

Chapter 4 Crystal Vibration

4.0 Elastic Waves

4.1 Elastic Waves in a **chain**






4.2 **Two Atoms** per Primitive Cell

4.3 **Quantization** of Elastic Waves & Phonon

Momentum

4.4 **3D Crystal Vibration**

Fields & “Elementary” Particles in Condensed Matter Physics

	Name	Field
	Electron	—
	Photon	Electromagnetic wave
	Phonon	Elastic wave
	Plasmon	Collective electron wave
	Magnon	Magnetization wave
—	Polaron	Electron + elastic deformation
—	Exciton	Polarization wave

Atoms are in a **perpetual movement** in solids:

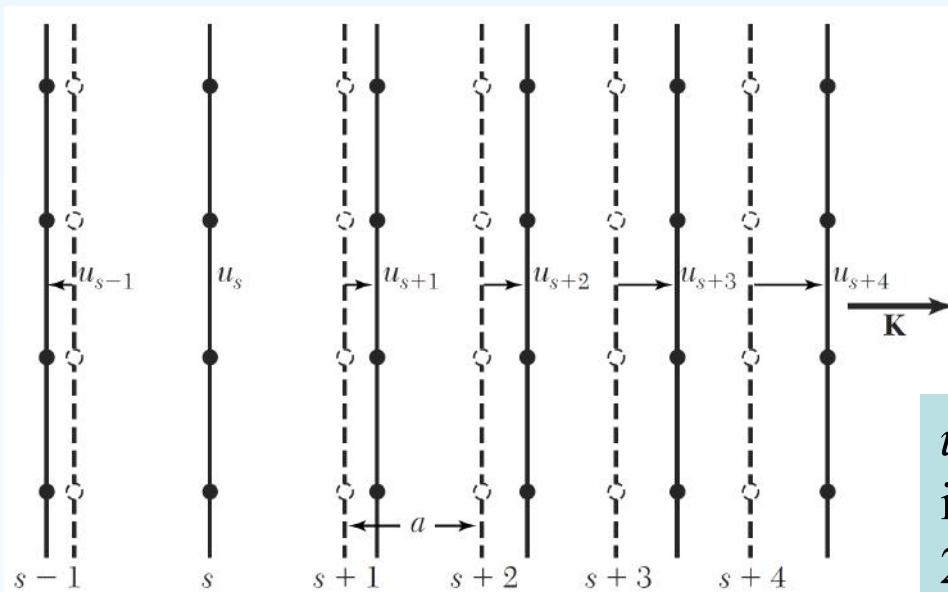
- ✓ **Low temperature:** thermal fluctuations are weak, vibration around its equilibrium position, elastic wave
- ✓ **High temperature:** strong thermal fluctuations, melting

Elastic Waves in solids

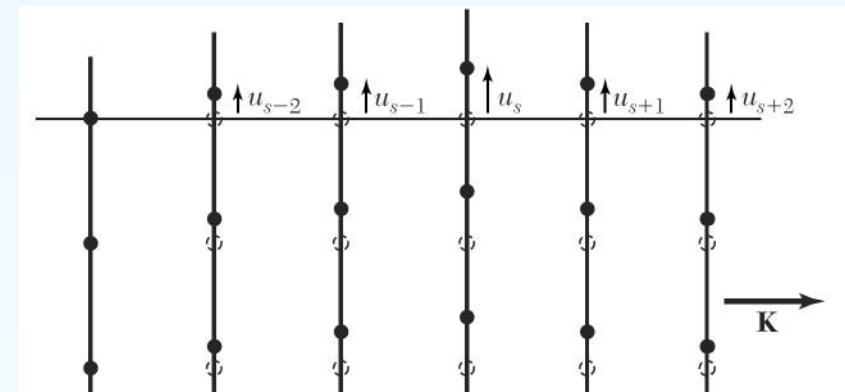
Propagates along, say, [100] direction, entire planes of atoms move in phase

Problem is reduced to 1D!

parallel to wave vector K



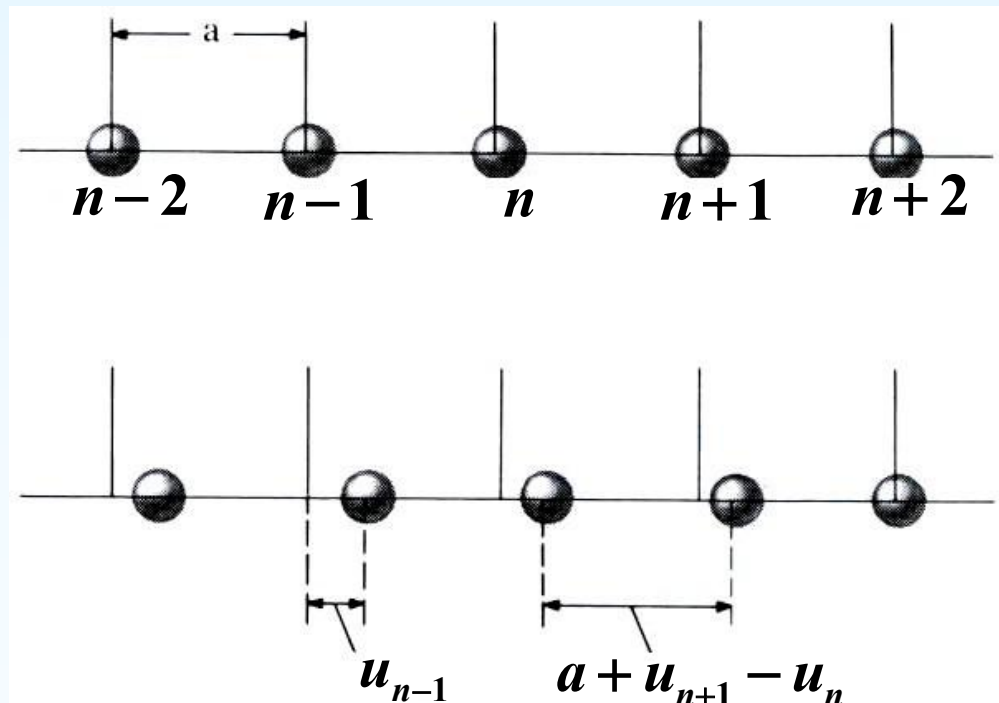
perpendicular to wave vector K



u_s is the *displacement* of the plane s from its equilibrium position, 1 **longitudinal** + 2 **transverse** modes.

