Solid State Physics
Lattice Vibration

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Books Recomended

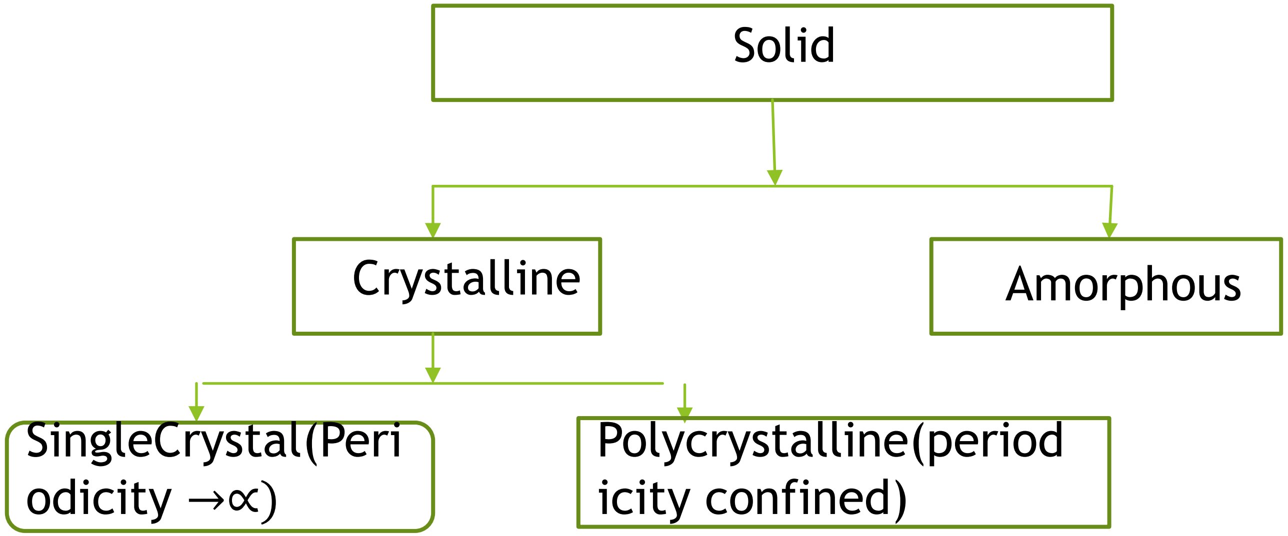
- 1] Solid state Physics by Dr. Jyotirmoy Guha
- 2] Introduction to Solid State Physics by Charles Kittel
- 2]Elements of Solid State Physics by J.P.Srivastava

Solid State Physics

- Solid State physics is one of the main & largest sub field of condense matter physics. It involves study of rigid matter called solid, employing well established laws of physics (for instance, Quantum Mechanics, Stat Mech, Electromagnetism & Crystallography.

- Solid state physics aims to describe how the large scale properties of solid (Ex: Magnetic Property, Electrical Property, Sp Heat, Optital Properties…) follow from the properties they possess on an atomic scale.

Classification of Solid



Solid

Crystalline

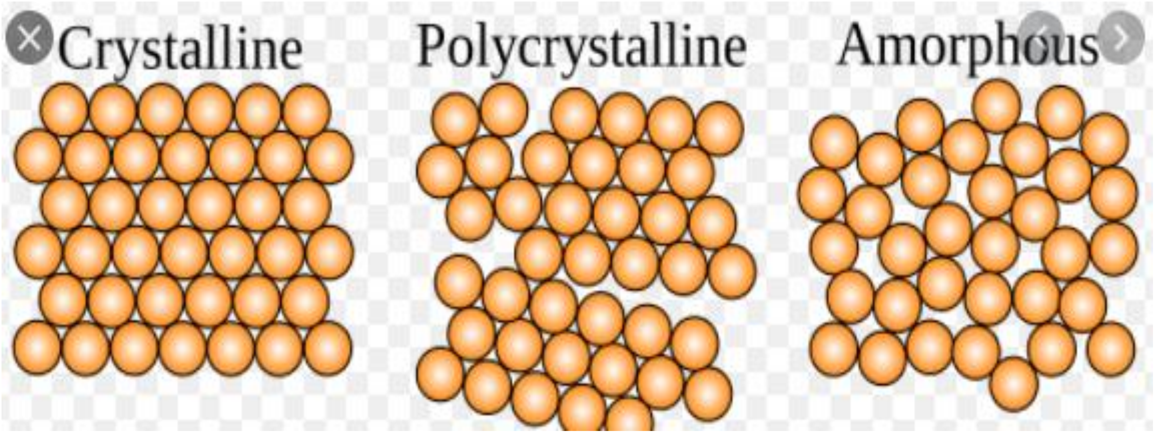
Amorphous

SingleCrystal(Periodicity →∝)

Polycrystalline(periodicity confined)

Crystal & Amorphous Solid

- **Crystal** A solid which has a regular (periodic) arrangement of atoms over 3 –D space
- **Amorphous** A solid has completely random(irregular/disordered) atomic arrangement

