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E-NOTES

SUBJECT: CONDENSED MATTER PHYSICS

SUBJECT CODE: DPH31

UNIT : 2

SYLLABUS:

Monoatomic lattices - Lattice with two atoms per primitive cell - First Brillouin zone - Group and phase velocities - Quantization of lattice vibrations - Phonon momentum - Inelastic scattering by phonons - Einstein‘s model and Debye‘s model of specific heat.

UNIT - II.

(8) GROUP VELOCITY AND PHASE VELOCITY

Waves can be in a group and
grp → waves = W.P
Such groups are called Wave packet.
so the velocity with which a wave
wp → velocity = G.V
packet travels is called group Velocity

The Velocity with which the phase of a wave Travels is called phase velocity velocity → phase = p.v

If we consider that k is much less then π/a (or) $k \ll \pi/a$

λ is much greater then $2a$. $2a < \lambda$

Then, $k \ll \pi/a \quad \lambda \gg 2a$

ω is approximately linear within k because

$\sin \frac{1}{2}ka = \frac{1}{2}ka$

$\omega = 2\pi f$

ω - angular velocity

$$\omega = \sqrt{\left(\frac{B}{m}\right)} ka$$

$k \quad \frac{2\pi}{\lambda}$

Where α is angular wavenumber

$k = 2\pi/\lambda$

Phase velocity $V_P = \frac{\omega}{k} = \sqrt{\frac{B}{m}} a =$

α constant

group Velocity $v_g = \frac{d\omega}{dk} = \sqrt{\left(\frac{\beta}{m}\right)} a = \text{const.}$

$\boxed{\omega = k v_p}$

Thus for long wavelength, the medium behaves as continuous and homogeneous elastic medium.

The phase velocity is now equal to the group of velocity.

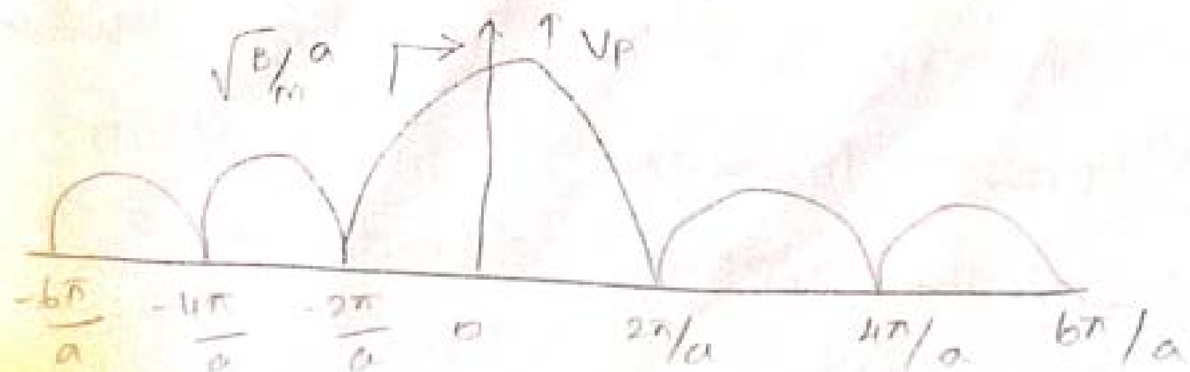
When k increases, the ω is not a linear fn of k and disperssion effects are more important

The group velocity and phase velocity are given by

$$v_p = \frac{\omega}{k} = \sqrt{\left(\frac{\beta}{m}\right)} a \left| \frac{\sin \frac{ka}{2}}{ka/2} \right|$$

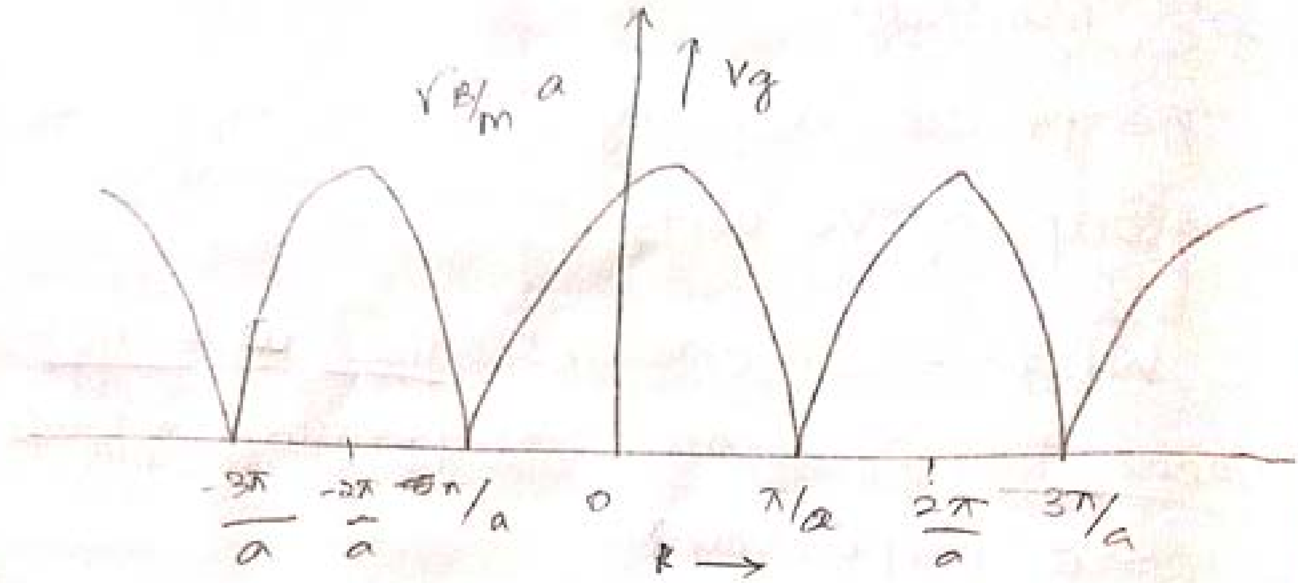
and

$$v_g = \frac{d\omega}{dk} = \sqrt{\left(\frac{\beta}{m}\right)} a \left| \cos \frac{ka}{2} \right|$$



The graph is drawn the plot V_p as a fn of k

The fig shows the phase velocity as a fn of propagation constant k



The graph is drawn the plot V_g, vs, k (ang wave number). This fig shows the group velocity as a function of propagation constant k. So in the frequency range both the velocities are function of frequency.

The result is lloly to light when it passes through a ~~fn~~ medium where the refractive index is a fn of frequency.

The phenomenon is known as dispersion & the medium behaves as a $\boxed{\text{dispersive}}$ medium so the medium is now dispersion one.

⑤ Phonon Momentum

A phonon does not have momentum but, for most practical purposes a phonon with wave vector $\vec{k}$ interacts with other particles and fields as if it had a momentum.

$\hbar\vec{k} \cdot \hbar\vec{k}$ is known as crystal momentum

The conservation law holds in case of wave vector and momentum in a crystal

The wave vector conservation law in case of Bragg diffraction of x-ray photon is given by

$$\vec{k}' = \vec{k} + \vec{G}$$

$\vec{k}' \Rightarrow$ wave vector of scattered photon

$\vec{k} \Rightarrow$ wave vector of incident photon.

