

\[ 2N = \# \text{element} \]
\[ N = \# \text{unit cells} \]

Still \( N \) distinct frequencies.

Consider 3D lattice. Any guesses?

Get \( N^3 \) discrete points.

Macrosopic: \( N \) is huge, of course.

- Specifying between \( k^3 \) values is tricky.

Problem 2: how do we convert sum into an integral?

Problem 3: how to make it an integral over \( k_x, k_y, k_z \)?

Solution: "Density of states."
What is "density of states"?

1) Simples case

\[ \text{Plot this log-log density} \]
\[ w \text{ vs. } k \]

1D atomic lattice

\[ w \text{ vs. } k \]

D(w) \text{ maybe this...}

2D square lattice done for homework.

Discuss this result?

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 fixed \( w \)!
See note: "Possible bad candidates" another way to justify discrete pts

General way 1: $\mathbf{O}(N)$

Point every $\left( \frac{2\pi}{V} \right)^3$

Dense pts: $\frac{1}{20\pi^3}$

Region of k-space with points inside

For a given $N$

Assume spherical symmetry.

\[ \int d^3k \rightarrow \int V_{4\pi k^2} \times \text{densify} = \text{pts} \]

Approx.: if linear dispersion

\[ N = \frac{V}{k^2} \rightarrow k = \frac{\omega}{V} \]

\[ \Delta k = \frac{\omega}{V} \]

\[ \int \frac{4\pi}{V} \left( \frac{\omega}{V} \right)^2 \left( \frac{d\omega}{V} \right) \frac{V}{(2\pi)^3} \]

\[ \mathbf{O}(\omega) \Delta \omega \]

So

\[ \mathbf{O}(\omega) = \frac{V}{(2\pi)^3} \left( \frac{\omega}{V} \right)^3 \]

2D:

\[ \int d^2k \rightarrow \int 2\pi \Delta k \times \frac{A_{2D}}{2\pi} = \int 2\pi \left( \frac{\omega}{V} \right) \frac{d\omega}{V} \frac{A_{2D}}{2\pi} \]

\[ \mathbf{O}(\omega) = \frac{A_{2D}}{(2\pi)^2} \cdot 2\pi \left( \frac{\omega}{V} \right) \]

1D:

\[ \int d\lambda \rightarrow \int \frac{d\lambda}{2\pi} = \int \frac{2 \left( \frac{\omega}{V} \right) \frac{1}{2\pi}}{2\pi} \]

\[ \mathbf{O}(\omega) = \frac{1}{2\pi} \cdot 2 \cdot \frac{1}{V} \]
If not linear dispersion, then as:

\[ \sigma_D = D(w) = \frac{1}{2\pi^2} \int \frac{1}{(\omega - \omega_k)^2} \, d\omega \]

or if not even spherical approximation:

\[ \frac{\text{Vol} \, \tau}{(2\pi)^3} \int \frac{dA}{|\mathbf{K}|} \int_{\text{solid cone}} \frac{d\Omega}{4\pi} \int_{\text{dwell time}} \frac{d\tau}{2\pi^2} \]

Back to main problem:

\[ U_{\text{disp}} = \sum_{\phi \in \phi} \left( \mathcal{R}_1 + \mathcal{R}_2 \right) \frac{\tau}{\omega} \mu_{\omega} = \sum_{\phi \in \phi} \left( \frac{1}{\mu_{\omega}/\kappa_T} + \frac{1}{\tau} \right) \mu_{\omega} \]

Translate to integral:

\[ U = \int \sigma_D(w) \, dw \cdot \frac{1}{\mu_{\omega}/\kappa_T - 1} \times \mu_{\omega} \]

Another problem!

Limits of integration?

Debye model

Use: w = k approximation

Only acoustic branch

\[ \text{we knew that } \int \sigma_D(w) \, dw = N \text{ (not sure) } \]

So cut off integral early to force that to be true