4.1 Elastic Waves in a chain

- ✓ Problem simplified as a chain in 1D, N.N. atoms (*equilibrium positions*) separated by a distance of a (*lattice constant*).
- ✓ The displacement of n -th atom is denoted as u_n .



The potential energy of a pair of N.N. atoms: $\phi(a)$

Relative displacement between n and $n+1$ atoms: $\delta = u_{n+1} - u_n$

Corresponding, the two-site potential changes to:

$$\phi(a + \delta)$$

Expand $\phi(a + \delta)$ around the equilibrium position:

$$\phi(a + \delta) = \underbrace{\phi(a)}_{\text{Minimal Value of Potential Energy at equil. position}} + \underbrace{\left(\frac{\partial \phi}{\partial X} \right)_a}_{\text{Vanishes at equilibrium position}} \delta + \frac{1}{2} \underbrace{\left(\frac{\partial^2 \phi}{\partial X^2} \right)_a}_{\text{Harmonic Term for Elastic Deformation}} \delta^2 + \dots$$

Minimal Value of Potential Energy at equil. position

Vanishes at equilibrium position

Harmonic Term for Elastic Deformation

1. E.O.M in the harmonic approximation

Consider a small δ , i.e., a weak vibration, expand the potential to the order of δ^2

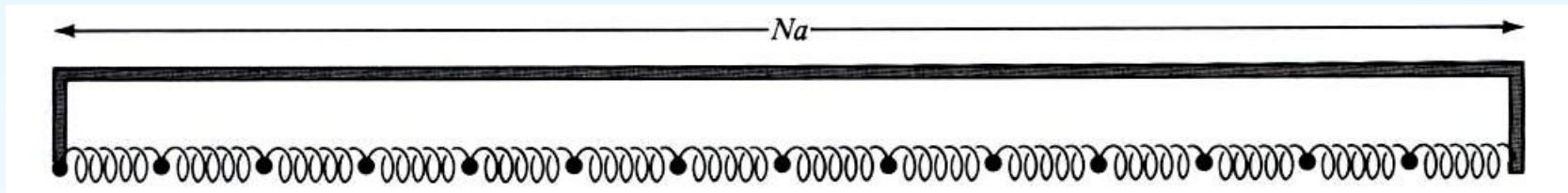
$$\phi(a + \delta) = \phi(a) + \frac{1}{2} \left(\frac{\partial^2 \phi}{\partial X^2} \right)_a \delta^2$$

Elastic force between two atoms:

$$f = - \frac{\partial \phi}{\partial \delta} = - \left(\frac{\partial^2 \phi}{\partial X^2} \right)_a \delta$$
$$\beta = \left(\frac{\partial^2 \phi}{\partial X^2} \right)_a \quad \text{—— elastic constant}$$

$$f = -\beta\delta = -\beta(u_{n+1} - u_n)$$

- In the *harmonic approx.*, the atoms are connected via “springs”.
- The 1d atomic chain can be regarded as *coupled harmonic oscillators*.
- (Elastic) *lattice wave* can propagate in the 1d atomic chain as collective excitation.



Consider only N.N. coupling, the total force on n -th atom:

$$\beta(u_{n+1} - u_n) - \beta(u_n - u_{n-1}) = \beta(u_{n+1} + u_{n-1} - 2u_n)$$

with corresponding e.o.m.:

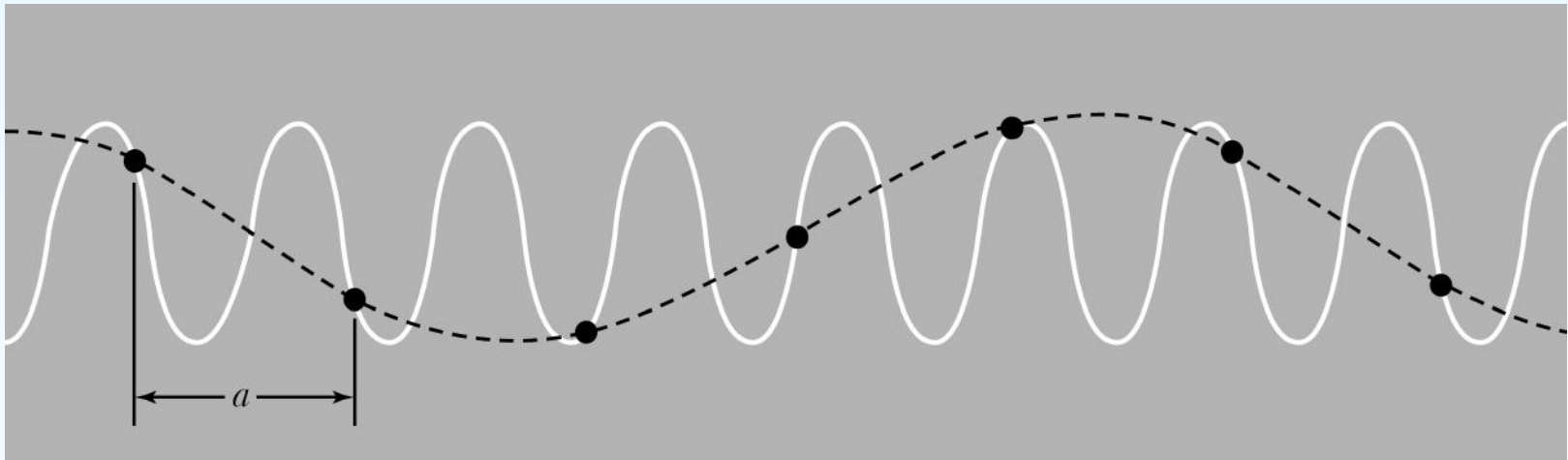
$$M \frac{d^2 u_n}{dt^2} = \beta(u_{n+1} + u_{n-1} - 2u_n)$$

2. Lattice Wave

There exists a e.o.m. for *each atom*, # of equations *equals*
of atoms.

