Phonons as excitations

THE PROBLEM OF QUANTUM MELTING

Second quantization:

Recall from quantum mechanics:

$$[x, p] = xp - px = i\hbar$$

based on this lets introduce 2 operators, which create and annihilate an excitation when applied to the ground state or vacuum.

$$\begin{cases} b = \dfrac{1}{\sqrt{2\hbar M\omega}} (M\omega x + ip) \\[4mm] b^{+} = \dfrac{1}{\sqrt{2\hbar M\omega}} (M\omega x - ip) \end{cases}$$

lets ~~very~~ verify that anti commutator is

$$[b, b^{+}] = 1$$

$$[bb^{+}] = \frac{1}{2\hbar M\omega} \left\{ (M\omega^2) \underbrace{[xx]}_{=0} + i M\omega \underbrace{[px]}_{=-i\hbar} - i M\omega \underbrace{[xp]}_{i\hbar} + \underbrace{[pp]}_{=0} \right\} = \frac{1}{2\hbar} i M\omega [px]$$

$$= \frac{1}{2\hbar} (-2i [xp]) = \frac{-2 i \cdot i \hbar}{2\hbar} = 1$$

inversely we can express x and p as

$$x = \sqrt{\frac{\hbar}{2M\omega}} (b^{+} + b) \qquad p = \frac{i \sqrt{2\hbar M\omega}}{2} (b^{+} - b)$$

Recall those $\overset{x}{\cancel{}}$ P are operators here! Just a different representation.

For the HARMONIC OSCILLATOR:

$$\mathcal{H} = \frac{p^2}{2M} + B\frac{x^2}{2} = -\frac{\cancel{2} \hbar M\omega}{2 \cancel{2} 2M} (b^{+} - b)^2$$

$$+ \frac{B\hbar}{2M\omega} (b^{+} + b)^2 = -\frac{\hbar\omega}{4} (b^{+} - b)^2 + \frac{B\hbar}{2M\sqrt{B/M}} (b^{+} + b)^2 =$$

$$\hookrightarrow B = \omega^2 M$$

$$H = \tfrac{1}{2}\hbar\omega\,(bb^\dagger + b^\dagger b) = \overline{LS}$$

$$= \hbar\omega\,\underbrace{b^\dagger b}_{[bb^\dagger]=1} + \tfrac{1}{2}\hbar\omega = \hbar\omega\,(n + \tfrac{1}{2})$$

where $n = b^\dagger b$ is the occupation number
(the number of ~~excitation~~ particles in the
ground state)

for the states with excitations present:

$$b\,|n\rangle = \sqrt{n}\,|n-1\rangle$$
$$b^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

the philosophy of
bosons the
more the marier!

the amplitude grows as $\sim\sqrt{n+1}$!

b – anihilation
$b^\dagger$ – creation   operators.

they increase (decrease) the # of bosons
by $+\,(-1)$.

for $n \equiv b^\dagger b \implies n\,|n\rangle = b^\dagger b|n\rangle = b^\dagger \sqrt{n}\,|n-1\rangle$

$$= \sqrt{n}\cdot\sqrt{n}\,|n\rangle = n\,|n\rangle$$

for the groun state: $b\,|0\rangle = 0$

$$|n\rangle = \tfrac{1}{\sqrt{n!}}\,(b^\dagger)^n\,|0\rangle.$$

Now we are ready for something
interesting.

Quantum Melting.

Recal that vibration amplitude

$$U \equiv \delta x = \sqrt{\frac{\hbar}{2M\omega}} \; (b^+ + b) \quad \text{for 1 phonon mode}$$

The average shift from eq. is $\langle U \rangle = 0$

but for:

$$\langle U^2 \rangle = \frac{\hbar}{2M\omega} \left\langle (b+b)^2 \right\rangle = \frac{\hbar}{2M\omega} \langle b b^{++} + b b +$$

$$\underbrace{b^+ b + b b^+}_{2 b^+ b - [b b^+] = 1} \rangle = \frac{\hbar}{2M\omega} \left(2 \langle b^+ b \rangle + 1\right) = \frac{\hbar}{2M\omega} \left(n + \frac{1}{2}\right)$$

and for the highest energy phonons

$$\omega = \omega_D \qquad \qquad \theta_D \equiv \hbar \omega_D$$

$$\langle U^2 \rangle = \frac{\hbar^2}{2M \theta_D} \left(n \pm \frac{1}{2}\right) \qquad n = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

$$= \frac{1}{e^{\theta_D/k_B T} - 1}$$

So for

$$T \to 0 \qquad \langle U^2 \rangle \approx \frac{\hbar^2}{2M\omega_D} \qquad \text{(zero point oscillations!)}$$

$$T \gg \theta_D : \qquad \langle U^2 \rangle \sim \frac{\hbar^2}{M \theta_D^2}$$

