# First reading assignment

**Difficulties:**

I) dispersion relation for sound, speed of sound, transverse and longitudinal sound modes

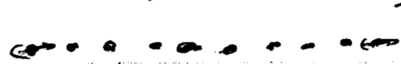
II) How to get the number of allowed frequencies in the interval $[\omega, \omega + d\omega]$ (the density of states) (7.66 & 7.67)

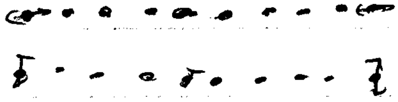
III) What is the density of states? How can it be measured by neutron scattering? What do sound modes have to do with the reaction of the system to physical changes?

IV) What happens at high frequencies? Why does Debye model break down? Is the model bad at high temperatures? Where does Debye frequency come from?

(I) modes on a 1-d solid:

open boundary → wavelength $\lambda$ is integer fraction of $2L$ $\quad \lambda = \frac{2L}{\ell}$, $\ell = 1, 2, 3, \ldots$

longitudinal 

transversal 

standing wave:
$$\left.\begin{aligned} \omega T = 2\pi &\Rightarrow T = \frac{2\pi}{\omega} \\ cT = \lambda = \frac{2L}{\ell} &\Rightarrow T = \frac{2L}{\ell c} \end{aligned}\right\} \quad \omega = \frac{\pi \ell c}{L}$$

3-d:
$$\omega^2 = c^2 \left[ \left( \frac{\pi \ell_x}{L_x} \right)^2 + \left( \frac{\pi \ell_y}{L_y} \right)^2 + \left( \frac{\pi \ell_z}{L_z} \right)^2 \right]$$

(II) see page (96) bottom

(III) density of states = # states per energy

neutron scattering: energy is conserved, look at energy difference between incoming and outgoing neutrons → information on the internal energy states

phonons are the only way to store internal energy in this solid, kick one atom → all others start to move

raise temperature → phonons take the energy

(IV)
- wave lengths shorter than lattice ~~distance~~ constant can not exist → no waves beyond certain k-vector → no waves beyond certain frequency → Debye frequency
- Debye model: continuous, isotropic, reality: discrete, anisotropic
- at high temperatures specific heat of harmonic oscillator is $k_B$ <u>independent of $\omega$</u>

⇒ $C_V$ is always correct as long as there is the correct number of oscillators

$$C_N \xrightarrow[k_BT \gg \hbar\omega]{} \frac{3N(\hbar\omega)^2}{k_BT^2} \frac{1}{\left(\frac{\hbar\omega}{k_BT}\right)^2} = 3Nk_B \quad ✓$$

$$C_N \xrightarrow[k_BT \ll \hbar\omega]{} \sim \frac{1}{T^2} e^{-\frac{\hbar\omega}{k_BT}} \longrightarrow 0$$

experimentally for small $T$: $C_N \sim \frac{1}{T^3}$

→ need better theory → coupled oscillators ↓ 11/20

**Model III**: Debye solid

consider solid as an <u>elastic medium</u> of size $L_x L_y L_z$

→ possible oscillation modes are standing waves

wavelengths $\frac{2L_x}{l_x}, \frac{2L_y}{l_y}, \frac{2L_z}{l_z}$ with integers $l_x, l_y, l_z$

frequency of the mode of type $i$ (2 transverse, 1 longitudinal)

$$\omega^2_{(l_x, l_y, l_z, i)} = c_i^2 \left[ \left(\frac{\pi l_x}{L_x}\right)^2 + \left(\frac{\pi l_y}{L_y}\right)^2 + \left(\frac{\pi l_z}{L_z}\right)^2 \right]$$

energy of the system

$$H = \sum_{(l_x, l_y, l_z, i)} \hbar\omega_{(l_x, l_y, l_z, i)} \left( n_{(l_x, l_y, l_z)} + \tfrac{1}{2} \right)$$

number of quanta in mode $(l_x, l_y, l_z)$

partition function:

$$Z(T) = \sum_{\{n_{(l_x, l_y, l_z, i)}\}} e^{-\beta \sum_{(l_x, l_y, l_z, i)} \hbar\omega_{(l_x, l_y, l_z, i)} \left(n_{(l_x, l_y, l_z)} + \frac{1}{2}\right)}$$