The solution is a traveling wave:

$$u(na, t) = Ae^{i(qna - \omega t)}$$



3. Dispersion Relation

$$u(na, t) = Ae^{i(qna - \omega t)}$$

Substitute it in the e.o.m.,

$$-M\omega^2 e^{iqna} = \beta \left[e^{iq(n+1)a} + e^{iq(n-1)a} - 2e^{iqna} \right]$$

$$M\omega^2 = 2\beta(1 - \cos qa)$$

$$\omega = \sqrt{\frac{2\beta(1 - \cos qa)}{M}} = 2\sqrt{\left(\frac{\beta}{M}\right)} \left| \sin \frac{qa}{2} \right|$$

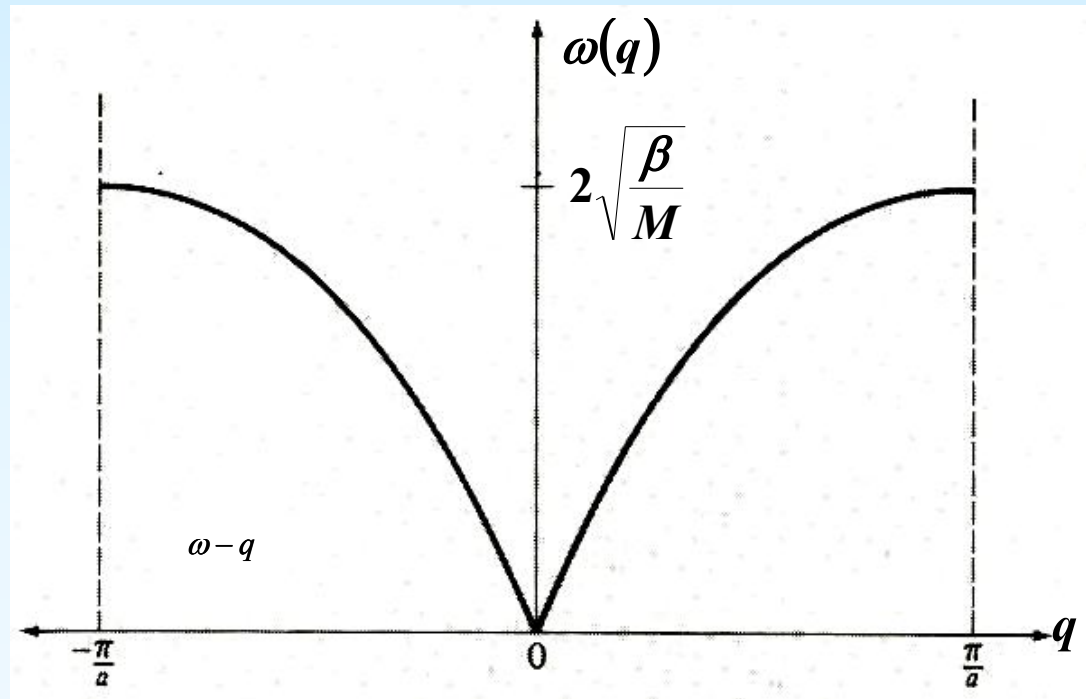
----dispersion relation

4.1 Elastic Waves in a chain

◆ $q \rightarrow 0, \lambda$ is large,
long wavelength appr.,

$$\sin \frac{qa}{2} \approx \frac{qa}{2}$$

$$\omega = \left(\frac{\beta}{M} \right)^{1/2} qa$$



ω shows a linear relation with q , the same as that of the elastic wave in the continuous medium. i.e., in the l.w.a. the discreteness of lattice site can be neglected. --*Acoustic branch*

◆ As q increases, $\omega - q$ deviates from linear relation.

◆ when $q = \pm \frac{\pi}{a}$, ω achieves its max value

$$\omega_{\max} = 2\sqrt{\left(\frac{\beta}{M}\right)}$$

recall:

$$\omega = \sqrt{\frac{2\beta(1 - \cos qa)}{M}} = 2\sqrt{\left(\frac{\beta}{M}\right)} \left| \sin \frac{qa}{2} \right|$$

3. Periodic functions of q

ω is a period wavefunction of q , $\omega\left(q + n\frac{2\pi}{a}\right) = \omega(q)$

n —integer, period $\frac{2\pi}{a}$ ———primitive reciprocal lattice vector

$n\frac{2\pi}{a} = G_h$ ———reciprocal lattice vector

$$\omega(q + G_h) = \omega(q)$$

$$u(q + G_h) = u(q)$$

The wave length (vector) related to a specific lattice wave is not unique, there exist a series of q , different from each other by $h \cdot 2\pi/a = G_h$.