According to the Lindermann criterion
when $\langle U^2 \rangle \sim a$ ~~the~~ melting occurs.
(precisely $\langle U^2 \rangle \sim 0.2 a$)

So one can introduce the melting
parameter $\Lambda \equiv \frac{\langle U^2 \rangle}{a}$ ← De Boer parameter

at $T=0$ $\quad \langle U^2 \rangle \sim \frac{\hbar}{M\omega}$ where $\omega = \sqrt{\frac{B}{M}}$ ← bulk modulus
or the stiffness of the lattice

Lets estimate B

If we shift an atom from the equilibrium bgra there will be o change in the pot. energy $\sim Ba^2 \sim V(a)$

↖ the interaction potential between atoms.

so $B \sim \dfrac{V(a)}{a^2} \Rightarrow \Lambda \approx \dfrac{\hbar}{a} \dfrac{1}{\sqrt{MV(a)}}$

and if $\Lambda \gtrsim 0.2 - 0.3$ the system is unstable against the quantum zero point motion and the xtal $\underline{\sqrt{\text{mets}}}$!!!

P: Does it really happen?

Well we need small M and weak $V(a)$

meet ^{4}He   He is very light and He interaction is very small.

That's why He is liquid down to $T=0$!

What do you think about H (hydrogen)?

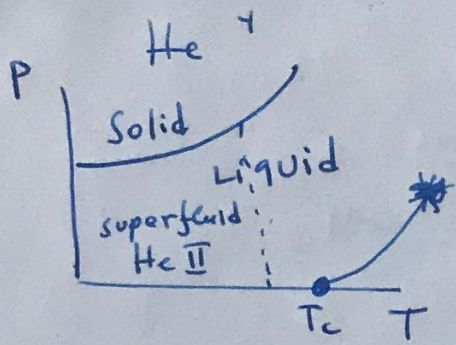Another way to "encorage" quantum melting is to apply pressure P but of course $a \downarrow$ but $V(a)$ goes up and then $\Lambda \approx V(a)a^2$ may change either way. For ^{4}He $V(a)$ goes up quick and it becomes SOLID. For electronic liquid it is opposite:
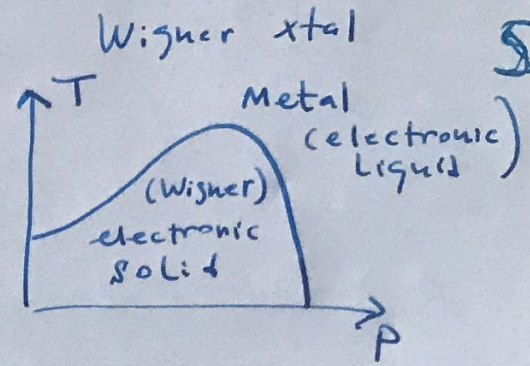
$V(a) = \dfrac{e^2}{a}$ and $\Lambda = \dfrac{\hbar}{a}\sqrt{\dfrac{Me^2}{a}} \sim \dfrac{1}{\sqrt{a}}$

so as $P \uparrow a \downarrow \Lambda \uparrow \Rightarrow$ cold melting of an electronic crystal (Wigner)

He^4

P

Solid

Liquid

superfluid

He II

T_c T

VS.

Wigner xtal

T

Metal
(electronic)
Liquid

(Wigner)
electronic
Solid

P

PHYSICAL QUANTITIES IN SEMICLASSICAL MODEL

| Phonons |. The 1st take on collective excitations

Consider a chain of identical atoms:
(ions)

← n a →Motion along the chain

Define the position of atoms as:

x_n — in the equilibrium $x_n^{eq} = n \cdot a$

If we allow the motion of the atoms:

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

○— Note since it is 1D we allow only <u>longitudinal</u>
<u>motion</u>.

- Let us also assume the potential is <u>quadratic</u>.
- Now its getting strange., We technically descibe
  the motion of balls connected with springs!!

$$V_{total} = \sum_j V(x_{j-1} - x_j) = \sum_j \frac{k}{2}(x_{j+1} - x_j - a)^2$$

$$= \sum_j \frac{k}{2}(\delta x_{j+1} - \delta x_j)$$

restoring
The Force on the mass n is

$$F_n = -\frac{\partial V_{tot}}{\partial x_n} \underset{\delta x_n = x_n - na}{=} -\frac{\partial}{\partial x_n}\left(\frac{k}{2}(x_{n+1} - x_n - a)^2\right) =$$

$$\underbrace{= k(\delta x_{n+1} - \delta x_n) + k(\delta x_{n-1} - \delta x_n)} = m \, \delta \ddot{x}_n$$

Newtonian Law.