$$= \prod_{l_x, l_y, l_z, i} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega_{(l_x, l_y, l_z, i)}\left(n + \frac{1}{2}\right)}$$

$$= \prod_{l_x, l_y, l_z, i} \frac{e^{-\beta \frac{\hbar}{2} \omega_{(l_x, l_y, l_z, i)}}}{1 - e^{-\beta \hbar \omega_{(l_x, l_y, l_z, i)}}}$$

$$\ln Z = \sum_{l_x, l_y, l_z, i} \left[ -\frac{\beta \hbar}{2} \omega_{(l_x, l_y, l_z, i)} - \ln\left(1 - e^{-\beta \hbar \omega_{(l_x, l_y, l_z, i)}}\right) \right]$$

$$U = -\left(\frac{\partial \ln Z}{\partial \beta}\right) = \sum_{l_x, l_y, l_z, i} + \frac{\hbar \omega_{(l_x, l_y, l_z, i)}}{2} + \frac{e^{-\beta \hbar \omega_{(l_x, l_y, l_z, i)}}}{1 - e^{-\beta \hbar \omega_{(l_x, l_y, l_z, i)}}} \hbar \omega_{(l_x, l_y, l_z, i)}$$

$$= \sum_{l_x, l_y, l_z, i} \hbar \omega_{(l_x, l_y, l_z, i)} \left[ \frac{1}{2} + \frac{1}{e^{\beta \hbar \omega_{(l_x, l_y, l_z, i)}} - 1} \right]$$

$$C_N = \frac{\partial U}{\partial T} = -\frac{1}{k_B T^2} \frac{\partial U}{\partial \beta} = \frac{1}{k_B T^2} \sum_{l_x, l_y, l_z, i} \left(\hbar \omega_{(l_x, l_y, l_z, i)}\right)^2 \frac{e^{\beta \hbar \omega_{(l_x, l_y, l_z, i)}}}{\left(e^{\beta \hbar \omega_{(l_x, l_y, l_z, i)}} - 1\right)^2}$$

How do we perform the sum over $l_x, l_y, l_z, i$?

If we know the density $n(\omega)$ of modes at frequency $\omega$

$$\rightarrow C_N = \frac{1}{k_B T^2} \int_0^\infty d\omega \, n(\omega) (\hbar \omega)^2 \frac{e^{\beta \hbar \omega}}{\left(e^{\beta \hbar \omega} - 1\right)^2}$$

How many modes are there at frequency $\omega$?

fix type $i$

modes with frequency less or equal to $\omega$

$$= \text{number of } (l_x, l_y, l_z) \text{ with } \left(\frac{\pi c_i l_x}{L_x}\right)^2 + \left(\frac{\pi c_i l_y}{L_y}\right)^2 + \left(\frac{\pi c_i l_z}{L_z}\right)^2 \leq \omega^2$$

$$= \frac{1}{8} \frac{4}{3} \pi \omega^3 \frac{L_x}{\pi c_i} \frac{L_y}{\pi c_i} \frac{L_z}{\pi c_i} = \frac{\omega^3 V}{6 \pi^2 c_i^3}$$

only positive $l_x, l_y, l_z$

density of modes in x-direction

→ density of modes ~~of~~ type $i$

$$n_i(\omega) = \frac{d}{d\omega}\,\frac{\omega^3 V}{6\pi^2 c_i^3} = \frac{\omega^2 V}{2\pi^2 c_i^3}$$

→ total density of modes

$$n(\omega) = n_1(\omega) + n_2(\omega) + n_3(\omega) = \frac{\omega^2 V}{2\pi^2}\left(\frac{2}{c_t^3} + \frac{1}{c_\ell^3}\right)$$

diverges for $\omega \to \infty \Rightarrow$ infinitely many modes?