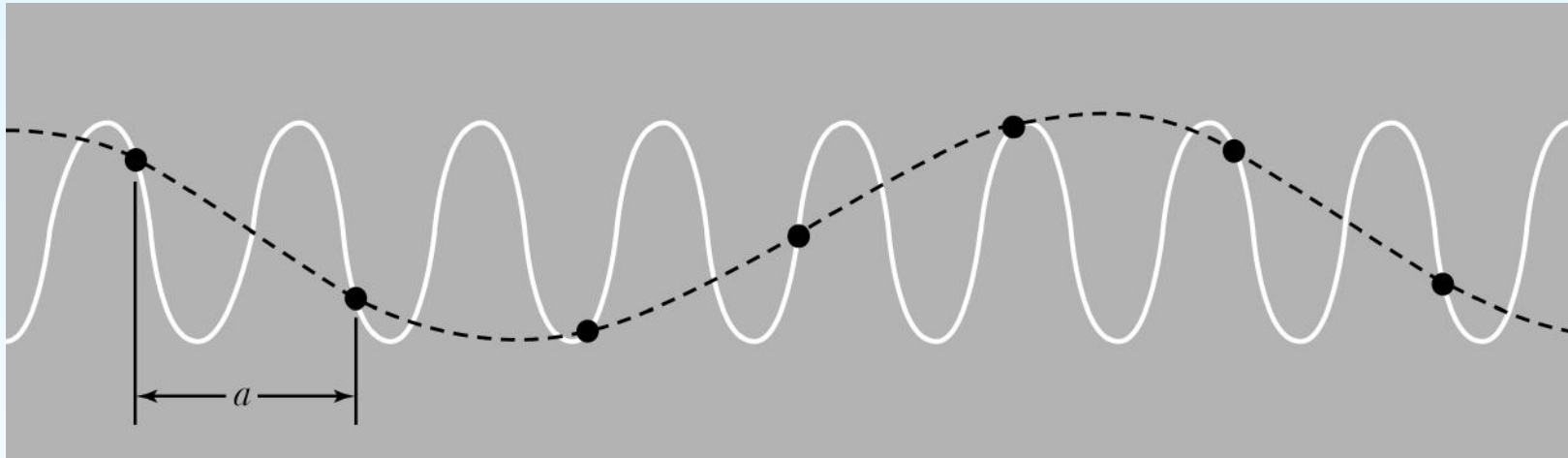
Only wavelengths *longer than $2a$* are *needed* to represent the motion.

Therefore, within the range of $-\pi/a \leq q \leq \pi/a$, q can fully characterize all allowed lattice waves.

—— *1st Brillouin zone*

q and $q+G_h$ correspond to exactly the same lattice waves

$$q = \frac{2\pi}{5a}, \quad \lambda = \frac{2\pi}{q} = 5a \quad \left| \quad q' = q + \frac{2\pi}{a} = \frac{12\pi}{5a}, \quad \lambda' = \frac{2\pi}{q'} = \frac{5}{6}a$$



- ✓ The wave represented by the solid curve conveys no information not given by the dashed curve.

4. Standing Wave

At the Brillouin zone boundary $q = \pm \pi/a$

$$u_s = u \exp(qsa)$$

$$u_s = u \exp(\pm is\pi) = u (-1)^s$$

Does not represent a traveling wave, but a standing wave

This situation is equivalent to **Bragg reflection** of x-rays!

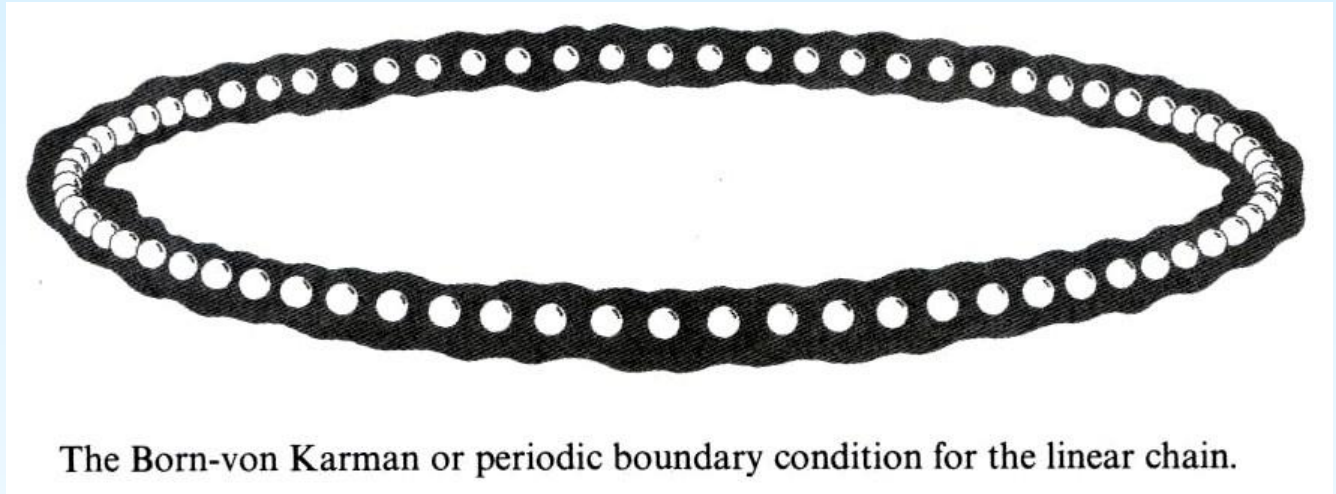
$$2d \sin \theta = n\lambda$$

a $\pi/2$ $2\pi/q$
 ↑ ↑ ↓
K is along
the atomic chain

$$\underline{n=1}$$

5. Periodic Boundary Condition

**Born-von
 Karman
 boundary
 condition**

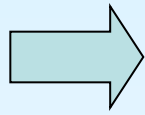


$$u(a) = u(Na + a) \quad u(na) = u(Na + na)$$

$$Ae^{i(qna - \omega t)} = Ae^{i(q(N+n)a - \omega t)} \quad \longrightarrow$$

$$e^{iqNa} = 1 \quad qNa = 2\pi l \quad \boxed{q = \frac{l}{N} \frac{2\pi}{a}} \quad l \text{ integer}$$

1st B.Z. $-\frac{\pi}{a} < q \leq \frac{\pi}{a}$



$$-\frac{N}{2} < l \leq \frac{N}{2}$$

q has N discrete values -- equals # of sites/atoms in the chain

All q values within 1st B.Z. describes *all vibration modes*, each q corresponds to a *lattice wave vector*.