Recap: A normal mode is a collective oscillation
where all particles move at the same frequency.

Lets attempt to solve it by assuming
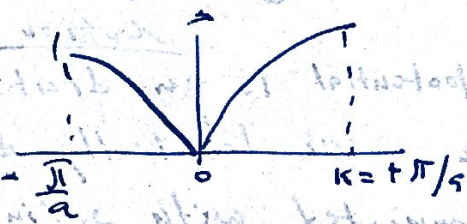that we have a wave propagating through
the chain

$$\delta x_n = A e^{i\omega t - ikx_n} = A e^{(i\omega t - ikna}$$

A is the amplitude of the wave.

$$-m\omega^2 A e^{i\omega t \cdot ikna} = k A e^{i\omega t} [e^{-ika(n+1)} +$$

$$+ e^{-ika(n-1)} - 2e^{ikan}] \quad or$$

$$m\omega^2 = 2k [1 - \cos(ka)] = 4k \sin^2(ka/2)$$

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

Not too surprizing again b/c of the
periodicity of the crystal we end up
with the same physics.

$$e^{iG \cdot x} = 1 \quad where \quad G_q = \frac{2\pi}{a} \cdot n$$

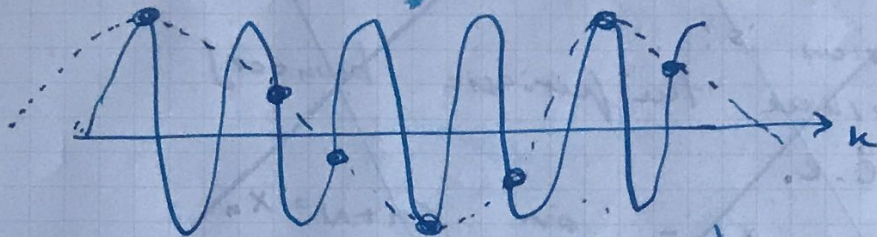Again the same issue as for electrons
k is defi'ed up to   k + Gu = k

But what k we should use say in

$$v_{phase} = \frac{\omega}{k} = ? = \frac{\omega}{k+G} ?$$

$$or \ do \ we \ say \ \frac{2\pi}{k} \gtrless \frac{2\pi}{k+G} ?$$

The resolution to this puzzle comes from the fact that:

We can define the wave only at the lattice points x_n

So $k + \frac{2\pi}{a} n$ and k are the same!

This is also known as _aliasing_ of waves.

● Properties of 1D chains.

Sound wave: always has λ much larger than a (e.g. human (c_s) $\sim 10 m$)

Large λ, small k so

the dispersion $\omega = v_{sound} k$
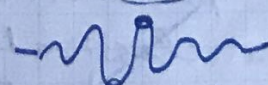
$$\omega = 2\sqrt{\frac{k}{m}} \left| \sin\left(\frac{ka}{2}\right)\right| \cong 2\sqrt{\frac{k}{m}} \cdot \left|\frac{ka}{2}\right|$$

$$v_{sound} = \frac{\omega}{k} \cong \sqrt{\frac{k}{m}} \cdot a$$

<u>Large λ, short k</u>:   We define the _group velocity_:

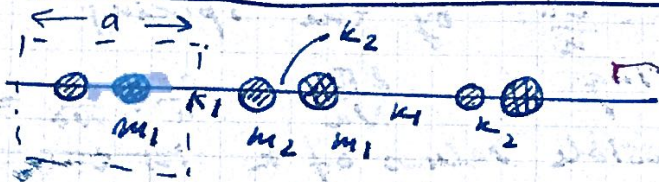$$\begin{cases} v_{group} = \frac{d\omega}{dk} \\ v_{phase} = \omega/k \end{cases}$$

v_{group}

how individual maxima and minima move.

if the dispersion is _linear_

$$v_{group} = v_{phase}$$

non-linear   they are different.