$\vec{G} \Rightarrow$ vector in the reciprocal lattice.

If in the inelastic scattering of phonon a photon is created than the conservation law becomes.

$$\vec{K'} = \vec{K} + \vec{K} + \vec{G} \longrightarrow (2)$$

Wave vector form of phonon.

If instead of creation a phonon is absorbed in the process, we have conservation law as -

$$\vec{K'} = \vec{K} + \vec{K} + \vec{G} \longrightarrow (3).$$

(4) In elastic Scattering of phonons → vibration

In elastic Scattering of photons by long wavelengths phonons:

Let us consider the case of crystal which is regarded as a continuum of refractive index μ and if a photon of frequency $v = \frac{\omega}{2\pi} = \frac{c}{\lambda}$ is propagated in this crystal, the wave vector of photon is determined by the relation

$$\omega = \frac{ck}{\mu} \text{ (or) } \lambda v = \frac{c}{\lambda} \longrightarrow (1)$$

where

c is the velocity of light.

Let the photon interact with the phonon beam or sound wave in the crystal

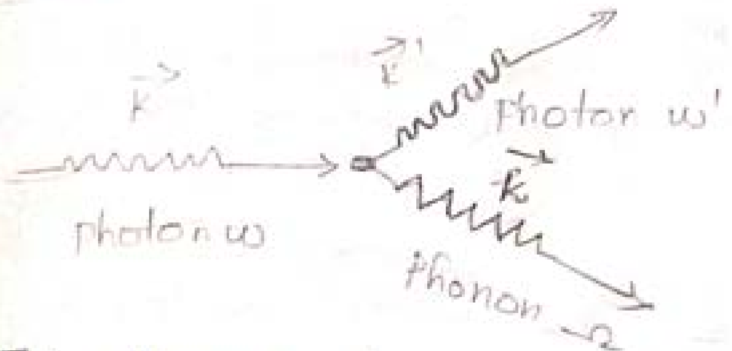
The photon will be scattered by the sound wave.
pressure

light scatter ih refractive index changes

This is due to the fact that the elastic strain field of sound wave changes the local conc. of atoms and thus the refractive index of the crystal is changed.

In other words the elastic field of light wave sets upto a periodic mechanical strain in the medium which changes the elastic properties of the medium.

In the inelastic scattering in a crystal a photon can either create or absorb a phonon.



The phonon is scattered in the process as shown in fig.

In the scattering, the wave vector $\vec{k}$ of the photon is changed to $\vec{k}'$ and the frequency is changed from ω to ω'.

Let the phonon be created being a wave vector $\vec{k}$ and angular frequency Ω. By the law of conservation of energy we have

$$\hbar\omega = \hbar\omega' + \hbar\Omega \longrightarrow (2)$$

$\downarrow$ Photon $\rightarrow$ photon o/p $\rightarrow$ phonon

By the conservation of wave vector

$$\hbar\vec{k} = \hbar\vec{k}' + \hbar\vec{K} \longrightarrow (3)$$

If the velocity of the sound is taken as constant, we have.

$V_s \vec{K}$

$$\Omega = V_s\vec{K} \longrightarrow (4)$$

$$\left(\text{because } \frac{\lambda\Omega}{2\pi} = V_s\right)$$

The phonon can carry off only a small fraction of the energy of incident photon.

Again $V_s \leq c$. The wave vector $\vec{K}$ of the phonon is comparable in magnitude to the photon wave vector $\vec{k}$ which shows that

$$c\vec{k} \simeq V_s\vec{K}.$$

We k. That 1/8

$\omega = c\vec{k}$

$\Omega = V_s\vec{k}$ —— (5)

as $c >> V_s$ so $\omega >> \Omega$

from eqn (2) & (3) it is observed

that $\omega = \omega'$

$\vec{k}' = \vec{k}$ —— (6).

The fig. shows the momentum balance diagram for this process.

Here ϕ is the scattering angle.

from the figure

$|\vec{K}|^2 = |\vec{k}|^2 + |\vec{k}'|^2 - 2|\vec{k}||\vec{k}'| \cos\phi$

$= k^2 + k^2 - 2k^2 \cos\phi$ $\quad k' = k$

$= 2k^2 - 2k^2 \cos\phi$

$= 2k^2 (1 - \cos\phi)$ $\quad 2\sin^2\phi/2$

$= 4k^2 \sin^2 \phi/2.$

$(\vec{K}) = 2|\vec{k}| \left(\frac{\sin\phi}{2}\right)$ —— (7).

Putting value of $k = \frac{\omega n}{c}$ we have x/y V_s

from eqn (5)

$V_s\vec{K} = \frac{2V_s\omega n}{c} \frac{\sin\phi}{2}$ $\quad \boxed{V_s\vec{K} = \Omega}$

$\Omega = \left(\frac{2V_s\omega n}{c}\right) \sin\phi/2$ —— (8).

expression ⑧ gives the frequency of phonon.

⑧

INELASTIC SCATTERING OF NEUTRONS BY PHONONS.

insert

Consider that a neutron impinges on a solid crystal and is scattered in-elasticitycally.

In this process, the neutron will lose or gain the energy and momentum.

Let loss or gain corresponds to creation or annihilation of one phonon. The conservative of wave vector is given by the relation.

$$\vec{K} = \vec{K}' + \vec{G} \pm \vec{k} \quad \text{——} \; ①$$

Here

$\vec{K}$ = Wave vector of incident neutron

$\vec{K}'$ = Scattered neutron.

$\vec{G}$ = Wave vector of reciprocal lattice

$\vec{k}$ = Wave vector of phonon +ve & -ve signs are used for the cases.

When a phonon is created (+) or gain

When a phonon is absorbed (-) ...

respectively

Mn - mass of the neutron than

K.E of the incident neutron $= \frac{p^2}{2Mn}$

p → Momentum of the Incident neutron

$= \hbar \vec{k}$.

K.E of The incident neutron

$$= \frac{\boxed{\hbar^2 k^2}}{2Mn} \rightarrow p^2$$

Let $\vec{K}'$ be the wave vector of scattered neutron, then.

K.E of the scattered neutron

$$= \frac{\hbar^2 k'^2}{2Mn}.$$

Applying the law of conservation of energy, we have

from eqn ① $\vec{G}$ is wave vector so does not exist

$$\frac{\hbar^2 k^2}{2Mn} = \frac{\hbar^2 k'^2}{2Mn} \pm \hbar\Omega \longrightarrow ②.$$

$\vec{K}$ $\vec{k}'$ $\vec{G}$ $\hbar\Omega$

$$E = E' \pm \hbar\Omega.$$

(+) Sign is used when phonon is created.

(-) Sign is used when phonon is absorbed $\hbar\Omega$ is the energy of phonon created.

In order to determine the dispersion relation using eqn ① & ②.

It is necessary to find the gain or loss of energy of scattered neutrons which will give $\hbar\Omega$ & hence Ω.