For 1D chain, all N q points are uniformly distributed:

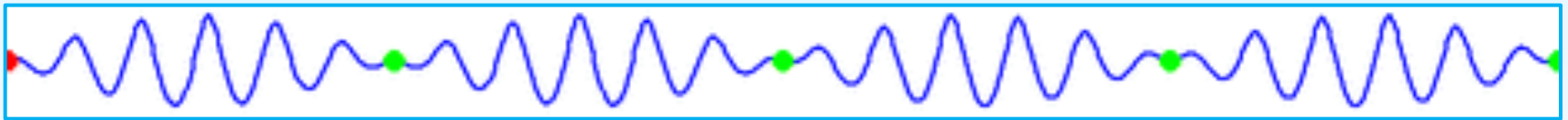
distance btw q points: $\frac{2\pi}{Na} = \frac{2\pi}{L}$

6. phase and group velocities

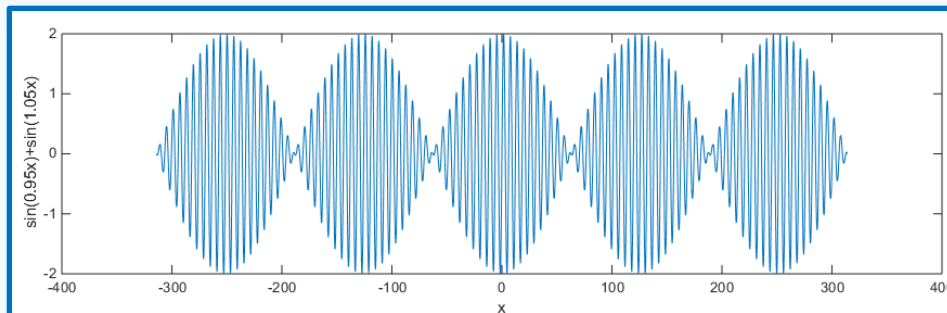
phase velocity: the rate at which the phase of the wave propagates in space, for a pure lattice wave with specific frequency ω and lattice vector q

$$v_p = \frac{\omega}{q}$$

$$v_p = \frac{\lambda}{T}$$



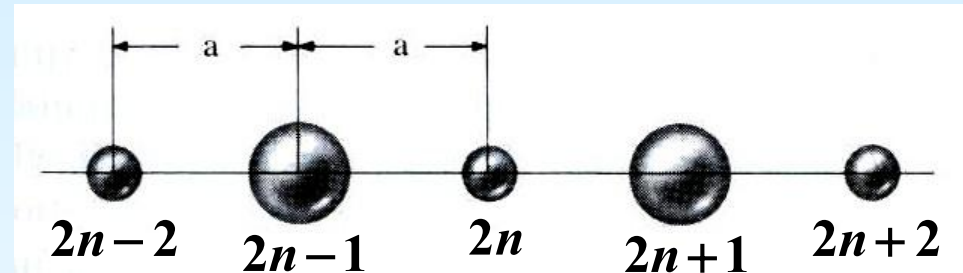
group velocity: describe the speed of the *envelope* of the wave packet (given *a small range of q* , such that the envelope *does not distort* too much during propagation).



$$v_g = \frac{\partial \omega}{\partial q}$$

4.2. 1D chain with two atoms per primitive cell

1. Equation of Motion



N primitive unit cell, each of which contains *two different atoms*, lattice constant $2a$, atom mass $M > m$.

atoms with mass m : $\dots, 2n-2, 2n, 2n+2, \dots$

atoms with mass M : $\dots, 2n-1, 2n+1, 2n+3, \dots$

Displacement of each atom (with respect to equil. position):

$$\dots, u_{2n-2}, u_{2n}, u_{2n+2}, \dots \quad \dots, u_{2n-1}, u_{2n+1}, u_{2n+3}, \dots$$

Consider only **inter. between N.N. atoms** & **hamornic approx.:**

$$\left\{ \begin{array}{l} m \frac{d^2 u_{2n}}{dt^2} = \beta (u_{2n+1} + u_{2n-1} - 2u_{2n}) \\ M \frac{d^2 u_{2n+1}}{dt^2} = \beta (u_{2n+2} + u_{2n} - 2u_{n+1}) \end{array} \right.$$

β — elastic constant between atoms

$2N$ atoms, $2N$ equations, the correlated motions of atoms constitute a *wave*.

2. dispersion relation

subs. $\begin{cases} u_{2n} = Ae^{i(2naq-\omega t)} \\ u_{2n+1} = Be^{i((2n+1)aq-\omega t)} \end{cases}$ into the E.O.M., we get

$\begin{cases} -m\omega^2 A = \beta(e^{iqa} + e^{-iqa})B - 2\beta A \\ -M\omega^2 B = \beta(e^{iqa} + e^{-iqa})A - 2\beta B \end{cases}$ reorganize it:

$\begin{cases} (2\beta - m\omega^2)A - (2\beta \cos qa)B = 0 \\ (-2\beta \cos qa)A + (2\beta - M\omega^2)B = 0 \end{cases}$

Condition of the existence of solutions

$$\begin{vmatrix} 2\beta - m\omega^2 & -2\beta \cos qa \\ -2\beta \cos qa & 2\beta - M\omega^2 \end{vmatrix} = 0$$

$$mM\omega^4 - 2\beta(m + M)\omega^2 + 4\beta^2 \sin^2 qa = 0$$

$$\begin{cases} \omega_-^2 = \frac{\beta}{mM} \left\{ (m + M) - [m^2 + M^2 + 2mM \cos(2qa)]^{\frac{1}{2}} \right\} \\ \omega_+^2 = \frac{\beta}{mM} \left\{ (m + M) + [m^2 + M^2 + 2mM \cos(2qa)]^{\frac{1}{2}} \right\} \end{cases}$$

two different ω - q relations, meaning *two branches* of lattice waves.