Note at $\pm \pi/a$: $v_{group} = 0$! the dispersion is flat.
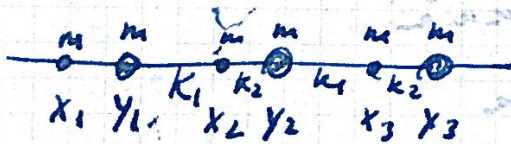
$$\boxed{\text{Two atoms per unit cell. — PHONON modes.}}$$

Lets for simplicity assume that $m_1 = m_2$
We are about to repeat the same algebra
as for the 1D chain with 1-type of atoms
where we found that the system will
have the energy dispersion $\omega(k) \sim |\sin\frac{ka}{2}|$

$$\begin{cases} m\,\delta\ddot{x}_n = k_2\,(\delta y_n - \delta x_n) + k_1\,(\delta y_{n-1} - \delta x_n) \\ m\,\delta\ddot{y}_n = k_1\,(\delta x_{n+1} - \delta y_n) + k_2\,(\delta x_n - \delta y_n) \end{cases}$$

again we will be
looking for a solution of
this kind:

$$\delta x_n = A_x\, e^{i\omega t - ikna}$$
$$\delta y_n = A_y\, e^{i\omega t - ikna}$$

We focus our attention on the 1st BZ.

$$-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}, \quad \text{with } N \text{ unit cells}$$

$$L = N\cdot a$$

k will be quantized $k = \dfrac{2\pi}{Na} = \dfrac{2\pi}{L}$

here we mean N
the number of u.c.
Not the number of atoms.

If we devide the range of k values in the 1st BZ $\frac{2\pi}{a}$ by the spacing between neighboring ks $\frac{2\pi}{Na}$: $\frac{2\pi}{a} : \frac{2\pi}{Na} \Rightarrow N$ we obtain N possible values of k ~~in the BZ.~~ or 1 value of k per unit cell.

But Debye states that there is only one more normal mode per degree of freedom and here we have 2 atoms but seemingly one mode!

What to do? Lets go ahead and solve the equations:

$$\begin{cases} -\omega^2 m A_x e^{-iwt - ikna} = \\ \quad k_2 A_y e^{iwt - ikna} + k_1 A_y e^{iwt - ik(n-1)a} \\ \quad - (k_1 + k_2) A_x e^{iwt - ikna} \\ \\ - \omega^2 m A_y e^{iwt - ikna} \\ \quad = k_1 A_x e^{iwt - ik(n+1)a} + k_2 A_x e^{iwt - ikna} \\ \quad - (k_1 + k_2) A_y e^{iwt - ikna} \end{cases}$$

$$\Rightarrow \begin{cases} -\omega^2 m A_x = k_2 A_y + k_1 A_y e^{ika} - (k_1 + k_2) A_x \\ \\ -\omega^2 m A_y = k_1 A_x e^{-ika} + k_2 A_x - (k_1 + k_2) A_y \end{cases}$$

or

$$m\omega^2 \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} (k_1 + k_2) & -k_2 - k_1 e^{ika} \\ -k_2 - k_1 e^{-ika} & (k_1 + k_2) \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix}$$

The solution is:

$$0 = \begin{vmatrix} (k_1 + k_2) - m\omega^2 & -k_2 - k_1 e^{ika} \\ -k_2 - k_1 e^{-ika} & (k_1 + k_2) - m\omega^2 \end{vmatrix} =$$

$$= |(k_1 + k_2) - m\omega^2|^2 - |k_2 + k_1 e^{ika}|^2 = 0$$

$$m\omega^2 = (k_1 + k_2) \pm |k_1 + k_2 e^{ika}|$$

$$|k_1 + k_2 e^{ika}| = \sqrt{(k_1 + k_2 e^{ika})(k_1 + k_2 e^{-ika})} =$$

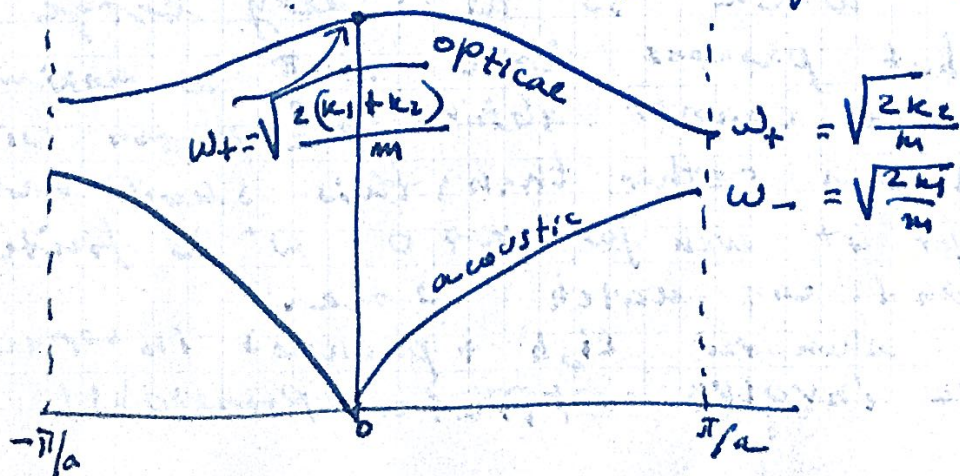$$= \sqrt{k_1^2 + k_2^2 + 2k_1 k_2 \cos ka}$$