Secondly, we have to determine the corresponding scattering direction which will give $\vec{K} - \vec{K}'$.

knowing the value of G from $\vec{K} - \vec{K}' = \vec{G}$ for the elastically scattered neutrons.

One can obtain $\vec{K}$.

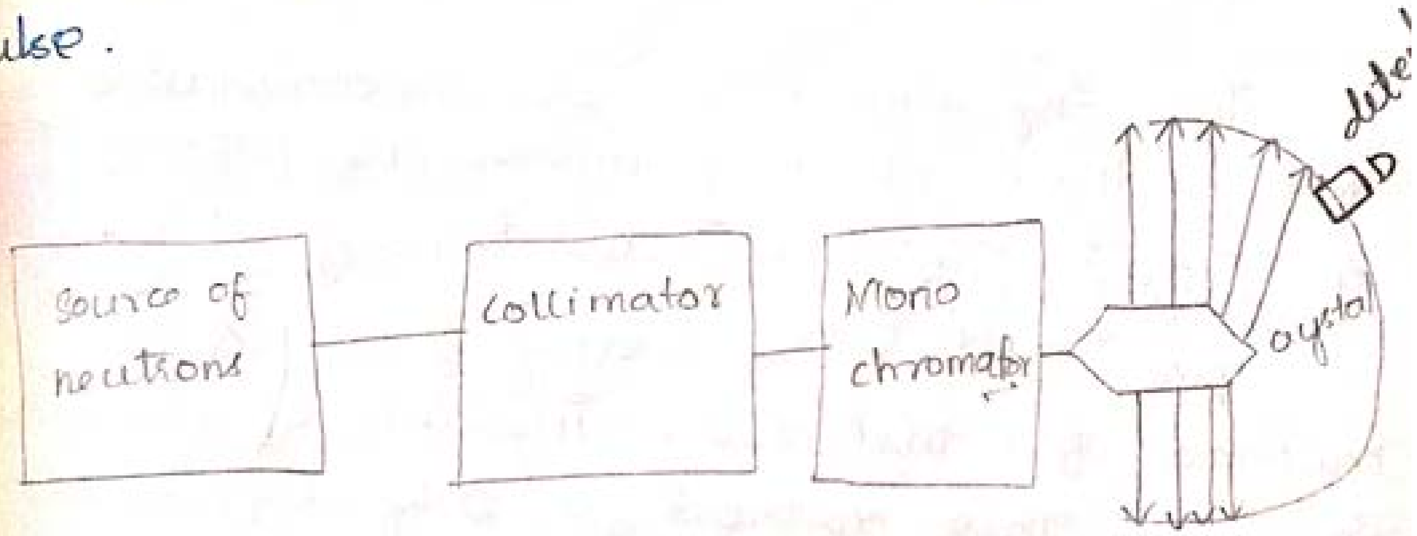
This vector is shown in fig.

We distinguish elastically scattered neutrons from inelastically scattered neutrons by the fact that they are more numerous and produce a peak in the intensity curve at Bragg angle.

A time of flight method is used for inelastic neutron scattering.

The experimental set up is shown in figure A. pulse of mono-energetic neutrons of proper energy $\vec{E}$ and wave neutron vector $\vec{K}$ is allowed to fall on the crystal.

The detector D measures the time of flight from the initiation of the pulse.

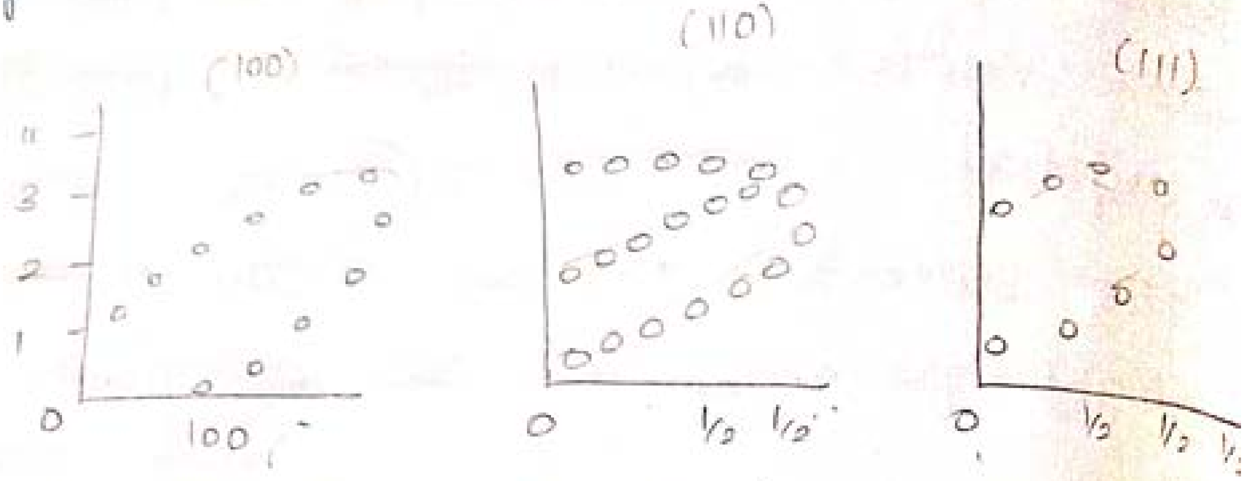


The time of flight gives the values of $\vec{E}'$ and the position of detector gives the direction of K'

Now $\hbar\Omega$ can be calculated, the neutron scattering occurs at many possible angles corresponding to different possible $\vec{K}$. vectors of the lattice vibrations ε_p hence the detectors is moved to another positions around the crystal

In this way different sets of $\vec{E}'$ & $\vec{k}'$ are obtained.

The accurate determination of phonon spectra for sodium is shown in fig.



The fig shows the dispersion waves for sodium when phonons are propagated in [100], [110], [111] directioning at 90°k

The neutron scattering is an ideal method for the determination of phonon spectra. This method is only applicable when the absorption of neutron by nuclei of the crystal is not high.

In some cases, considering the angular width of scattered neutron beam some important data about the phonon life time can be obtained.

③

EINSTEIN'S THEORY OF SPECIFIC HEAT.

Einstein, in 1907, applied quantum principles to the thermal vibrations of atoms in Solids

Einstein consideration as a solid of NA atom to behave as 3NA independent harmonic oscillators each of frequency ν.

The classical mechanics, a mode of oscillators can have any of a continuous range of energies, the only restriction being that the energy is half kinetic & half potential.

The meaning of quantisation is that only certain discrete value of energy are allowed.

In other words, quantum theory assume that atom are again identical independent harmonic oscillator all of which vibrate independently with the same natural frequency, but have discrete energy levels.

These values are given by planck's formula

$$E_n = nh\nu = n\hbar\omega \longrightarrow ①$$

If dN oscillator have energies lying b/w E and $E+dE$, then the mean energy of atomic oscillator is given by

$$\vec{E} = \frac{\sum E\,dN}{\sum dN} \longrightarrow (2)$$

$\frac{\sum E\,d_N}{\sum d_N}$

$3N_A$

dN

from statistical mechanics.