3. First B.Z.

$\omega_{\pm}^2(q)$ is a periodic function of q , with period $2\pi/2a$.

$$\omega_{\pm}^2\left(q + s\frac{\pi}{a}\right) = \omega_{\pm}^2(q)$$

reciprocal lattice vector: $\frac{2\pi}{2a} = \frac{\pi}{a}$ $s\frac{\pi}{a} = G_h$

$$\omega_{\pm}^2(q + G_h) = \omega_{\pm}^2(q)$$

one can also prove:

$$u_{2n}(q + G_h) = u_{2n}(q)$$

$$u_{2n+1}(q + G_h) = u_{2n+1}(q)$$

therefor q and $q + G_h$ describe **exactly the same vibration mode**, we can restrict q within a peorid π/a , i.e., a primitive reciprocal lattice vector.

A symmetric choice: $-\frac{\pi}{2a} < q \leq \frac{\pi}{2a}$ $2a$ ———lattice constant
 ———first Brillouin zone

4. optical and acoustic branches

(1) extreme values $-\pi < 2qa \leq \pi$

➤ short wavelength limit $q \rightarrow \pm \frac{\pi}{2a}$

$$(\omega_-)_{\max} = \left(\frac{\beta}{mM} \right)^{\frac{1}{2}} \{ (m + M) - (M - m) \}^{\frac{1}{2}} = \left(\frac{2\beta}{M} \right)^{\frac{1}{2}}$$

$$(\omega_+)_{\min} = \left(\frac{\beta}{mM} \right)^{\frac{1}{2}} \{ (m + M) + (M - m) \}^{\frac{1}{2}} = \left(\frac{2\beta}{m} \right)^{\frac{1}{2}}$$

$$M > m, \omega_- < \omega_+$$

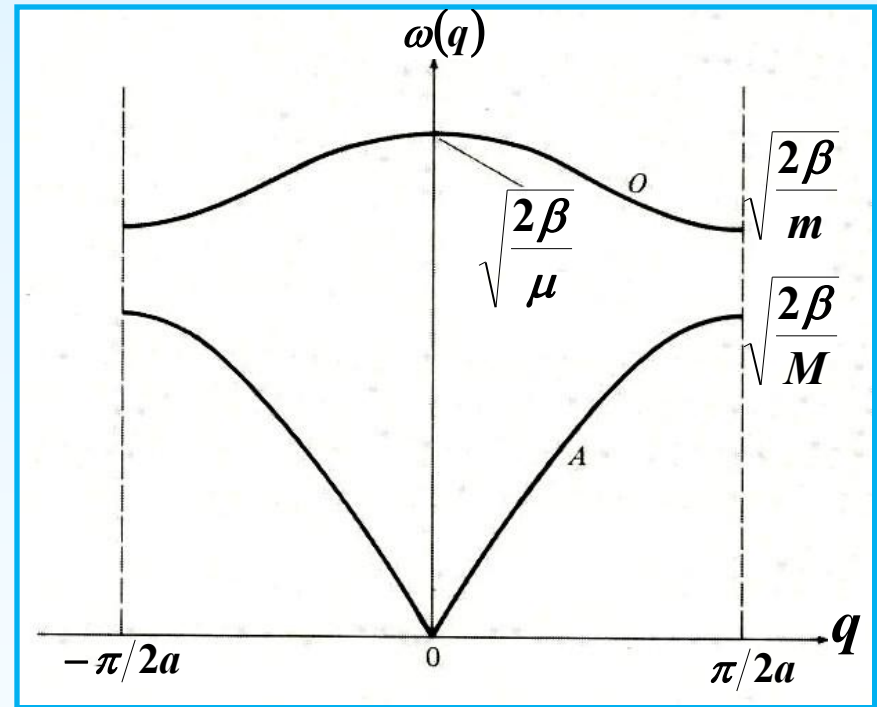
ω_- low frequency—acoustic

ω_+ high frequency—optic

- ✓ There exist a **gap** between the top of acoustic branch and the bottom of optic branch.

➤ A forbidden region.

- ✓ The gap depends on β , the difference between m and M .



➤ long wavelength limit ($q \rightarrow 0$)

acoustic branch:

$$\begin{aligned}\omega_-^2 &= \frac{\beta}{mM} \left\{ (m + M) - \left[(m + M)^2 - 2mM(1 - \cos(2qa)) \right]^{\frac{1}{2}} \right\} \\ &= \frac{\beta}{mM} (m + M) \left\{ 1 - \left[1 - \frac{4mM}{(m + M)^2} \sin^2(qa) \right]^{\frac{1}{2}} \right\}\end{aligned}$$

when $\frac{4mM}{(m + M)^2} \sin^2(qa) \ll 1$

utilize $X \ll 1 \quad (1 - X)^{1/2} = 1 - \frac{1}{2}X \quad \Rightarrow$

$$\omega_- = \sqrt{\frac{2\beta}{m + M}} |\sin(qa)| = \sqrt{\frac{2\beta}{m + M}} a |q|$$

Same as simple atomic chain, linear dispersion relation in the LWA, $\omega_- \rightarrow 0$, if $q \rightarrow 0$, $\omega_- \rightarrow 0$

optic branch:

$$\omega_+^2 = \frac{\beta}{mM} \left\{ (m + M) + \left[(m + M)^2 - 2mM(1 - \cos(2qa)) \right]^{\frac{1}{2}} \right\}$$

$$= \frac{\beta}{mM} (m + M) \left\{ 1 + \left[1 - \frac{4mM}{(m + M)^2} \sin^2(qa) \right]^{\frac{1}{2}} \right\}$$

in $\frac{4mM}{(m + M)^2} \sin^2(qa) \ll 1$ approx.

$$\omega_+^2 = \frac{2\beta}{mM} (m + M) \left\{ 1 - \frac{mM}{(m + M)^2} \sin^2(qa) \right\}$$

if $q \rightarrow 0$, $(\omega_+)_{\max} = \sqrt{\frac{2\beta}{\mu}}$ $\mu = \frac{mM}{m+M}$