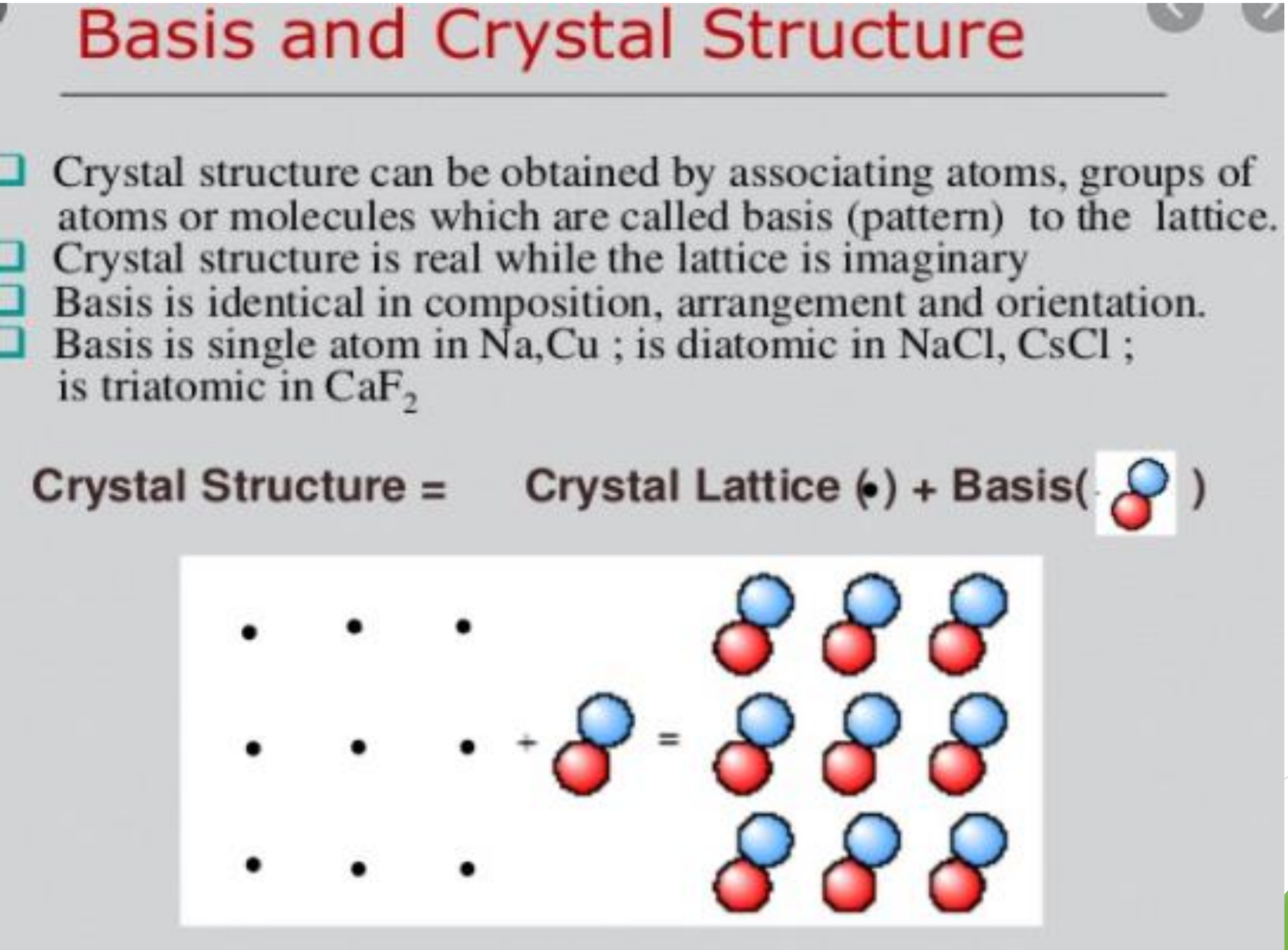


Distinction between Crystalline & Amophous

Properties	Crystalline	Amorphous
Geometry	Definite/Regular	Irregular
Order of Arrangement	Long Range	Short Range
Nature	True Solids	Pseudo – Solids or super-cooled liquids
Melting	Sharp	No particular M.P
Heat of Fusion	Definite	No Definite
Isotropism	Anisotropic	Isotropic
Cleavage	When cutting with a sharp edge, the two new halves will have smooth surfaces	When cutting with a sharp edge, the two resulting halves will have irregular surfaces
Rigidity	Rigid	Not Rigid , May Change Shape
Example	NaCl,KCl,Sugar	Glass,Wax,Plastic

Lattice

- **Lattice:**An array of points in space such that the environment about each point is same or as an infinite 3-D array of points showing how atoms or molecules are arranged in a crystal.

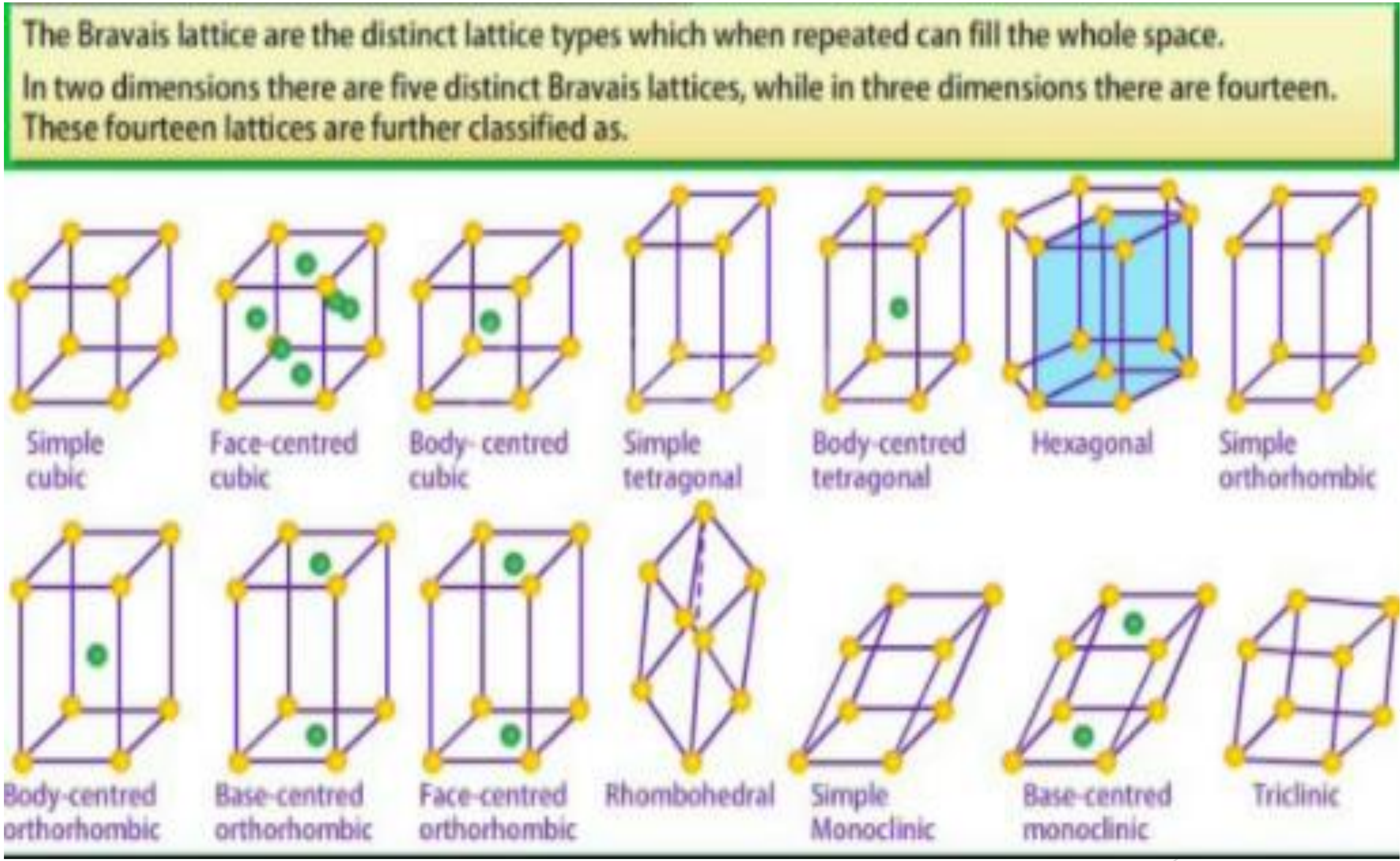


Basis and Crystal Structure

- Crystal structure can be obtained by associating atoms, groups of atoms or molecules which are called basis (pattern) to the lattice.
- Crystal structure is real while the lattice is imaginary
- Basis is identical in composition, arrangement and orientation.
- Basis is single atom in Na,Cu ; is diatomic in NaCl, CsCl ; is triatomic in CaF_2

Crystal Structure = Crystal Lattice (•) + Basis( )

Bravais Lattice



The Bravais lattice are the distinct lattice types which when repeated can fill the whole space.

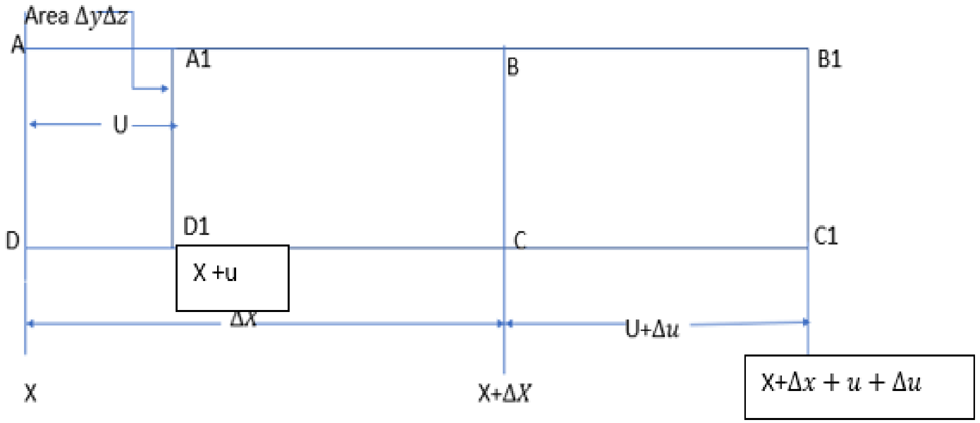
In two dimensions there are five distinct Bravais lattices, while in three dimensions there are fourteen. These fourteen lattices are further classified as.