One know that the no. of atomic oscillation dN_a having energies lying b/w E and $(E+dE)$ at a temp T_1 is proportion to $\exp(-E/k_BT) = dN$.

Thus,

$$\vec{E} = \frac{\sum_{n=0}^{\infty} nh\nu \exp[-nh\nu/k_BT]}{\sum \exp[-nh\nu/k_BT]}$$

$$\vec{E} = \frac{h\nu[e^{-h\nu/k_BT} + 2e^{-2h\nu/k_BT} + 3e^{-3h\nu/k_BT} + \ldots}{[1+e^{-h\nu/k_BT} + e^{-2h\nu/k_BT} + e^{-3h\nu/k_BT} \ldots}$$

$$x = \frac{-h\nu}{k_BT}$$

$$\vec{E} = \frac{h\nu[e^{x} + 2e^{2x} + 3e^{3x} + \ldots \infty]}{[1+e^{x} + e^{2x} + e^{3x} + \ldots \infty]}$$

$$\vec{E} = h\nu\left[\frac{d}{dx}\log(1+e^{x}+e^{2x}+e^{3x}+\ldots\right]$$

$\vec{E} = h\nu \left[\frac{d}{dx} \log \frac{1}{(1-e^x)}\right.$ $e^{-h\nu/k_BT}$

$= h\nu \left[\frac{d}{dx} \{\log 1 - \log(1-e^x)\}\right.$

$= -h\nu(-e^x)/(1-e^x)$ $-h\nu\left[\frac{-e^x}{1-e^x}\right]$

$= h\nu\left[\frac{e^x}{1-e^x}\right] = \frac{h\nu}{e^{-x}(1-e^x)}$ $e^{-x} - e^{-x}.e^{x}$

$$= \frac{h\nu}{e^{-x}-1}$$

$$\vec{E} = \frac{h\nu}{e^{h\nu/K_BT}-1} \quad \text{——— (3)}$$

The total internal energy of a k mol of a solid therefore becomes.

$\frac{1}{\theta} = \theta$

Ru

$$U = 3N_A \vec{E}.$$

$$U = \frac{3N_A h\nu}{e^{h\nu/K_BT}-1}$$ and ∴ Molar

Specific heat.

$K_B\theta_E$

$$C_V = \left(\frac{du}{dT}\right) = \frac{-3N_A h\nu \exp[h\nu/K_BT][-h\nu/K_BT]^2}{[\exp(h\nu/K_BT-1]^2}.$$

Let $h\nu = K_B\theta_E$ is known as einstein temperature.

Ru θ_E $\left(\frac{h\nu}{K_B}\right)$

Thus.

$$C_V = \frac{(3N_A K_B)\exp[h\nu/K_BT][h\nu/K_BT]^2}{[\exp[h\nu/K_BT)-1]^2}$$

$3N_A\vec{E}$

$$\frac{C_V}{3R_u} = \left[\frac{h\nu}{K_B T}\right]^2 \left\{\frac{\exp(h\nu/K_B T)}{\exp(h\nu/K_B T - 1)^2}\right.$$

$$= \left[\frac{\theta_E}{T}\right]^2 \frac{\exp \theta_E/T}{\exp(\theta_E/T - 1)^2} \longrightarrow 4$$

$$= F_E\left(\frac{\theta_E}{T}\right) \longrightarrow 49.$$

$\boxed{\text{P(E) is called einstein function}}$.

case (i)

At high temperature $h\nu << K_B T$

Now eqn 3 is written as

$$\vec{E} = \frac{h\nu}{(e^x - 1)} \quad \text{with } x = \frac{h\nu}{K_B T}$$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \simeq 1 + x$$

Hence at ↑ tem.

$$\vec{E} = \frac{h\nu}{(1+x-1)} = \frac{h\nu}{x}.$$

$$\vec{E} = \frac{h\nu}{h\nu/K_B T} = \boxed{K_B T} \qquad x = \frac{h\nu}{K_B T}$$

$$U = 3N_a \vec{E} = 3\overset{R_u}{N_A K_B} T$$

$$= 3R_u T$$

$$C_V = \frac{dU}{} = 3R_u.$$

In for large value. T the expression reduces to classical expression.

case (ii)

At low temperature $h\nu >> K_BT$ at hence $\exp(h\nu / K_BT) >> 1$

$$\bar{E} = \frac{h\nu}{\exp(h\nu/K_BT)}$$

Thus at low ↓ term the total energy of k mol of a solid is given by

$$U = 3N_A h\nu \exp(-h\nu/K_BT).$$

$$C_V = \left(\frac{dU}{dT}\right) = (3N_A h\nu)\left[\exp\left(\frac{-h\nu}{K_BT}\right)\right]\left[\frac{h\nu}{K_BT^2}\right]$$

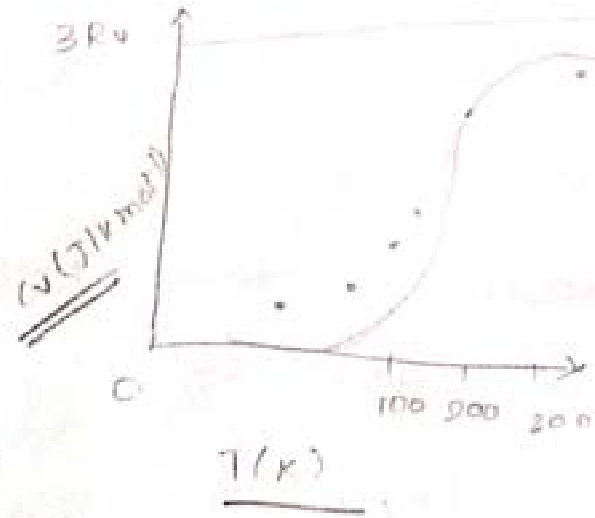
$$= 3N_A \left[\frac{h\nu}{K_BT}\right]^2 K_B \exp\left[-\frac{h\nu}{K_BT}\right]$$

$$C_V = 3R_V\left[\frac{h\nu}{K_BT}\right]^2 \exp\left[-\frac{h\nu}{K_BT}\right] \quad \text{—(5)}$$

equ (5) indicate at ↓ term, the exponential term is more important then the $\left[\frac{h\nu}{K_BT}\right]^2$ term in determining the term vecition of C_V

Thus with decreasing terms, C_V drops exponentially eqn (5) is plotted in fig for aluminium with $\nu = 6.4 \times 10^{12}$ Hz.