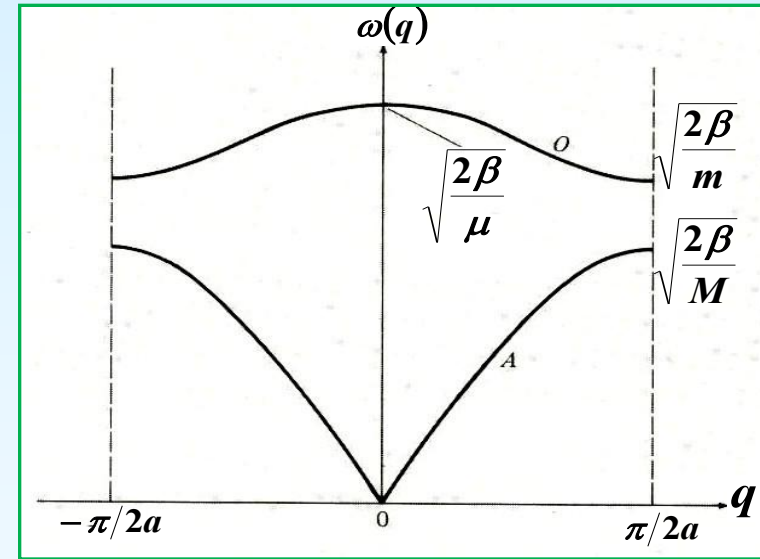
	acoustic branch	optical branch
$q = \pm \frac{\pi}{2a}$	$(\omega_-)_{\max} = \sqrt{\frac{2\beta}{M}}$	$(\omega_+)_{\min} = \sqrt{\frac{2\beta}{m}}$
$q \rightarrow 0$	$(\omega_-)_{\min} = 0$	$(\omega_+)_{\max} = \sqrt{\frac{2\beta}{\mu}}$

(2) vibration amplitude

$$\frac{A}{B} = \frac{2\beta \cos qa}{2\beta - m\omega^2} = \frac{2\beta - M\omega^2}{2\beta \cos(qa)}$$

acoustic branch:

$$\left(\frac{A}{B}\right)_- = \frac{2\beta - M\omega_-^2}{2\beta \cos(qa)} \quad \omega_-^2 \leq \frac{2\beta}{M}$$



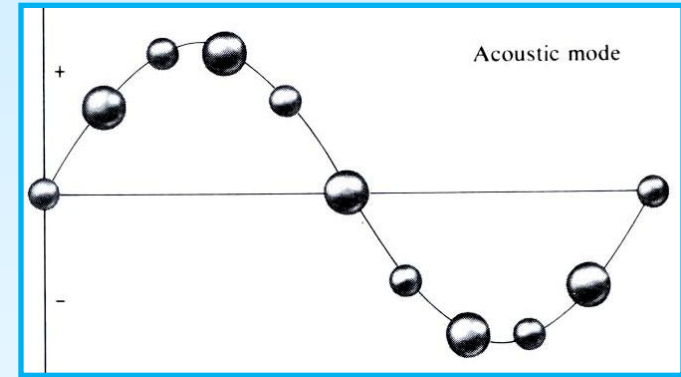
1st Brillouin zone: $\cos(qa) \geq 0$

$$\left(\frac{A}{B}\right)_- \geq 0$$

two N.N. atoms have *displacements*
always in *the same direction*

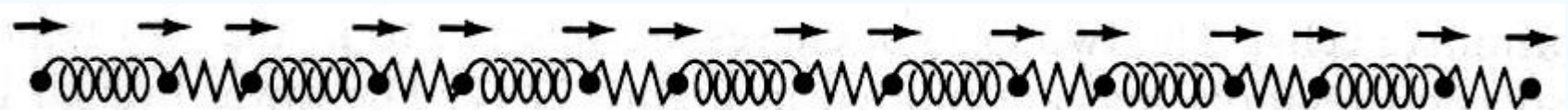
Longwave length approx.

$$q \rightarrow 0, \left(\frac{A}{B} \right)_- \approx 1$$



Two atoms in the same primitive cell have the same amplitude & phase, i.e., their motions are exactly the same.

—— **long wavelength acoustic wave** represents the vibration of mass center.

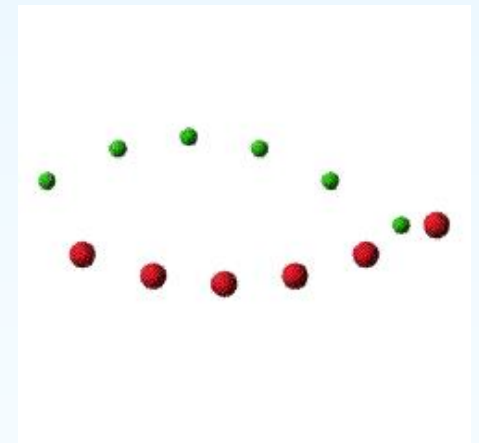
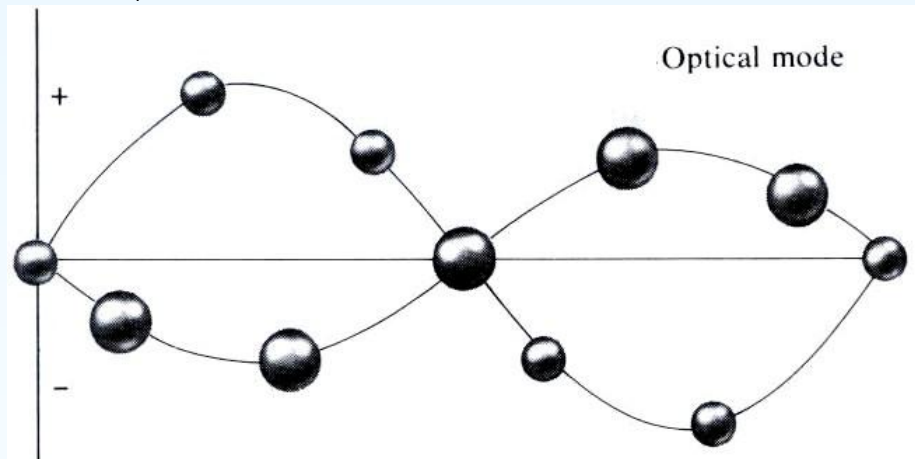