so finally

$$\omega_\pm = \sqrt{\frac{k_1 + k_2}{m} \pm \frac{1}{m} \sqrt{k_1^2 + k_2^2 + 2k_1 k_2 \cos(ka)}}$$

$$= \sqrt{\frac{k_1 + k_2}{m} \pm \frac{1}{m} \sqrt{(k_1 + k_2)^2 - 4k_1 k_2 \sin^2\left(\frac{ka}{2}\right)}}$$

for each k we have 2 solutions $\pm$
or 2 branches of the dispersion

~~Since there are 2 branches~~ or we have
2N modes! Exactly as Debye predicted
one excitation mode for degree of freedom.

$$\omega_+ = \sqrt{\frac{2(k_1 + k_2)}{m}} \qquad \text{optical}$$

$$\omega_+ = \sqrt{\frac{2k_2}{m}}$$

$$\omega_- = \sqrt{\frac{2k_1}{m}}$$

acoustic

$-\pi/a \qquad 0 \qquad \pi/a$

LIS

Long wavelength show linear dispersion
= acoustic branch. $= \omega_-(k)$

Def: any mode which $\omega = \alpha k$ for $k \to 0$
is called acoustic

and if we assume $\sin\frac{ka}{2} \sim \frac{ka}{2}$ and $\sqrt{1+x} \cong 1+x/2$

we get $\omega_- = \sqrt{\dfrac{k_1+k_2}{m} - \dfrac{1}{m}\sqrt{(k_1+k_2)^2 - \dfrac{4k_1k_2}{4}(ka)^2}} \Rightarrow$

$$V_{sound} = \frac{d\omega_-}{dk} = \sqrt{\frac{a^2 \, k_1 k_2}{2m \, (k_1 - k_2)}}$$

The high energy branch is more
interesting:

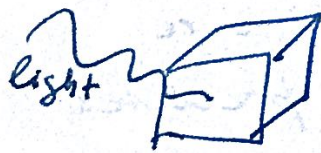for $k=0$ $\qquad \omega_+ = \sqrt{\dfrac{2(k_1+k_2)}{m}}$

and

$$V_{group} = \frac{d\omega}{dk} = 0 \bigg|_{at\ k=0} !$$

This branch is called OPTICAL.
Here is why.

during the light absorption
energy and momentum must
be conserved, i.e.

$\omega = ck$ so ω is very large

but phonons have $k \sim \frac{\pi}{a}$ as maximum
and cannot absorb the photon with
anything rather than this small value.
But for ω^+ even for $k \to 0$ ω^+ is finite
and can match $\omega = ck$.
So whenever light + phonons interact
we involve OPTICAL PHONONS.

L15

Lets look a little more carefully
at the opt. and. acoustic mode for $k \to 0$

$$m\omega^2 \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} k_1 + k_2 & -k_2 - k_1 \\ -k_2 - k_1 & k_1 + k_2 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix}$$
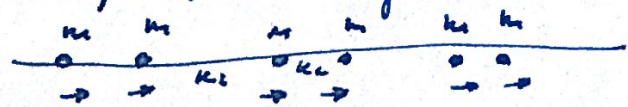
or

$$\omega^2 \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix} \cdot \frac{k_1 + k_2}{m}$$

For the acoustic mode $\omega = 0$ at $k = 0$

$$\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix} = 0 \quad \Rightarrow \quad \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

masses at position x and y move
together

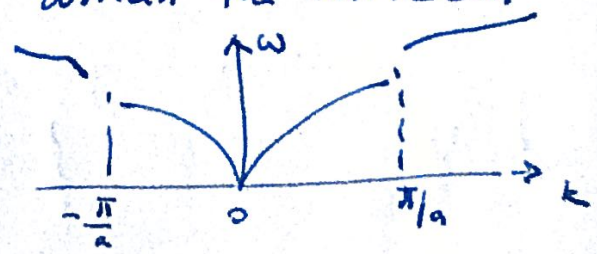In Short the atoms within the unit cell
always move together