Lattice Vibration

- When the lattice is at equilibrium each atom is positioned exactly at its lattice site Being at a temperature an atom of the solid oscillate continuously about its mean position and energy is communicated to neighbouring atom of the solid (which also are in oscillation). So there is communication / exchange /coupling of energy between the atoms And all the atoms of the crystal vibrate as a whole. Such Oscillation is called **lattice vibration.**
- We first consider elastic vibrational motion of a continuous, homogeneous medium, we then study characteristics of elastic vibrational motion of a crystal lattice in 1 D (= a linear chain of discreate atoms) and generalise result in 2D & 3D.

Elastic vibration in Continuous vibration

- Let us consider an element of homogeneous , isotropic elastic substance of length Δx having uniform cross sectional area $\Delta y \Delta z$ placed along x axis. When there is no elastic strain, let the element ABCD extend from x to x +Δx as shown in fig. When the elastic strain is produced, the new position of the element become $A1B^1C^1D^1$ie, the left end AD is shifted to A^1D^1 through a distance u. when right end of BC is shifted to is shifted to B^1C^1 through a distance u + Δu . When elastic medium is linear the applied stress & strain related by Hooke’s law.
- Change in length= A1B1 – AB= $[(x+\Delta x + u + \Delta u) - (x + u) \; - [(x + \Delta x) - x] = \Delta x + \Delta u - \Delta x = \Delta u$
- Oiginal length = AB= $(x+\Delta x) \; - x = \; \Delta x$
- Strain= s(x) = change in length / original length
- lim $\lim_{\Delta x \to 0} \Delta u / \Delta x = \frac{\partial u}{\partial x}$ (1)
- Stress/Strain = constant of elasticity
- F(x) / $\Delta y \Delta z$s(x) = C
- F(x) = C s(x) $\Delta y \Delta \Delta z$ (2)



Contd…..

- Similarly F$(x + \Delta x)$
- ∴F(x+Δx) – F(x) = C s(x+$\Delta x)\Delta y\Delta z$ $-$ $C\ s(x)\Delta y\Delta z$ = m a
- ∴C [$s(x + \Delta x) - s(x)]\Delta y\Delta z$ = m a (3)
- Where m is the mass and a is the acceleration, Expanding $s(x + \Delta x)$ by Taylor's series about x and neglecting higher terms in Δx, we have
- C $\frac{\partial s}{\partial x}\Delta x\Delta y\Delta z = m\ a$ (4)
- Substituting value of s(x) in eq(4) from (1)
- $C\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right)\Delta x\Delta y\Delta z = m\ \frac{\partial 2u}{\partial t2}$ where a=$\frac{\partial 2u}{\partial t2}$ (5)
- $\boldsymbol{\frac{\partial 2u}{\partial x2}} = \boldsymbol{\frac{\rho}{C}\frac{\partial 2u}{\partial t2}}$[density =$\rho = \frac{m}{\Delta x\Delta y\Delta z}$] (6)

Contd…..

- From (6) ,we have
- $\frac{\rho}{C}$ =1/$v_p{}^2$
- Eq 6 represents a wave eq for the amplitude of elastic waves in linear homogeneous medium as a function of x & t. The solution can be written as
- U (x,t) = A $e^{i(wt-kx)}$ (7)
- Where k = $2\pi/\boldsymbol{\lambda}$ **,** is known as propagation constant.
- Eq (7) represent a sinusoidal disturbance of wavelength **λ and** ω propagated along x axis.To obtain a relation between ω & k we differentiate eq (7) twice and then substitute it in (6) we get

Contd……

- $\frac{\partial 2u}{\partial x2} = -A\ k^2 e^{i(\ wt-\ kx)} \& \frac{\partial 2u}{\partial t2} = -A\omega^2 e^{i(\ wt-\ kx)}$
- $A\ k^2 e^{i(\ wt-\ kx)} = A\frac{\rho}{C}\omega^2 e^{i(\ wt-\ kx)}$
- $k^2 = \frac{\rho}{c}\omega^2$
- $\boldsymbol{\omega = k\sqrt{(c/\rho)}}$ **(8)**
- **The above relation is known as dispersion relation because it relates frequency and wavelength.**

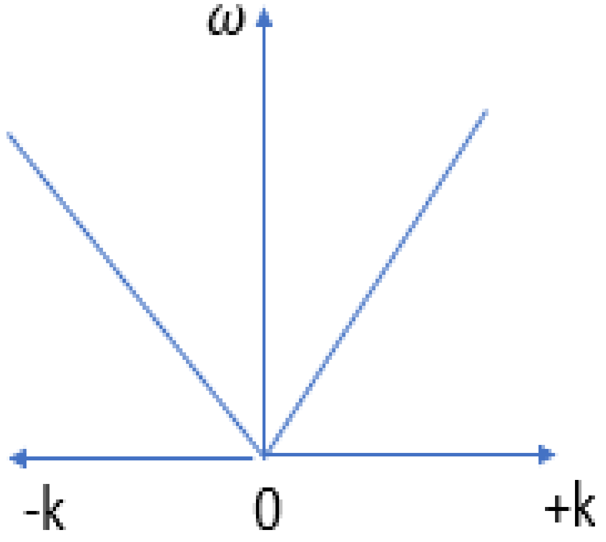


Fig 2

Phase Velocity

- **The rate of advancement of a point of constant phase of a wave in a medium along the direction of wave propagation is defined as phase velocity v_{ph} of the wave. It is the velocity with which pure wave moves.**

- **Considering the point of constant phase to be point of zero phase, we put phase angle of eq (7)**

- $\boldsymbol{\omega t - kx = 0 \rightarrow x = \frac{\omega t}{k} = \frac{2\pi\nu}{2\pi/\lambda} t = \nu\lambda\, t = V_{ph}\, t}$ **(9)**

- $\boldsymbol{V_{ph} = \nu\lambda = \frac{\omega}{k} = \sqrt{\frac{C}{\rho}} = constant}$ **(10)**

- **Phase velocity is constant independent of frequency &wavelength , depends on modulus of elasticity C and density ρ of the medium.**