There is evidentally good agreement with data at very low temperature where C_V is more nearly proportional to T^3 then to eqn (B)



Debye's model of lattice specific heat

In 1912 Debye pointed out that the einstein's assumption that the atoms of the crystals vibrate independetly at the same frequency is not justifiable and suggested that the oscillations are coupled together and are capable of producing a spectrum of frequencies

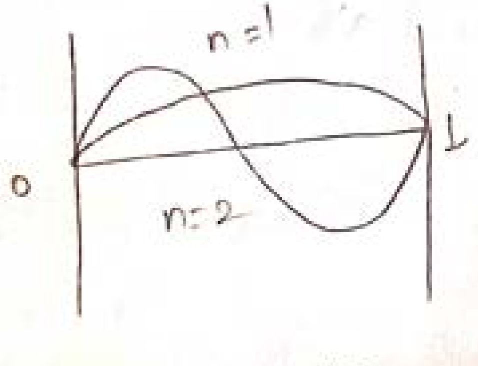
Debye considered the vibrational modes of a crystal as a whole, whereas einstein considered the vibration of single atom with the assumption that atomic vibrations are independent of each other.

As the atoms of the crystal no longer vibrate independently, it is convenient to work with the vibrational are mode of a system rather than vibrational modes of a single atom.

Vibrational modes of a continuous medium

In order to consider the vibrational modes of a continuous medium.

Let us first consider the simple case of 1-D continuous string of length L fixed at two ends as shown in fig.



In this case, stationary waves are set up with specific wavelength such that $n\left(\frac{\lambda}{2}\right)=L$.

It should be remembered that if only one end is fixed, then any

Wavelength can propagate.

Let $u(x,t)$ represent the displacement of the string at a distance x at any instant t.

The wave eqn is given by

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{C_s^2}\frac{\partial^2 u}{\partial t^2} \quad \text{——— } ①$$

where C_s is the Velocity of propagation.

The soln of eqn ① is given by

$$u(x,t) = A \sin\left(\frac{n\pi x}{L}\right)\cos 2\pi \nu_n t, \quad \text{— } ②$$

where

n is the +ve integer ≥ 1.

The Wavelength and frequencies are given by

$$\lambda_n = \frac{2L}{n} \text{ and } \nu_n = \frac{C_s}{\lambda_n}$$

all V

$$= \frac{C_s}{\frac{2L}{n}}$$

$$\nu_n = \frac{C_s n}{2L} \quad \text{——— } ③$$

By cross multiplication 4th eqn appear

$$\nu_1 = \frac{C_s}{2L}$$

$$\nu_2 = \frac{2C_s}{2L} = \frac{C_s}{L}$$

$$\nu_3 = \frac{3C_s}{2L}$$

i.e frequency spectrum is discrete

The No. of possible modes of Vibration in frequency interval $d\nu$ is given by

$$dn = \left(\frac{2L}{c_s}\right) d\nu$$

because $n = \frac{2L}{c_s} \nu_n \longrightarrow (4)$

Expanding the above case for three dimensions, the wave eqn is.

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = \frac{1}{c_s^2} \frac{\partial^2 u}{\partial t^2} \quad \text{——} (5)$$

The soln of eqn is (5) is

$$u(x,y,z) = A \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right) \cos 2\pi\nu t \quad \text{——} (6)$$

where n_x, n_y, n_z are +ve integer ≥ 1

Sub eqn (6) into eqn (5) we have

$$\left(\frac{\pi^2}{L^2}\right)(n_x^2 + n_y^2 + n_z^2) = \frac{4\pi^2 \nu^2}{c_s^2}$$

$$n_x^2 + n_y^2 + n_z^2 = R^2 = \frac{4L^2\nu^2}{c_s^2} \longrightarrow (7)$$

So, in three dimensional case. the wavelength and frequencies are determined by three integers

n_x, n_y, n_z.

from eqn ⑦ we can say that in three dimensional case the wavelengths and frequencies are determined by three integers n_x, n_y and n_z. The case is similar to the electromagnetic waves in a box of Volume V.

The no. of possible modes of vibrations $Z(\nu)\,d\nu$ in frequency range ν and $\nu + d\nu$ can be calculated as follows:

The problem is now to find out the no. of points in the frequency range ν and $\nu + d\nu$

All the points will lie in the volume of the octant of the Sphere of radius R corresponding to frequency ν, and $(R+dR)$ corresponding to frequency $\nu + d\nu$ because the box lies in 1/8 th Volume of the Sphere, so constructed. Hence,

$$dN = \frac{1}{8}(4\pi R^2 dR) \longrightarrow ⑧$$

is as each point corresponds to a set of three integers n_x, n_y and n_z; each set of integers determines a possible mode of vibration

eqn⑧ immediately gives the no. of modes in this frequency range :

$$Z(\nu)\,d\nu = \frac{1}{8}\left[4\pi\left[\frac{4L^2\nu^2}{C_s^2}\right]\right]\underbrace{\left[\frac{2L\,d\nu}{C_s}\right]}_{dR}$$

$$\cancel{= \frac{4\pi V\nu^2 d\nu}{C_s^3}}$$

$$= \frac{1}{8}\left[4\pi\left[\frac{8L^3\nu^2 d\nu}{C_s^3}\right]\right] \quad \therefore L^3 = V$$

$$Z(\nu)\,d\nu = \frac{4\pi V\nu^2 d\nu}{C_s^3} \longrightarrow ⑨.$$

Where V is the volume of the solid

The possible frequencies vary btwn. 0 and ∞. Incase of elastic waves in a solid both transverse and longitudinal waves are possible but their Velocities are different

For each frequency there are two transverse mode corresponding to the deflection ⊥r to the direction of propagation and one longitudinal mode corresponding to the deflection along the direction of propagation.

Thus,

$$z(\nu)d\nu = 4\pi V \left[\frac{2}{C_t^3} + \frac{1}{C_l^3}\right]\nu^2 d\nu \quad \text{--- (10)}$$

$\downarrow$ Transverse Velocity $\quad \downarrow$ longitudinal.

Debye Approximation:

The crystals are made up of atoms is discrete "mass points".

Consider an elastic wave propagated in a crystal

As long as the wavelength of the wave is large compared with the interatomic distances the crystal can be regarded as a continum from the point of view of wave.

Hence according to Debye the continum model may be employed for all possible vibrational modes of crystal.

The total no. of vibrations in a crystal spectrum can be obtained by integrating $z(\nu)\,d\nu$ with in the power limits.

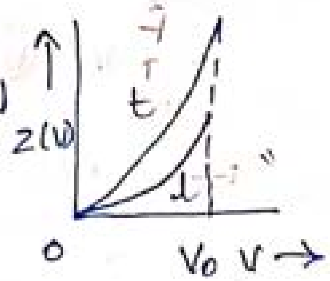
The lower limit of integration may be taken as $\nu=0$ because the density of states in the frequency spectrum increases very rapidly with increasing frequency.