For optical branch $k = 0$ $\quad \omega_+^2 (k=0) = \frac{2(k_1 + k_2)}{m}$

$$\frac{2(k_1 + k_2)}{m} \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix} \frac{k_1 + k_2}{m} \Rightarrow$$

$$\begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

describes two masses
moving in _opposite_
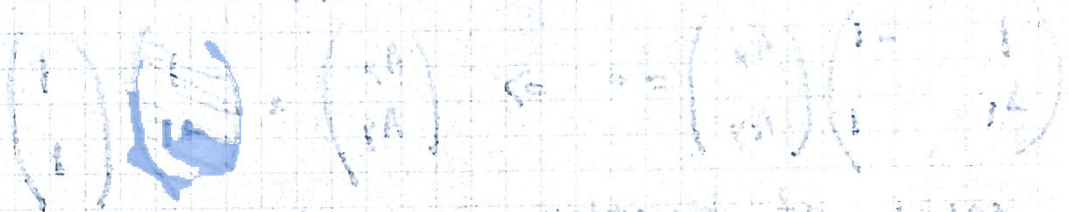_direction_
within the unitcell.

L15

Now lets study our nodes close to the
zone boundary. $\pm @ \frac{\pi}{a}$

$$\omega_+ = \sqrt{\frac{2\varepsilon_2}{m}}$$
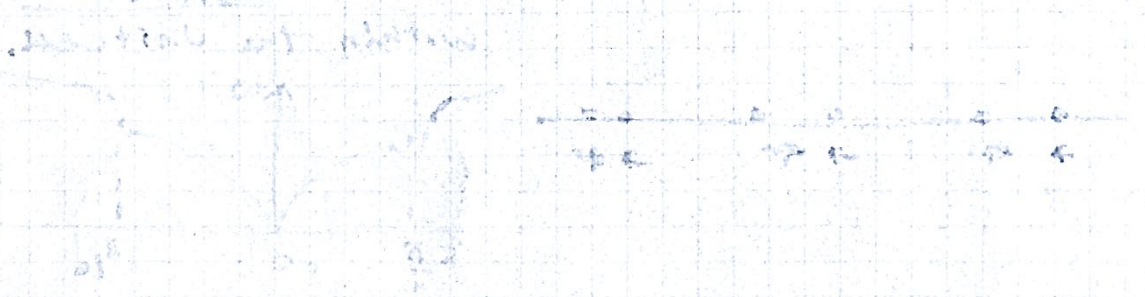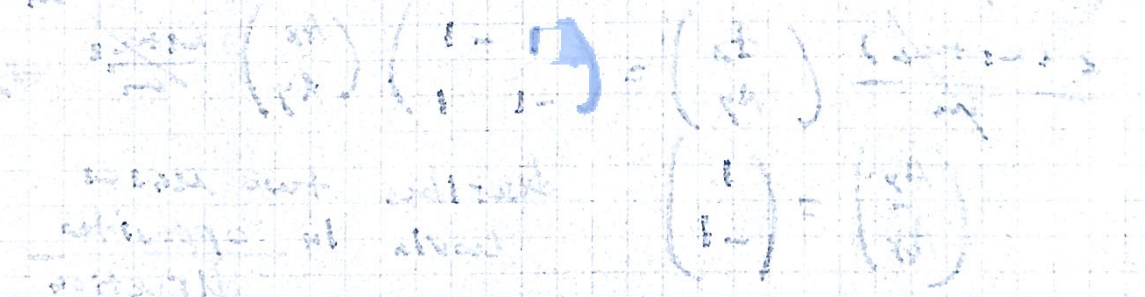
$$\omega_- = \sqrt{\frac{2\varepsilon_1}{m}} \; ; \quad \frac{d\omega}{dk} = 0 \text{ at the Z.B.}$$

when the phonon k approaches
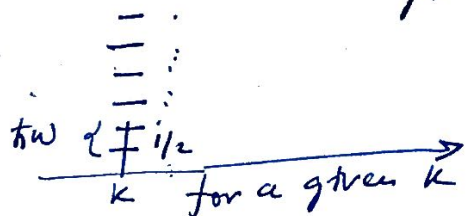the z.b. the plane wave turns into
a standing wave, with antiphase motion

L 15

For $h = 0$ we get $\hbar w(k)/2$

The lowest energy of excitation for $\hbar w(k) \Rightarrow n = 1$

$$\hbar w \left\{ \mp \tfrac{i}{2} \right.$$

k for a given k

Phonon is a descrete quantum of vibration
(photon is a quantum of light)

All known excitations are bosons
except for exotics like spinons, Majonas
etc.

Temperature shakes atoms and the phonons
can occupy higher and higher energy states.