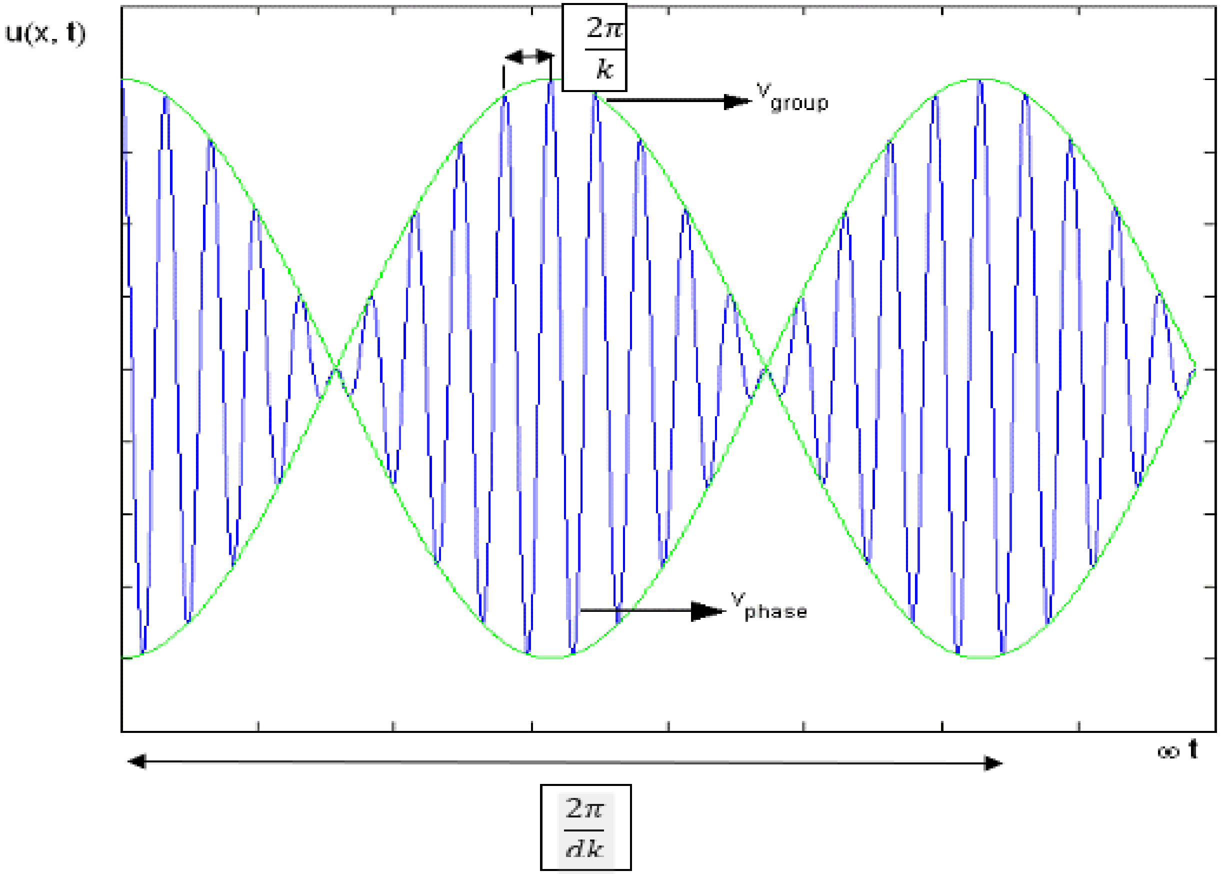
- **Eq (6) become**

- $\boldsymbol{\frac{\partial 2u}{\partial x2} = \frac{\rho}{C}\frac{\partial 2u}{\partial t2} = \frac{1}{Vph2}\frac{\partial 2u}{\partial t2}}$ (11)

Group Velocity

- **The group velocity is the velocity with which the energy is transmitted via pulses or packet rather than by pure wave . It is the velocity with which the overall shape of the wave amplitudes, known as modulation of enveloip of the wave propagates through space**.
- Let us consider the superposition of two wave train of same amplitude but different frequencies $\omega \ and \ \omega + d\omega$ and propagation constant k & k+dk. The two wave can be represented as
- $u_1 = A\cos(\omega t - kx)$ (1)
- $u_2 = A\cos\,[(\omega + d\omega)t - (k + dk)x]$ (2)
- $u_1 + u_2 = A(\cos\alpha + \cos\beta)$
- $= 2A\cos\left(\frac{\alpha+\beta}{2}\right)\cos\left(\frac{\alpha-\beta}{2}\right)$ (3)
- Where $\alpha + \beta = 2\omega t - 2kx + td\omega - xdk \approx 2\omega t - 2kx$ (4)
- $\alpha - \beta = xdk - td\omega$ (5)

- The eq (5) shows the superposition of wave having frequency ω & propagation constant k.
- The wave packet is modulated by an envelop $\cos(\frac{xdk-td\omega}{2})$, where $d\omega/2$ is the modulating frequency



- $v_g = \frac{d\omega}{dk}$
- $v_{ph} = \frac{\omega}{k} \rightarrow \omega = v_{ph}\, k$
- $v_g = d(v_{ph}k)/dk = v_{ph} + k(dv_{ph}/dk) = v_{ph} + \frac{2\pi}{\lambda} \frac{dvph}{d\left(\frac{2\pi}{\lambda}\right)}$
- $= v_{ph} + \frac{1}{\lambda} \frac{dvph}{-\frac{1}{\lambda 2} d\lambda}$
- $\boldsymbol{v_g = v_{ph} - \lambda \frac{dvph}{d\lambda}}$
- If ω is a linear function of k ie, =constant k
- then v_{ph} = constant & $dv_{ph}/d\lambda = 0$
- **$v_g = v_{ph}$ this is true for electromagnetic wave in vacuum which travels with velocity c**
- **independent of frequency & wavelength. This is the case for nondispersive medium.**
- **In dispersive medium Refractive index is non linear function of frequency ie non linear function of k. so ω/k $=v_{ph}$ is not constant but varies with λ, so v_{ph} & v_g differ.**

Normal mode of vibration in a finite length of continuous medium of 1-D

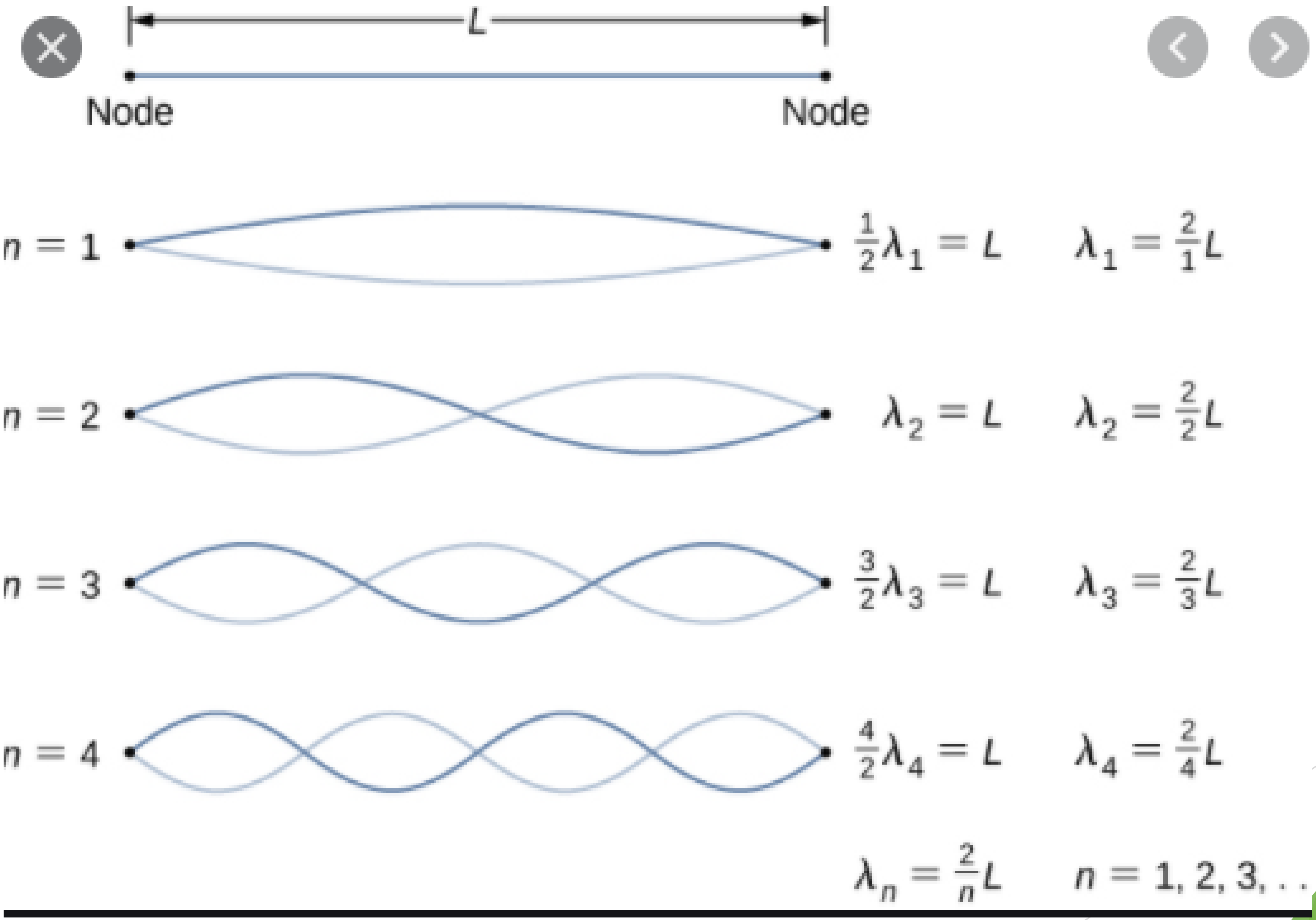
- Consider a 1D medium of finite length L.
- Boundary condition : no motion at x=0 & x=L
- When the medium is set into vibration 2 sets of travelling wave satisfying wave equation eq (11)
- $\frac{\partial 2u}{\partial x2} = \frac{\rho}{C}\frac{\partial 2u}{\partial t2} = \frac{1}{\mathrm{Vph2}}\frac{\partial 2u}{\partial t2}$
- Are generated that travel in opposite direction . We take them to be
- A sin(wt + kx) moving along x & B sin(wt-kx) along -x direction
- **u(x,t) = Asin (wt+kx) +B sin (wt-kx) (12)**

Contd…..