In case of a crystal having N atoms the no. of vibrations cannot exceed 3N because each atom vibrates with the three degrees of freedom, hence upper limit ν_D must be defined in such a way as to satisfy the relation,

$$\int_0^{\nu_D} z(\nu)\, d\nu = 3N \longrightarrow (11)$$

Where ν_D is called the Debye cut off frequency. the situation is shown in figure

$$\therefore \int_0^{\nu_D} z(\nu) d\nu = \int_0^{\nu_D} 4\pi V \left(\frac{2}{C_t^3} + \frac{1}{C_l^3}\right) \nu^2 d\nu = 3N$$



$$\Rightarrow 4\pi V \left(\frac{2}{C_t^3} + \frac{1}{C_l^3}\right) \int_0^{\nu_D} \nu^2 d\nu = 3N.$$

$$\Rightarrow 4\pi V \left(\frac{2}{C_t^3} + \frac{1}{C_l^3}\right) \frac{\nu_D^3}{3} = 3N$$

$$\Rightarrow 4\pi V \left(\frac{2}{C_t^3} + \frac{1}{C_l^3}\right) \nu_D^3 = 9N.$$

$$\nu_D^3 = \frac{9N}{4\pi V}\left[\frac{2}{C_t^3} + \frac{1}{C_l^3}\right]^{-1} \longrightarrow (12).$$

Taking $\left(\frac{N}{V}\right) = 10^{28}$ per m^3 and velocity of sound as 1000 m/s we have,

$$\nu_D^3 = \frac{9 \times 10^{28}}{4 \times 3.14}\left[\frac{2}{(1000)^3} + \frac{1}{(1000)^3}\right]^{-1}$$

$$\nu_D^3 = \frac{9 \times 10^{28}}{4 \times 3.14}\left[\frac{3}{(1000)^3}\right]^{-1}$$

or

$$\boxed{\nu_D = 10^{13}\ Hz.}$$

The corresponding minimum wavelength is given by. $v : \nu_D \lambda m.$

$$v = \nu_D \lambda m.$$

$$\lambda m = v/\nu_D$$

$$= (1000) \times 10^{-13}$$

$$\lambda m = 0.1\ nm.$$

0.9×10^{-9}

This shows that wavelength are greater than inter- atomic distances. So, the continum theory may not work especially in high frequency region.

The internal energy E can be calculated by the formula,

$$E = \int_0^{\nu_D} \vec{E}\, z(\nu)\cdot d\nu$$

$$= \int_0^{\nu_D} z(\nu)\cdot d\nu \times \frac{h\nu}{\left(\exp\left(\frac{h\nu}{K_B T}\right)-1\right)} \quad \text{——} (13)$$

Where, $\frac{h\nu}{\exp\left(\frac{h\nu}{K_B T}\right)-1}$ is the average energy $(\vec{E})$ of an oscillator having frequency ν.

$$E = \int_0^{\nu_D} 4\pi V \left(\frac{2}{C_t^3} + \frac{1}{C_l^3}\right) \nu^2 d\nu \times \frac{h\nu}{\exp\left(\frac{h\nu}{K_B T}\right)-1}$$

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = \int_0^{\nu_D} 4\pi V \left(\frac{2}{C_t^3} + \frac{1}{C_l^3}\right) \nu^2 d\nu \left[\frac{h\nu(-1)\exp\left(\frac{h\nu}{K_B T}\right)\left(\frac{-h\nu}{K_B T^2}\right)}{\left[\exp\left(\frac{h\nu}{K_B T}\right)-1\right]^2}\right]$$

$$C_V = \int_0^{\nu_D} 4\pi V \left(\frac{2}{C_t^3} + \frac{1}{C_l^3}\right) \nu^2 d\nu \; \frac{\exp\left(\frac{h\nu}{K_B T}\right)\left(\frac{h^2\nu^2}{K_B T^2}\right)}{\left[\exp\left(\frac{h\nu}{K_B T}\right)-1\right]^2}$$

$$= K_B \int_0^{\nu_D} 4\pi V \left(\frac{2}{C_t^3} + \frac{1}{C_l^3}\right) \nu^2 d\nu \times \frac{\exp\left(\frac{h\nu}{K_B T}\right)}{\left[\exp\left[\frac{h\nu}{K_B T}-1\right)\right]^2} \times \left(\frac{h\nu}{K_B T}\right)^2$$

Putting

$\left(\frac{h\nu}{K_B T}\right) = x$ $\left(\frac{h\nu_D}{K_B T}\right) = x_m$ and using above eqn (12) we get

$$= k_B \int_0^{\nu_D} 4\pi\nu \left(\frac{2}{c_t^3} + \frac{1}{c_l^3}\right) \nu^2 d\nu \times \frac{e^x}{(e^x-1)^2} \times x^2$$

$$C_V = 9Nk_B \frac{1}{x_m^3} \int_0^{x_m} \frac{x^4 e^x . dx}{(e^x-1)^2} \longrightarrow (14)$$

Let us define θ_D as the debye temp. given by the relation

$$\theta_D = \frac{h\nu_m}{k_B} \longrightarrow (15)$$

In terms of θ_D, the expression for C_V becomes.

$$C_V = 9Nk_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{e^x x^4 . dx}{(e^x-1)^2} \longrightarrow (16)$$

$$= 3R F_D \frac{\theta_D}{T} \longrightarrow (17)$$

$$F_D = 3\left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{e^x x^4 . dx}{(e^x-1)^2}$$

$\therefore \frac{1}{x_m} = \frac{T}{\theta_D}$

$x_m = \frac{\theta_D}{T}$

$Nk_B = R$

and is known as debye fn.

eqn (16) is known as debye formula for heat capacities of solid.

Debye's result for Silver at $\theta_D = 225k$ is shown in figure. It is observed from the graph that heat capacity approaches classical value at high temp & zero value at low temp.

At high temp.

for high Temp $T >> \theta_D$ and x is small as compared with unity from eqn (13)

$$E = \int_0^{\nu_D} Z(\nu) \frac{h\nu \, d\nu}{\exp\left[\frac{h\nu}{k_B T} - 1\right]} = 9N \left[\frac{k_B T}{h\nu_D}\right]^3 kT \int_0^{x_m} \frac{x^3 \, dx}{e^x - 1} \quad \text{--- (18)}$$

where $x = \frac{h\nu}{k_B T}$; $x_m = \frac{h\nu_D}{k_B T}$

at high temp $e^x - 1 = x$

$$E = 9N \frac{1}{x_m^3} k_B T \int_0^{x_D} x^2 . dx = 3Nk_B T \quad \text{--- (19)}$$

$$C_v = \frac{\partial E}{\partial T} = 3Nk_B \quad \text{--- (20)}$$

The result is in accordance with classical results

At low temp:

$T << \theta_D$

Upper limit of integration will be infinity hence from eqn (16)

$$C_v = 9NK_B\left(\frac{T}{\theta_D}\right)^3 \int_0^\infty \frac{e^x x^4 . dx}{(e^x - 1)^2}$$

$$= \cancel{9}^{3} NK_B\left[\frac{T}{\theta_D}\right]^3 . \frac{4}{\cancel{15}_5}\pi^4 .$$

$$C_v = \frac{12}{5}\pi^4 NK_B\left(\frac{T}{\theta_D}\right)^3 \text{———} (21)$$

This is well known debye T^3 low and is in good agreement with the experiment data for many substances.

An important result can be seen with the help of debye formula at low temp

$$E = 9NK_BT\left[\frac{K_BT}{hV_D}\right]^3 \int_0^{x_m} \frac{x^3 dx}{e^x - 1}$$

$$E \propto T^4 \longrightarrow (22)$$

This result is analogues to stefen's law for density of blackbody radiation. This we can say that phonons & photons obey the same statistic with the difference that phonons obey T^4 law only at low temp while photon only by T^4 low at all temp. althrough.