Based on the Bose statistics:

$$n_\beta \left(\beta \hbar w \right) = \frac{1}{e^{\beta \hbar w} - 1} \qquad \beta = \frac{1}{k_B T}$$

Thus the energy expectation :

$$E_k \doteq \hbar w(k) \left(n_\beta + \tfrac{1}{2} \right) \text{ for finite } T_s$$

From this we can calculate
many thermodynamical quantities, including
say the heat capacity :

$$U_{total} = \sum_k \hbar w(k) \left(n_\beta + \tfrac{1}{2} \right)$$

↳ sum over all normal modes

$$k = \frac{2\pi}{Na} \cdot m \qquad \text{for } -\frac{\pi}{a} \le k \le \frac{\pi}{a}$$

As we did for electrons:

$$\sum_k \rightarrow \frac{Na}{2\pi} \int_{-\pi/a}^{\pi/a} dk$$

Note the Total number of modes is
$$\frac{Na}{2\pi} \int_{-\pi/a}^{\pi/a} dk = N$$

LIST

Now let's calcute the total internal energy
due to phonons

$$U_{total} = \frac{N_a}{2\pi} \int_{-\pi/a}^{\pi/a} dk \, \hbar \omega(k) \left(n_B \left(\beta \hbar \omega(k) \right) + \frac{1}{2} \right)$$

$$\hookrightarrow \frac{dU}{dT} = C_V.$$

Recal the difference betwee Debye
and what we got is in wk
for Debye $\omega = v \cdot k$, but in our
case $\omega(k) \propto \sqrt{\frac{k}{m}} \sin\left(\frac{ka}{2}\right)$

In fact what Einsteid did he just
introduced the same idea stating how
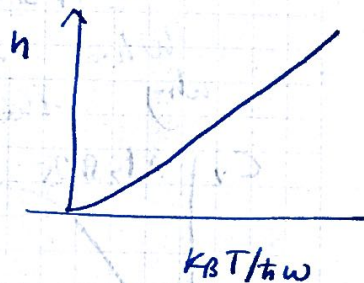ω depends on k.

THERMODYMICS OF PHONONS.

We state without a proof that bosons should obey to the Bose-Einshtein statistics: , i.e.

$$n = \frac{1}{e^{\epsilon/k_B T} - 1}$$ and if consider

the thermal vibrations of the frequency ω
(or $E = \hbar\omega$)

$$n(\omega, T) = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

for high temperatures
$k_B T > \hbar\omega$

$$\frac{1}{2} + n = \frac{1}{2} + \frac{1}{e^{\beta\epsilon} - 1} \underset{\underset{=\frac{1}{k_B T}}{\uparrow}}{=} \frac{e^{\beta\epsilon} + 1}{2(e^{\beta\epsilon} - 1)} =$$

$$= \frac{(1 + \beta\epsilon + \ldots) + 1}{2(1 + \beta\epsilon + (\beta\epsilon)^2/2 + \ldots)(-1)} = \frac{2 + \beta\epsilon + \ldots}{\beta\epsilon(2 + \beta\epsilon + \ldots)}$$

$$\approx \frac{1}{\beta\epsilon} = \frac{k_B T}{\hbar\omega} \implies \text{for high } T \text{ we have}$$

$$E = \hbar\omega\left(\frac{1}{2} + n(\omega, T)\right) = \hbar\omega\left(\frac{1}{2} + \frac{k_B T}{\hbar\omega}\right) =$$

$$= \underset{\underset{\text{"0" motion}}{\uparrow}}{\frac{\hbar\omega}{2}} + k_B T = k_B T \quad (\text{This is for 1D})$$

for 3D = 3 deg. of freedom

$$E = \sum \ldots = 3 k_B T \quad \text{which is equivalent to the internal energy of a gas.}$$

Heat capacity:
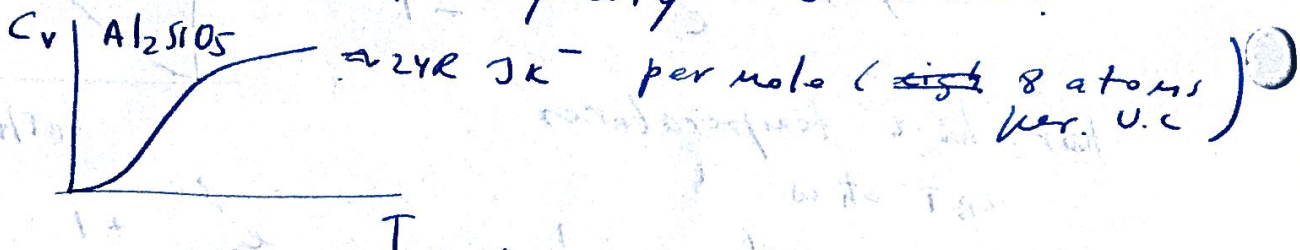
$$c_V = \left(\frac{\partial E}{\partial T}\right)_V = \sum \hbar\omega \frac{\partial n}{\partial T} =$$

$$= \sum k_B \left(\frac{\hbar\omega}{k_B T}\right)^2 \frac{e^{\hbar\omega/k_B T}}{\left(e^{\hbar\omega/k_B T} - 1\right)^2}$$