- **Applying Boundary condition u(x=0,t) & u(x=L,t) =0**
- **So we get Asin (wt) +B sin (wt) = 0**
- A = -B
- Again A sin (wt+kL) – A sin (wt-kL) =0
- 2 sin [(wt+kL)-(wt-kL)]/2 cos [(wt+kL)+(wt-kL)]/2 = 0
- sin kL cos wt = 0
- sin kL =0 [cos wt $\neq$ 0]

Contd……

- kL = nπ, n=0,1,2……..
- so eq 12 become
- u (x,t) = A sin (wt +kx) – A sin (wt-kx)
- **u (x,t) = 2A sin kx cos wt [k = nπ/L, n=1,2,3,……**
- dropping n=0 **]**
- **In the nth mode the string vibrates in n segments, the neighbouring segments are in opposite phases.**
- **So every values of k=** $\frac{\pi}{L}, \frac{2\pi}{L}, \frac{3\pi}{L}, \dots\dots$ **represent a normal mode of vibration.**
- **Frequency spectrum is discrete & is given by**
- $\omega_n = k\sqrt{\frac{C}{\rho}} = = n\pi/L\sqrt{\frac{C}{\rho}}$ **n = 1,2,3……**
- $\nu_n = \omega_n/2\pi = n\pi/L\sqrt{C/\rho} = n/2L\, v_{ph}$



$$\tfrac{1}{2}\lambda_1 = L \qquad \lambda_1 = \tfrac{2}{1}L$$

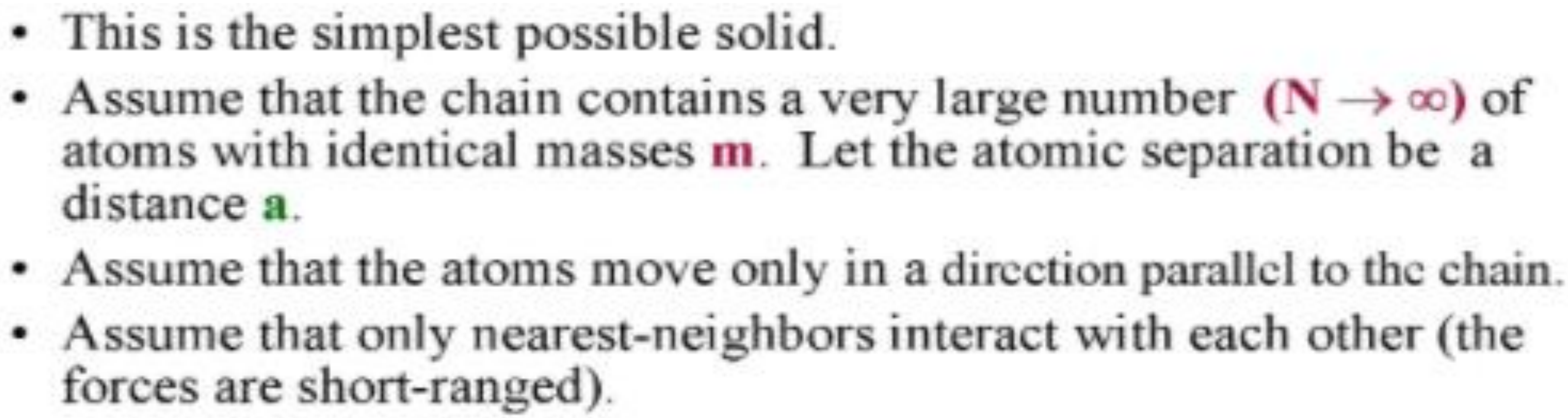
$$\lambda_2 = L \qquad \lambda_2 = \tfrac{2}{2}L$$

$$\tfrac{3}{2}\lambda_3 = L \qquad \lambda_3 = \tfrac{2}{3}L$$

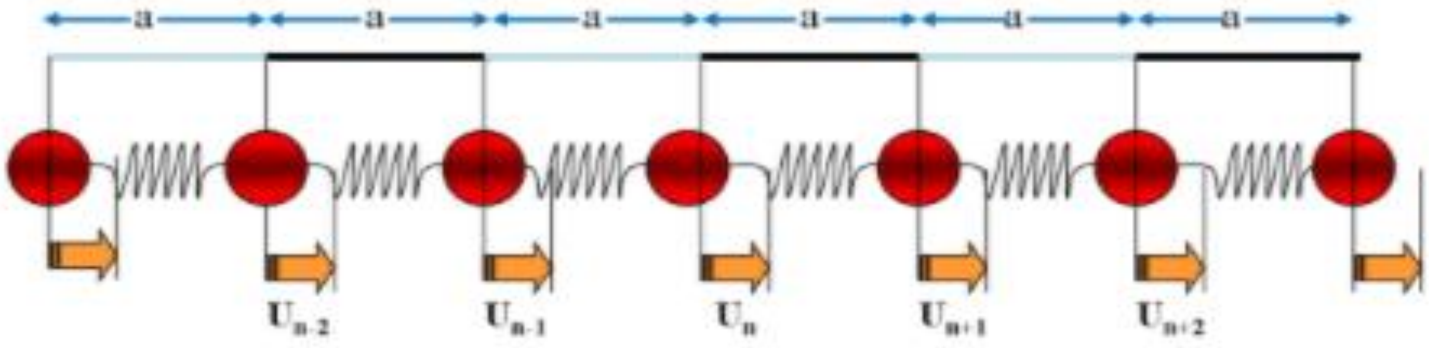
$$\tfrac{4}{2}\lambda_4 = L \qquad \lambda_4 = \tfrac{2}{4}L$$

$$\lambda_n = \tfrac{2}{n}L \qquad n = 1, 2, 3, \ldots$$

Vibration of 1D monoatomic linear lattice (spring model)



- This is the simplest possible solid.
- Assume that the chain contains a very large number $(N \to \infty)$ of atoms with identical masses **m**. Let the atomic separation be a distance **a**.
- Assume that the atoms move only in a direction parallel to the chain.
- Assume that only nearest-neighbors interact with each other (the forces are short-ranged).