Debye Approximation met a great success but accuato measurement show deviation from theoretical prediction in low term region.

According to dbye the T^3 law term region. According to debye should hold in the temp region $T \leq 0$. $1\theta D$ but bla paper should that is not always true but T^3 law hold for tem region $T \leq \theta D/50$, at consideraly low tem then predicted by debye.

Quantization of lattice Vibrations :-

The energy of a lattice vibration is quantized

The quantum of energy is called a phonon in analogy with the photon of the electromagnetic wave.

Elastic waves in crystals are made up of phonons.

Thermal vibrations in crystals are thermally excited phonons, like the thermally excited photons of black body electromagnetic radiation in a cavity

The energy of an elastic mode of angular frequency ω is

$$E = \left(n + \tfrac{1}{2}\right)\hbar\omega \longrightarrow ①$$

When the mode is excited to quantum ~~numbr~~ number n; that is when the mode is occupied by n phonons.

The term $\frac{1}{2}\hbar\omega$ is the zero point energy of the mode.

It occurs for both phonons and photons as a consequence of their equivalence to a quantum harmonic oscillator of frequency ω, for which the energy eigen values are also $(n+1/2)\hbar\omega$

Consider the standing wave mode of amplitude

$$u = u_0 \cos kx \cos\omega t$$

$u \rightarrow$ displacement of a volume element from its equilibrium position at x in the crystal.

The energy in the mode as in any harmonic oscillator, is half K.E and half potential energy, when averaged over time.

The kinetic energy density is

$$\frac{1}{2}\rho\,(\partial u/\partial t)^2$$

Where ρ is the mass density.

In a crystal of volume V, the volume integral of the kinetic energy is

$$\frac{1}{4}\rho V \omega^2 u_0^2 \sin^2\omega t$$

The time average kinetic energy is

$$\frac{1}{8}\rho V \omega^2 u_0^2 = \frac{1}{2}(n+1/2)\hbar\omega$$

and square of the amplitude is

$$u_0^2 = 4(n+1/2)\hbar / \rho V\omega.$$

This relates the displacement in a given mode to the phonon occupancy n of the mode.

The eqn of motion such as ω^2 and if this is +ve then ω can have either + or −

But the energy of a phonon must be +ve. so it is conventional and suitable to view ω as +ve. (phonon +ve → ω +ve)

If the crystal structure is unstable or becomes unstable through an unusual temperature dependence of the force constants

then ω^2 will be −ve

$\omega \rightarrow$ imaginary

A mode with ω imaginary will be unstable, at least if the real part of ω is −ve.

The crystal will transform spontaneously to a more stable structure, An optical mode with ω close to zero is called

Soft mode, and these are often involved in phase transitions, as in ferroelectric crystals.

cell:

$$F_{2n+1} = \frac{m_1 d^2 x_{2n+1}}{dt^2} = \beta\left[x_{2n+2} + x_{2n} - 2x_{2n+1}\right] \quad \text{— ①}$$

$$F_{2n} = \frac{m_2 d^2 x_{2n}}{dt^2} = \beta\left[x_{2n+1} + x_{2n-1} - 2x_{2n}\right] \quad \text{— ②}$$

soln of the eqn.

$$x_{2n} = \eta \exp[i(\omega t - 2kna)] \longrightarrow ③$$

$$x_{2n+1} = \xi \exp[i\{(\omega t - (2n+1)ka\}] \text{ — ④}$$

differentiating eqn ③ and ④ w.r to 't'

$$\frac{d^2 x_{2n}}{dt^2} = -\omega^2 \eta \exp[i\omega t - 2kna] \longrightarrow ⑤$$

$$\frac{d^2 x_{2n+1}}{dt^2} = -\omega^2 \xi \exp[i\{[\omega t - 2n+1)ka\}] \text{ — ⑥}$$

Again from eqn ③ and ④

$$x_{2n+2} = \eta \exp[i\{(\omega t - (2n+2)ka\}]$$
$$= \eta \exp[i(\omega t - 2nka - 2ka)]$$
$$x_{2n+2} = x_{2n}\, e[-2ika] \text{ — ⑦}$$
$$x_{2n-1} = \xi \exp[i\{\omega t - (2n-1)ka\}]$$
$$= x_{2n+1} \exp[2ika] \text{ — ⑧}$$

Sub these values in eqn ① we get

$$F_{2n+1} = \frac{m_1 d^2 x_{2n+1}}{dt^2} = \beta\left[x_{2n+2} + x_{2n} - 2x_{2n+1}\right]$$

$$m_1[-\omega^2 \xi \exp[i(\omega t - (2n+1)ka)]$$

$$= \beta[[\eta \exp[i\omega t - 2kna)] \exp[-2ika] +$$

$$\eta \exp[i\omega t - 2kna)] - 2\xi \exp[i\{\omega t - (2n+1)ka\}$$

(5) Lattice with two atoms per primitive cell:

$$F_{2n+1} = \frac{m_1 d^2 x_{2n+1}}{dt^2} = \beta\left[x_{2n+2} + x_{2n} - 2x_{2n+1}\right] \rightarrow (1)$$

$$F_{2n} = \frac{m_2 d^2 x_{2n}}{dt^2} = \beta\left[x_{2n+1} + x_{2n-1} - 2x_{2n}\right] \rightarrow (2)$$

soln of the eqn.

$$x_{2n} = \eta \exp[i(\omega t - 2kna)] \longrightarrow (3)$$

$$x_{2n+1} = \xi \exp[i\{(\omega t - (2n+1)ka\}] \longrightarrow (4)$$

differentiating eqn (3) and (4) w.r to 't'

$$\frac{d^2 x_{2n}}{dt^2} = -\omega^2 \eta \exp[i\omega t - 2kna] \longrightarrow (5)$$

$$\frac{d^2 x_{2n+1}}{dt^2} = -\omega^2 \xi \exp[i\{(\omega t - 2n+1)ka\}] \longrightarrow (6)$$

Again from eqn (3) and (4)

$$x_{2n+2} = \eta \exp[i\{(\omega t - (2n+2)ka\}]$$

$$= \eta \exp[i(\omega t - 2nka - 2ka)]$$

$$x_{2n+2} = x_{2n}\, e[-2ika] \longrightarrow (7)$$

$$x_{2n-1} = \xi \exp[i\{\omega t - (2n-1)ka\}]$$

$$= x_{2n+1} \exp[2ika] \longrightarrow (8)$$

Sub these values in eqn (1) we get

$$F_{2n+1} = \frac{m_1 d^2 x_{2n+1}}{dt^2} = \beta\left[x_{2n+2} + x_{2n} - 2x_{2n+1}\right]$$

$$m_1 \cdot -\omega^2 \xi \exp[i(\omega t - (2n+1)ka)]$$

$$= \beta\left[[\eta \exp[i\omega t - 2kna]] \exp[-2ika] + \right.$$

$$\eta \exp[i\omega t - 2kna] - 2\xi \exp[i\{\omega t - (2n+1)