For the high T lim $c_V = 3R$ ($J K^{-1}$)

$\equiv$ Dulong - Petit.

What classical stat. physics cannot explain
why the heat capacity $\to 0$ $T \to 0$?

$c_V \mid Al_2SiO_5$ $\approx 24R$ JK^- per mole ($\xcancel{eigh}$ 8 atoms per. u.c)

Density of states for phonons

$g(\omega)$ the number of vibration mode
between ω and $\omega + d\omega$ $\Rightarrow$ $g(\omega) d\omega$

$$U = \int \left(n(\omega) + \frac{1}{2}\right) \hbar\omega\, g(\omega)\, d\omega$$

$$c_V = \int \frac{dn}{dT} \hbar\omega\, g(\omega)\, d\omega$$

Now lets apply the idea of DOS to
acoustic phonons:

~~lets~~ To determine $g(\omega)$ we note

$g(\omega)\, d\omega = g(k)\, dk$ sing $\cancel{\not{}}$ $\omega = v_{ac} . k$

In the xtal with N unit cells, the volume per u.c.
$\frac{V}{N}$ and the volume of B.Z. $= \frac{2\pi^3 N}{V}$

So in the 1st BZ there will be N available
values of the k-vector, and ~~volume for~~
the number of k -values per unit volume
$N / V_{BZ} = V/(2\pi)^3$ $\therefore$ the Reciprocal $\frac{\cancel{2\pi^3 N}}{\cancel{V}} / N$ space

or in Sperical coordinates:

$$g(\omega)\, d\omega = \frac{V}{(2\pi)^3} \cdot 4\pi k^2 \, dk \qquad k = \omega/\bar{v}_a \quad dk = \frac{d\omega}{v_a} =$$

$$\Rightarrow g(\omega)\, d\omega = 3 \times \frac{V}{(2\pi)^3} \cdot 4\pi \left(\frac{\omega}{v_a}\right)^2 \frac{d\omega}{v_a} = \frac{3V\omega^2}{2\pi^2 v_a^3} \cdot d\omega$$

3 comes from the fact that there are 3 branches of acoustic waves for 3D.

so $f(\omega) \sim \omega^2$

HEAT CAPACITY

The total energy due to phonons:

$$E = \int_0^{\omega_D} \frac{3V\omega^2}{2\pi^2 v_a} \cdot \underbrace{\frac{1}{e^{\hbar\omega/k_B T} - 1}}_{= n(\omega, T)} \, d\omega$$

where ω_D is called the Debye frequency, a cut-off parameter.

$$\Rightarrow \frac{dE}{dt} = C_V = \int_0^{\omega_D} \frac{3V\omega^2}{2\pi^2 v_a} \cdot \hbar\omega \frac{dn}{dT} \, d\omega$$

1) Low T limit: At low T only low ω phonons exists since $n(\omega, T) \to 0 \; T \to 0$ also those $\omega \ll \omega_D$ so ω_D looks like ∞.

Substituding $x \equiv \hbar\omega/k_B T$ $\omega^3 d\omega = \left(\frac{k_B T}{\hbar}\right)^4 x^3 dx$

$$E = \frac{3V\hbar}{2\pi^2 v_a} \left(\frac{k_B T}{\hbar}\right)^4 \int_0^{\infty} x^3 (e^x - 1)^{-1} dx \Rightarrow$$

$$= \pi^4/15$$

$$E = \frac{V\pi^2 (k_B T)^4}{10 (v_a \hbar)^3} \Rightarrow E \sim T^4 \Rightarrow C_V = \frac{dE}{dT} \sim T^3$$

or $C_V = \frac{2V\pi^2 k_B}{5(v_a \hbar/k_B)^3} \cdot T^3$ if we introduce the Debye temperature

$$\theta_D = \frac{\hbar\omega_D}{k_B} \Rightarrow \theta_D = \frac{\hbar v_a}{k_B} \left(\frac{16\pi N^2}{V}\right)^{1/2} \text{(not shown here} \atop \text{read A\&M)}$$