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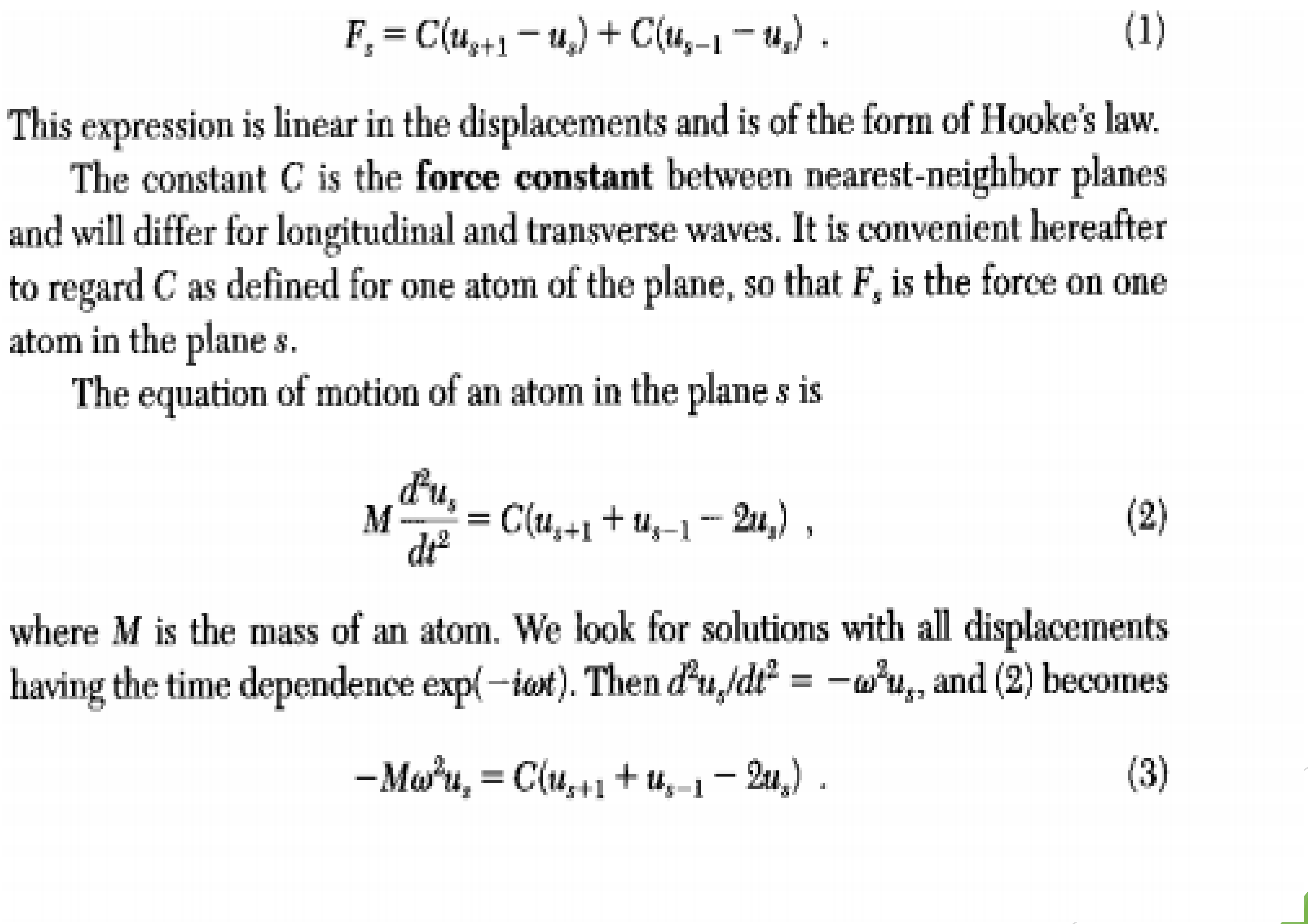
- The *monatomic chain* model represents a crystal in one dimension where all atoms are identical, equally spaced in equilibrium and connected by bonds of equal strength. The mass of an atom is m, the *spring constant*, C, describes the strength of the bond between atoms, and we enumerate the atoms along the chain using a variable s as a counter. The coordinate of atom s along the chain is u_s
- The force F_s acting on an atom s at any given moment is the product of its mass and its acceleration:
- $F_s=m\frac{d2Us}{dt2}$
- As long as the displacement of the atom is *elastic*, *i.e.* no permanent deformation takes place, we can apply *Hooke's law* and express the force as the displacement times the spring constant, C. Since the neighbouring atoms $s-1$ and $s+1$are also displaced from their equilibrium position, we need to consider the relative displacement between pairs



$$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s) \ . \tag{1}$$

This expression is linear in the displacements and is of the form of Hooke's law.

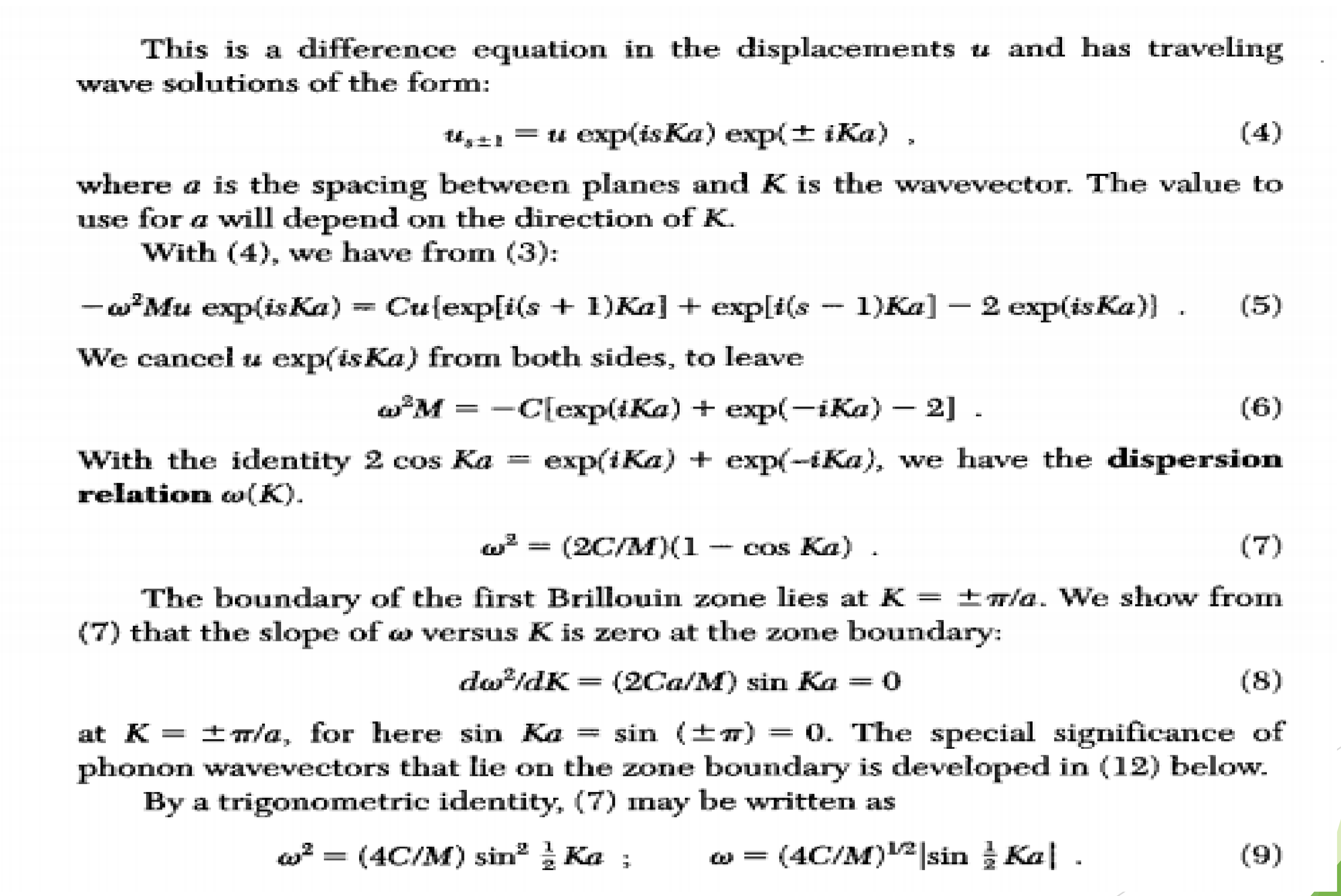
The constant C is the **force constant** between nearest-neighbor planes and will differ for longitudinal and transverse waves. It is convenient hereafter to regard C as defined for one atom of the plane, so that F_s is the force on one atom in the plane s.