There can be no modes with a wavelength shorter than the distance between two atoms → cutoff

$$n(\omega) = \begin{cases} \frac{\omega^2 V}{2\pi^2}\left(\frac{2}{c_t^3} + \frac{1}{c_\ell^3}\right) & \omega \le \omega_D \\ 0 & \omega > \omega_D \end{cases}$$

How to find $\omega_D$? There have to be $3N$ modes total

$$\Rightarrow 3N = \int_0^\infty d\omega\, n(\omega) = \int_0^{\omega_D} d\omega \frac{\omega^2 V}{2\pi^2}\left(\frac{2}{c_t^3} + \frac{1}{c_\ell^3}\right) = \frac{\omega_D^3 V}{6\pi^2}\left(\frac{2}{c_t^3} + \frac{1}{c_\ell^3}\right)$$

$$\Rightarrow \quad \omega_D = \left(\frac{18\pi^2 N}{V\left(\frac{2}{c_t^3} + \frac{1}{c_\ell^3}\right)}\right)^{1/3}$$ "Debye frequency" material constant

$$n(\omega) = \begin{cases} \frac{9N\omega^2}{\omega_D^3} & \omega \le \omega_D \\ 0 & \omega > \omega_D \end{cases}$$

$$\Rightarrow C_N = \frac{1}{k_B T^2}\int_0^\infty d\omega\, n(\omega)\,(\hbar\omega)^2 \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$$

$$= \frac{\hbar^2}{k_B T^2}\int_0^{\omega_D} d\omega \frac{9N}{\omega_D^3}\,\omega^4 \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2} = \frac{9N\hbar^2 k_B^5 T^5}{k_B T^2 \omega_D^3 \hbar^5}\int_0^{\beta\hbar\omega_D} dx\, x^4 \frac{e^x}{(e^x-1)^2}$$

$$= \frac{9 N k_B^4}{(\hbar\omega_D)^3} T^3 \int_0^{T_D/T} dx\, x^4 \frac{e^x}{(e^x-1)^2} \qquad T_D \equiv \frac{\hbar\omega_D}{k_B}$$

<u>for $T \to 0$:</u>

$$C_N \approx \frac{9 N k_B^4}{(\hbar\omega_D)^2} T^3 \int_0^{\infty} dx\, x^4 \frac{e^x}{(e^x-1)^2} = \frac{12 N k_B \pi^4}{5 T_D^3} T^3 \quad \checkmark$$

<u>for $T \to \infty$:</u>

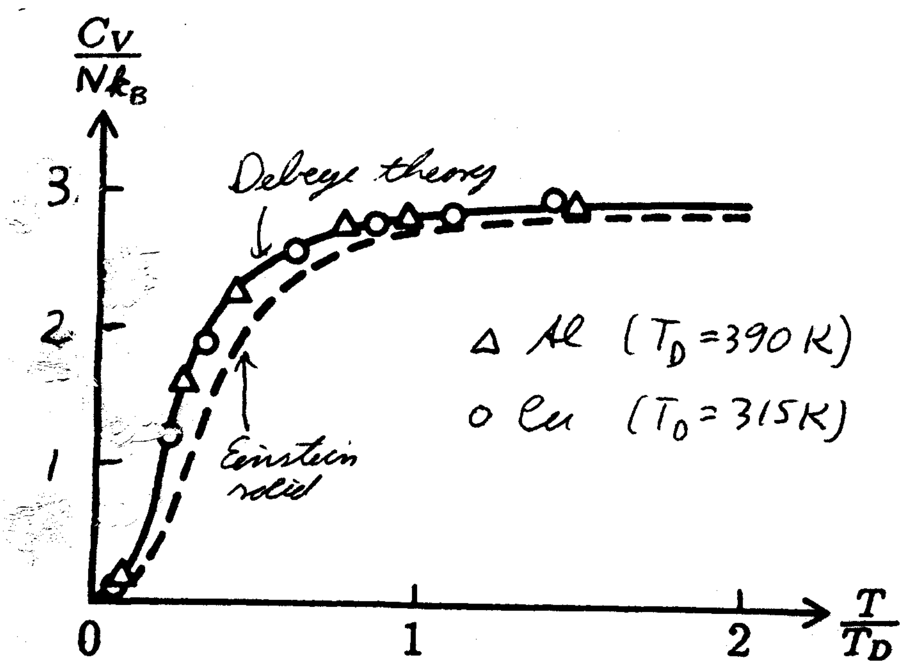
expand integrand around $x=0$:

$$\int_0^{T_D/T} dx\, x^4 \frac{e^x}{(e^x-1)^2} \approx \int_0^{T_D/T} dx\, x^4 \frac{1}{x^2} = \frac{1}{3}\left(\frac{T_D}{T}\right)^3$$

$$\Rightarrow \quad C_N \approx \frac{9 N k_B T^3}{T_D^3} \frac{1}{3}\left(\frac{T_D}{T}\right)^3 = 3 N k_B \quad \checkmark$$