$-m_1\omega^2\xi = \beta\eta\,[\exp(ika) + \exp(-ika) - 2\xi\beta$.

sub $\frac{\cos ka}{2}$

$(-m_1\omega^2 + 2\beta)\xi - 2\beta\eta\cos ka = 0$

$(2\beta - m_1\omega^2)\xi - 2\beta\eta\cos ka = 0 \longrightarrow (9)$

sub these values in eqn (2) we get.

$$F_{2n} = \frac{m_2\, d^2 x_{2n}}{dt^2}$$

$$= \beta\,[x_{2n+1} + x_{2n-1} - 2x_n]$$

$$F_{2n} = m_2 - \omega^2\eta\exp[(i\omega t - 2kna]$$

$$= \beta\,[\xi\exp[i\omega t - (2n+1)ka]] + \xi\exp$$

$$[i(\omega t - 2n+1)ka]\,e(-2ika).$$

$$e[-2ika] - 2\eta\exp(i(\omega t - 2kna)]$$

Next step back page

$$-m^2\omega^2\eta = \beta\,\xi\,[(\exp - ika)(\exp ika)] - 2\eta\beta$$

$$(2\beta - m_2\omega^2)\eta - 2\beta\xi\cos ka = 0 \quad (10)$$

eqn (9) & (10) Imaginary parts

$$\begin{vmatrix} 2\beta - m_1\omega^2 & -2\beta\cos ka \\ -2\beta\cos ka & 2\beta - m_2\omega^2 \end{vmatrix} = 0 \longrightarrow (11)$$

$(2\beta - m\omega^2)\,(2\beta - m_2\omega^2) - (-2\beta\cos ka) - (2\beta\cos ka)$

$(2\beta - m_1\omega^2) - (-2\beta\cos ka) - (2\beta\cos ka)$

$(2\beta - m_1\omega^2)\,(2\beta - m_2\omega^2) - (4\beta^2\cos^2 ka) = 0.$

$4\beta^2 - 2\beta m_2 \omega^2 - 2\beta m_1 \omega^2 + m_1 m_2 \omega^4 - 4\beta^2 \cos^2 ka$

$m_1 m_2 \omega^4 - 2\beta\omega^2 (m_1 + m_2) + 4\beta^2 (1 - \cos^2 ka) = 0$

$m_1 m_2 \omega^4 - 2\beta\omega^2 (m_1 + m_2) + 4\beta^2 \sin^2 ka = 0$

$$\omega^4 - 2\beta\omega^2 \frac{m_1 + m_2}{m_1 m_2} + \frac{4\beta^2 \sin^2 ka}{m_1 m_2} = 0$$

$$\omega^4 - \frac{2\beta (m_1 + m_2)\omega^2}{m_1 m_2} + \frac{4\beta^2 \sin^2 ka}{m_1 m_2} = 0 \rightarrow (12)$$

Let $\omega^2 = x$

$\omega^4 = x^2$; $x^2 - 2\beta\left(\frac{m_1 + m_2}{m_1 m_2}\right)x + \frac{4\beta^2}{m_1 m_2}\sin^2 ka = 0$

$$ax^2 + bx + c = 0$$

$a = 1$, $b = -2\beta \frac{m_1 + m_2}{m_1 m_2}$

$c = \frac{4\beta^2}{m_1 m_2} \sin^2 ka$

$\frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$

Soln of this quadratic eqn will be equa

$$\text{Roots} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$\omega_{\pm}^2 = \frac{-\left\{-\frac{2\beta(m_1 + m_2)}{m_1 m_2} \pm \sqrt{\left(-2\beta\frac{m_1 + m_2}{m_1 m_2}\right)^2 - 4 \times 1 \times \frac{4\beta^2 \sin^2 ka}{m_1 m_2}}\right.}{2(1)}$$

$2 \times 2 \sin \sqrt{\frac{ka}{m_1 m_2}}$

$$\omega^2_{\pm} = \frac{\beta(m_1+m_2)}{m_1m_2} \pm \sqrt{\beta^2}\left[\left(\frac{m_1+m_2}{m_1m_2}\right)^2 - \frac{4\beta\sin^2 ka}{m_1m_2}\right]^{1/2} \rightarrow (13)$$

ω^2_{+} - optical branch

ω^2_{-} - Acoustic branch (sound)

$$\omega^2_{+} = 2\beta\left[\frac{m_1+m_2}{m_1m_2}\right] \text{ optical branch} \rightarrow (14)$$

first brillouin zone:

$\frac{-\pi}{2a} \le k \le \frac{\pi}{2a}$ roots are at

$k_{max} = \pm \pi/2a$

$$\omega^2_{+} = \frac{2\beta}{m_2} \text{ (or) } \omega_{+} = \sqrt{\frac{2\beta}{m_2}} \longrightarrow (15a)$$

Since term becomes.

$\frac{-1}{m_1m_2}$ (or) $\sin^2 ka = \sin^2\frac{\pi}{2} = 1$ -ve root

cannot neglect since

ω_{-}; $k \to 0$.

$$\frac{4\sin^2 ka}{m_1m_2} = \frac{4k^2a^2}{m_1m_2}.$$

Its value is $\frac{4k^2a^2}{m_1m_2}$.

$$\omega^2_{-} = \frac{\beta(m_1+m_2)}{m_1m_2} - \beta\left[\left(\frac{m_1+m_2}{m_1m_2}\right)^2 - \frac{4k^2a^2}{m_1m_2}\right]^{1/2}$$

$$= \beta\left[\frac{m_1+m_2}{m_1m_2}\right] - \beta\left[\frac{m_1+m_2}{m_1m_2}\right]\left[1-\frac{m_1m_2}{(m_1+m_2)^2}\right.$$

$$\omega^2 = \beta\left[\frac{m_1+m_2}{m_1m_2}\right] - \beta\left[\frac{m_1+m_2}{m_1m_2}\right]\left[1-\frac{4k^2a^2}{m_1m_2}\left(\frac{m_1m_2}{m_1+m_2}\right)^2\right]^{1/2}$$

$$= \beta\left[\frac{m_1+m_2}{m_1m_2}\right]\left[1-\left(1-\frac{4k^2a^2}{m_1m_2}\left(\frac{m_1m_2}{m_1+m_2}\right)^2\right]^{1/2}\right.$$

$$= \beta\left[\frac{m_1+m_2}{m_1m_2}\right]\left[1-1-\frac{1}{2}\frac{4k^2a^2}{m_1m_2}\left(\frac{m_1m_2}{m_1+m_2}\right)^2\right]$$

Binomial theorem.

$$= \frac{2\beta(m_1+m_2)k^2a^2}{(m_1+m_2)^2}$$

$$= \frac{2\beta k^2a^2}{m_1+m_2}$$

$$\omega_- = ka\left[\frac{2\beta}{m_1+m_2}\right]^{1/2}$$

$$k \rightarrow \frac{\pi}{2a}$$

$$\boxed{\omega_-^2 = \sqrt{\frac{2B}{m_1}} \longrightarrow \text{Acoustic Branch}}$$