The equation of motion of an atom in the plane s is

$$M \frac{d^2 u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s) \ , \tag{2}$$

where M is the mass of an atom. We look for solutions with all displacements having the time dependence $\exp(-i\omega t)$. Then $d^2u_s/dt^2 = -\omega^2 u_s$, and (2) becomes

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s) \ . \tag{3}$$



This is a difference equation in the displacements u and has traveling wave solutions of the form:

$$u_{s\pm1} = u \exp(isKa) \exp(\pm iKa) \ , \tag{4}$$

where a is the spacing between planes and K is the wavevector. The value to use for a will depend on the direction of K.

With (4), we have from (3):

$$-\omega^2 Mu \exp(isKa) = Cu\{\exp[i(s+1)Ka] + \exp[i(s-1)Ka] - 2\exp(isKa)\} \ . \tag{5}$$

We cancel $u \exp(isKa)$ from both sides, to leave

$$\omega^2 M = -C[\exp(iKa) + \exp(-iKa) - 2] \ . \tag{6}$$

With the identity $2\cos Ka = \exp(iKa) + \exp(-iKa)$, we have the **dispersion relation** $\omega(K)$.

$$\omega^2 = (2C/M)(1 - \cos Ka) \ . \tag{7}$$

The boundary of the first Brillouin zone lies at $K = \pm\pi/a$. We show from (7) that the slope of ω versus K is zero at the zone boundary:

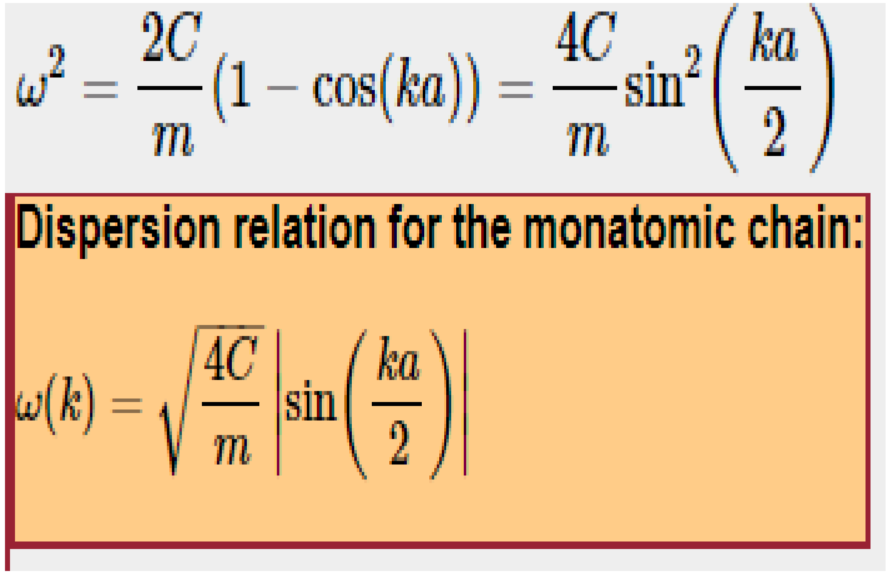
$$d\omega^2/dK = (2Ca/M)\sin Ka = 0 \tag{8}$$

at $K = \pm\pi/a$, for here $\sin Ka = \sin(\pm\pi) = 0$. The special significance of phonon wavevectors that lie on the zone boundary is developed in (12) below.

By a trigonometric identity, (7) may be written as

$$\omega^2 = (4C/M)\sin^2 \tfrac{1}{2}Ka \ ; \qquad \omega = (4C/M)^{1/2}|\sin \tfrac{1}{2}Ka| \ . \tag{9}$$

Dispersion relation for monoatomic Chain



$$\omega^2 = \frac{2C}{m}(1-\cos(ka)) = \frac{4C}{m}\sin^2\left(\frac{ka}{2}\right)$$

Dispersion relation for the monatomic chain:

$$\omega(k) = \sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

Plot Of ω VS k

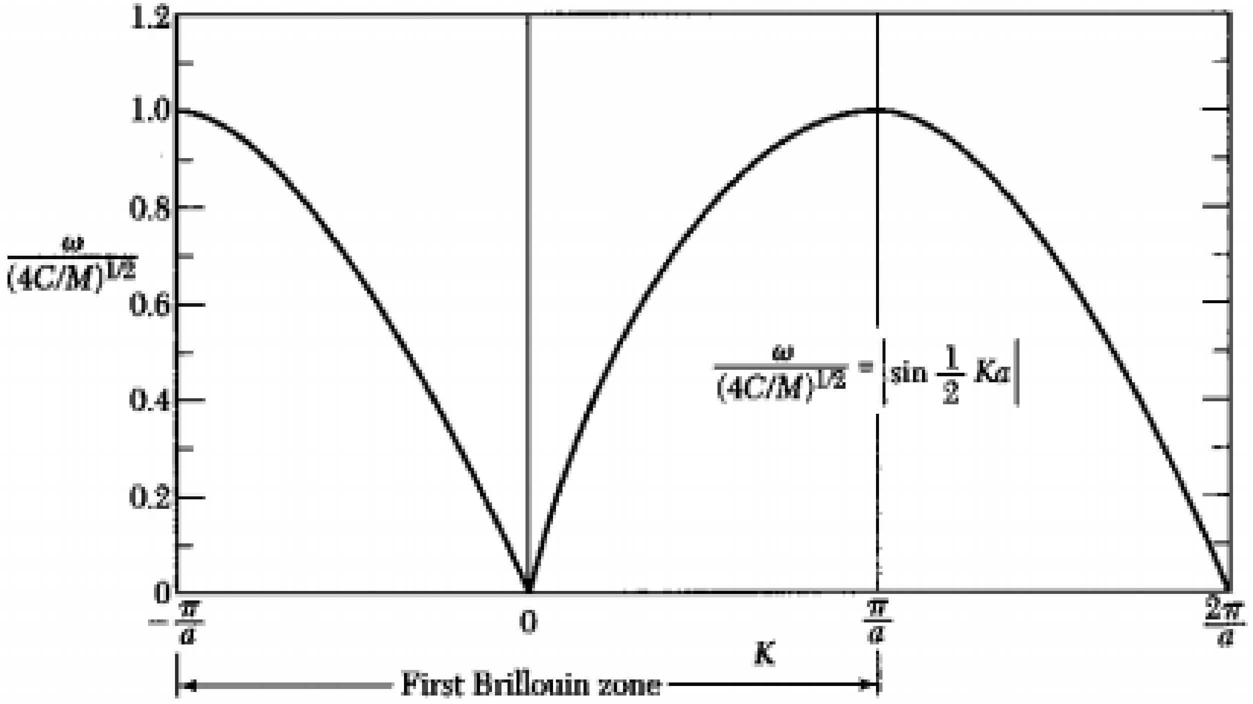


Figure 4 Plot of ω versus K. The region of $K \ll 1/a$ or $\lambda \gg a$ corresponds to the continuum approximation; here ω is directly proportional to K.

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- so $\boldsymbol{\omega} = \boldsymbol{\omega 0 \sin k a/2}$ & $\nu = \nu 0 \sin ka/2$
- $\omega o = 2\sqrt{c/m}$ & $\nu 0 = \frac{\omega 0}{2\pi} = \frac{1}{\pi}\sqrt{c/m}$
- So ω depends on k the relation between ω & k is know as dispersion relation & the plot of w vs k is dispersion curve. Dispersion curve is periodic & symmetric around origin.

First Brillouin Zone

- What range of K is physically significant for elastic waves?
- Only those in 1st Brillouin Zone
- From relation (4)

$= u_{s+1}/u_s = e^{i(s+1)ka}/ e^{iska} = e^{ika}$

- The range $-\pi\ to + \pi$ for the phase ka covers all the independent values of the exponential.
- We need both +ve & -ve values of K as wave propagates to the right or to left'
- The range of independent values of k is specified by
- $-\pi < ka < \pi$ or $-\frac{\pi}{a} < k < \frac{\pi}{a}$
- This is the 1st B. Zone of the linear lattice
- There is a real difference here from an elastic continuum;in the continuum limit a→ $0\ \&\ kmax \rightarrow \propto$.