<u>for intermediate T:</u>

good agreement with experiment



# V.3 Magnetic systems

## V.3.1 Overview and models

Goal: Describe magnetic properties of a solid

Model: - d-dimensional lattice with N sites
- a spin $\vec{S}_i$ on each lattice site
- spins interact with each other
- external magnetic field B in z-direction interacts with spins of moment $\mu$

Hamiltonian:

$$H = \sum_{1 \le i < j \le N} \varepsilon_{ij} \vec{S}_i \vec{S}_j - \mu B \sum_{i=1}^{N} (\vec{S}_i)_z$$

$\varepsilon_{ij}$ describes interaction of spin i with spin j

$\varepsilon_{ij} < 0 \Rightarrow$ spin $\vec{S}_i$ and $\vec{S}_j$ like to be parallel
$\varepsilon_{ij} > 0 \Rightarrow$ spin $\vec{S}_i$ and $\vec{S}_j$ like to be anti parallel

spin-spin interaction decays with spatial distance

$$\rightarrow \quad \varepsilon_{ij} = \begin{cases} \varepsilon_{ij} & i,j \text{ are neighbors} \\ 0 & i,j \text{ are not neighbors} \end{cases}$$

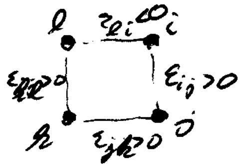
$$H = \sum_{\{i,j\}} \varepsilon_{ij} \vec{S}_i \vec{S}_j - \mu B \sum_{i=1}^{N} (\vec{S}_i)_z$$

$\leftarrow$ i,j neighbors

sometimes: include next nearest neighbors etc.

<u>disordered magnets</u>: $\varepsilon_{i,j}$ stochastic variables
"impurities in the crystal"

→ frustration




i wants to be parallel to j
j " " " " " k
k " " " " " l
but l wants to be antiparallel to i ↯

→ spin glasses → open research area

<u>no disorder</u>:

$$H = -\varepsilon \sum_{\{i,j\}} \vec{S}_i \cdot \vec{S}_j - \mu B \sum_{i=1}^{N} (\vec{S}_i)_z$$

$\varepsilon < 0$ ⇒ energy wants to align all spins
$\varepsilon > 0$ ⇒ energy wants to anti-align all spins

Warning: $\vec{S}_i$ are quantum-mechanical variables
(e.g., $[(\vec{S}_i)_x, (\vec{S}_i)_y] \neq 0$)

⇒ have to do real quantum statistics

⇒ Heisenberg model
- in $d=1$ physics depends on spin ($s = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$)
- not even solved in $d=1$ for arbitrary spin

Approximate spins as classical vectors:

$\vec{S}_i$ three dimensional vector: $O(3)$ model
$\vec{S}_i$ two dimensional vector: XY model

none can be solved exactly, some theory on phases / phase transitions available

Extra assumption:

The spins are oriented in $z$ direction by crystal.

$$\Rightarrow \quad H = -\varepsilon \sum_{\{i,j\}} s_i s_j - \mu B \sum_{i=1}^{N} s_i$$

with $s_i \in \{\pm 1\} \rightarrow$ everything commutes

"Ising model"

$\downarrow$ 1/22

Reminder:

want to explain

at $B=0$

ferromagnet | paramagnet
$0$ ——— $T^*$ ———→ $T$
$M \neq 0$ | $M = 0$

$H = -\varepsilon \sum_{\{i,j\}} s_i s_j$ with $\varepsilon > 0$ promising:

- at low $T$ energy dominates, energy wants either all spins $+1$ or all spins $-1$
  $\Rightarrow$ ferromagnet
- at high $T$ entropy dominates, entropy wants spins to be "random"
  $\Rightarrow$ $M=0$, paramagnet

Results:

$d=1$: – Ising model can be solved exactly
– no ferromagnetism

$d=2$: – Ising model can be solved exactly
– very technical, Onsager 1944
– has phase transition as expected
– ~~one~~ of the few exactly solvable models in [illegible] with a phase transition

$d=3$: – no exact solution

large $d$: – approximate solution "mean field theory"
– phase transition