- Values of k outside 1st B.Zone merely reproduce lattice motion described by values within limt of$\frac{\pm\pi}{a}$
- Suppose k lies outside the first zone, but related by a web vector k1 defined by k1= k-2nπ/a lies within the first zone, where n is a integer. Then displacement ratio becomes .
- Us+1/Us = exp ika [as exp $2\pi n i = 1$]
- We note that 2n$\frac{\pi}{a}$ is a reciprocal lattice vector as 2$\frac{\pi}{a}$ is a reciprocal lattice vector.Thus by subtraction of an appropriate reciprocal vector from k, we always obtain an equivalent vector in the 1st zone.
- Thus the displacement always be described by a web vector within the first zone.

Contd….

- At the boundary Kmax = +-π/a of the B zone the solution Us represents a standing web.
- At the Zone boundary s Kmax a= $\pm s\pi$ so Us = U exp(+-isπ) = U (-1)^s
- This is a standing wave as alternate atoms oscillate in opposite phases, as U=+-1
- This situation is equivalent to Bragg reflection of X-rays, when Bragg condition satisfies, a travelling web can not propagate in a lattice but a standing web is set up.
- The critical value Kmax= +-π/a found here satisfies Bragg's condition

$$2d \sin\theta = n\lambda \; when\ \theta = \frac{\pi}{2}, \&\ d = a, k = \frac{2\pi}{\lambda}, n = 1\ so\ \lambda = 2a$$

BRILLOUIN ZONES

- A Brillouin zone is defined as Wigner-Seitz primitive cell in a reciprocal lattice.
- Wigner-Seitz cell: smallest possible primitive cell, which consist of one lattice point and all the surrounding space closer to it than to any other point. The construction of the W-S cell in the reciprocal lattice delivers the first Brillouin zone (important for diffraction)

- The value of the Brillouin zone is a vivid geometrical interpretation of the diffraction condition.
- Brillouin zones are nothing but allowed energy regions in momentum space for electrons present in periodic crystals. The electrons present in periodic crystals are commonly referred as ‘Bloch electrons or Bloch waves’.
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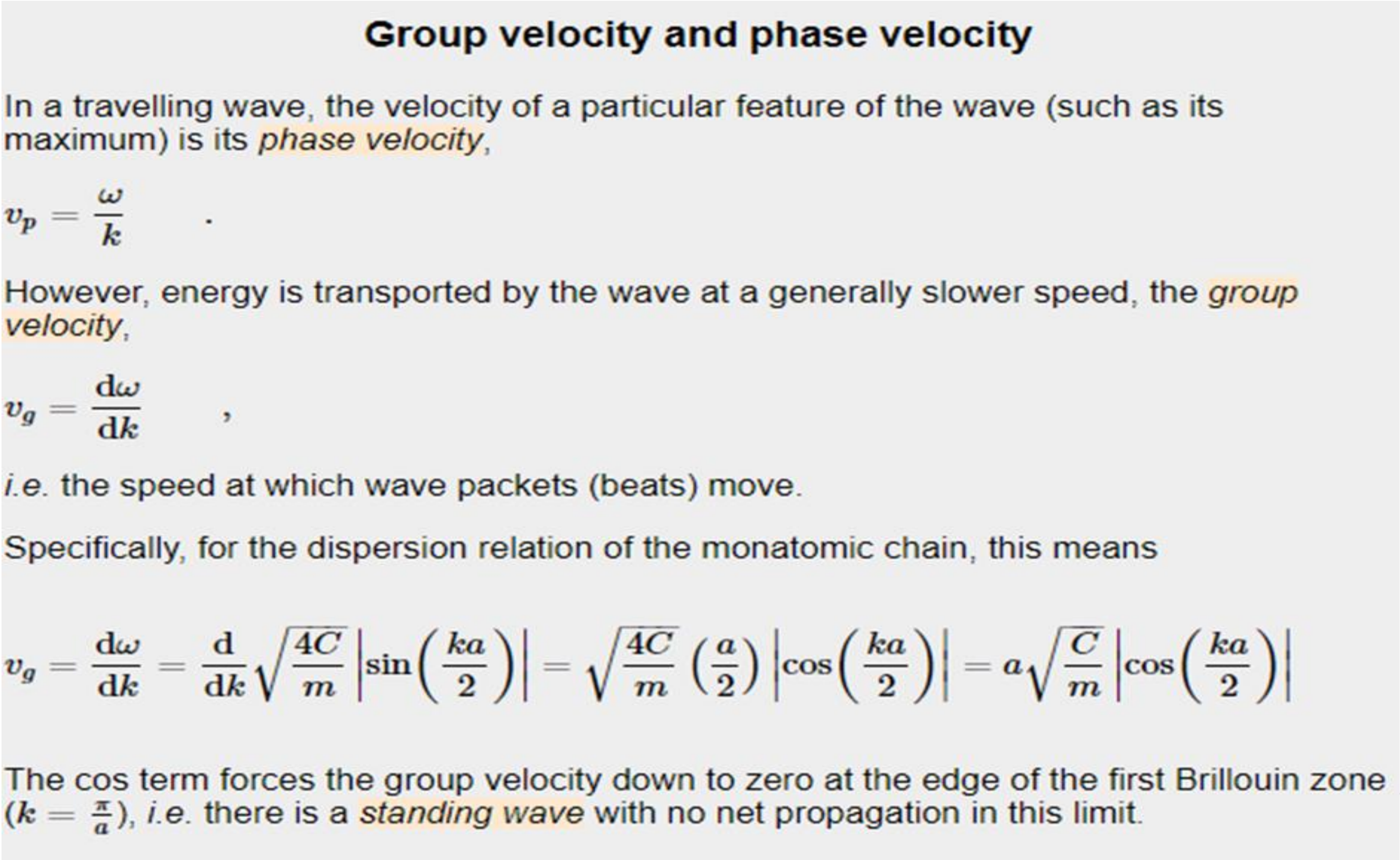

Group velocity and phase velocity

In a travelling wave, the velocity of a particular feature of the wave (such as its maximum) is its *phase velocity*,

$$v_p = \frac{\omega}{k} \quad .$$

However, energy is transported by the wave at a generally slower speed, the *group velocity*,

$$v_g = \frac{\mathrm{d}\omega}{\mathrm{d}k} \quad ,$$

i.e. the speed at which wave packets (beats) move.

Specifically, for the dispersion relation of the monatomic chain, this means

$$v_g = \frac{\mathrm{d}\omega}{\mathrm{d}k} = \frac{\mathrm{d}}{\mathrm{d}k}\sqrt{\frac{4C}{m}}\left|\sin\left(\frac{ka}{2}\right)\right| = \sqrt{\frac{4C}{m}}\left(\frac{a}{2}\right)\left|\cos\left(\frac{ka}{2}\right)\right| = a\sqrt{\frac{C}{m}}\left|\cos\left(\frac{ka}{2}\right)\right|$$

The cos term forces the group velocity down to zero at the edge of the first Brillouin zone ($k = \frac{\pi}{a}$), *i.e.* there is a *standing wave* with no net propagation in this limit.

Long wavelength limit

- When Ka≪ 1 we expand cos Ka≅1-1/2(Ka)^2 so the dispersion relation

  become

$$\omega^2 = \left(\frac{C}{M}\right)k^2a^2$$

The result that the frequency is directly proportional to the wavevector in the long wavelength limit is equivalent to the velocity of sound is independent of frequency in this limit. Thus v $=\frac{\omega}{k}$, exactly as in the continuum theory of elastic waves-in the continuum limit a=0 and thus Ka=0