Optical Branch:

$$\left(\frac{A}{B}\right)_+ = \frac{2\beta \cos qa}{2\beta - m\omega_+^2} \quad \omega_+^2 \geq \frac{2\beta}{m}$$

1st B.Z.: $\cos(qa) > 0$

$\left(\frac{A}{B}\right)_+ < 0$ N.N. atoms vibrate in *opposite* directions

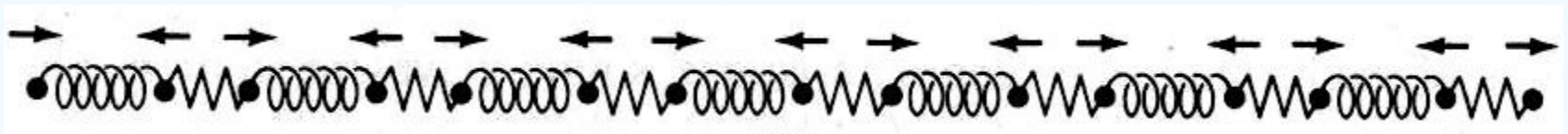


long wavelength limit

$$q \rightarrow 0, \quad \left(\frac{A}{B} \right)_+ \approx -\frac{M}{m}$$

$$mA + MB = 0$$

- ✓ The center of mass (in the primitive cell) is stationary, two atoms move in opposite direction (*relative to the center of mass*).



5. Periodic Boundary Condition

q values are within the 1st B.Z. $-\frac{\pi}{2a} < q \leq \frac{\pi}{2a}$

N primitive cells, each contains *two different* atoms:

PBC: $u_1 = u_{2N+1}$

$$e^{i2Nqa} = 1 \quad \Rightarrow$$

$$2qNa = 2\pi l, \quad l\text{--integer}$$

$$q = \frac{l\pi}{Na} \quad -\frac{\pi}{2a} < q \leq \frac{\pi}{2a} \quad \Rightarrow \quad \boxed{-\frac{N}{2} < l \leq \frac{N}{2}}$$

l is an integer in $-N/2 \sim N/2$, N different values \rightarrow # of q values is also N (equals # of primitive cells).

For each q , there are **two** modes (acoustic & optical).

First B.Z., $2N$ independent modes.

Generally, N primitive cells, P atoms in each cell.

of q values = N (# of primitive cells)

of vibration **branches**: $\propto P$

of vibration **modes**: $\propto PN$

4.3 Normal coordinate, Phonon

I. normal mode and collective excitation

1D atomic chain: N primitive cells, N independent modes, consider only N.N. coupling, under the harmonic approx.

potential:
$$U = \frac{\beta}{2} \sum_n (u_{n+1} - u_n)^2$$

kinetic:
$$T = \frac{1}{2} M \sum_n \dot{u}_n^2$$

Total energy of the system:

$$H = \frac{1}{2} M \sum_n \dot{u}_n^2 + \frac{\beta}{2} \sum_n (u_{n+1} - u_n)^2$$

$$H = \sum_{l=1}^N \frac{1}{2} \left(M\omega_l^2 \varphi_l^2 + \frac{\pi_l^2}{M} \right)$$

Hamiltonian becomes a sum of that of ***N harmonic oscillators***
new coordinate and momentum — **Normal Coordinate**.

- ✓ Summation over l contains N terms, each of which describes a linear Harmonic oscillator with frequency ω_l .
- ✓ ***We establish the equivalence*** between the ***vibration of N interacting atoms*** and ***N independent hamornicl oscillators***.

Quite general conclusion, also valid for 3D crystals.

II. Phonon

phonon: energy quanta in the crystal vibration.

According to the quantum theory, the energy of harmonic oscillator is quantized as

$$\varepsilon_l = \left(\frac{1}{2} + n_l \right) \hbar \omega_l$$

Total energy of crystal vibration: $\varepsilon = \sum_l \left(\frac{1}{2} + n_l \right) \hbar \omega_l$

Each vibration mode's energy takes $\hbar \omega_l$ as its unit, one adds integer times of $\hbar \omega_l$ to the system when exciting a lattice wave.

—— *energy* of the phonon

✓ Each lattice wave is a mode, corresponds to a kind of phonon.

excite from ground state to $\left(\frac{1}{2} + n_l\right)\hbar\omega_l$ excited state, one costs energy $n_l\hbar\omega_l$, and creat n_l **phonons** of frequency ω_l .

- Quasi particle:**
- energy: $\hbar\omega$
 - quasi momentum (**crystal momentum**): $\vec{p} = \hbar\vec{q}$
 - average number of q -state phonon:

$$\bar{n}(q) = \frac{1}{e^{\hbar\omega_q/k_B T} - 1}$$

——phonon is boson,
obey Bose-**Einstein** Stat.

Lattice wave scattered when propagating in the crystal→

phonon-phonon scattering;

Phonon number does no conserve, it can be *created* or *annihilated*.

4.4 Vibration of 3D lattices

I. three-dimensional simple lattice

One-dimension (1D):

$$\text{E.O.M.:} \quad m \frac{d^2 u_n}{dt^2} = \beta (u_{n+1} + u_{n-1} - 2u_n)$$

$$\text{Solution:} \quad u_n = A e^{i(qx_n - \omega t)} = A e^{i(qna - \omega t)}$$

3D: suppose the motion of each atom follows the form below,

$$\vec{u}_n = \vec{A} e^{i(\vec{q} \cdot \vec{R}_n - \omega t)}$$

\vec{q} indicates the direction where the wave propagates;

\vec{A} offers the vibration amplitude and its direction (polarization)

$\vec{A} // \vec{q}$: longitudinal; $\vec{A} \perp \vec{q}$: transverse

substitute $\vec{u}_n = \vec{A} e^{i(\vec{q} \cdot \vec{R}_n - \omega t)}$ into the E.O.M., and get 3 associated equations on \vec{A} (with components A_x, A_y, A_z).

equivalent to a 3×3 matrix equations

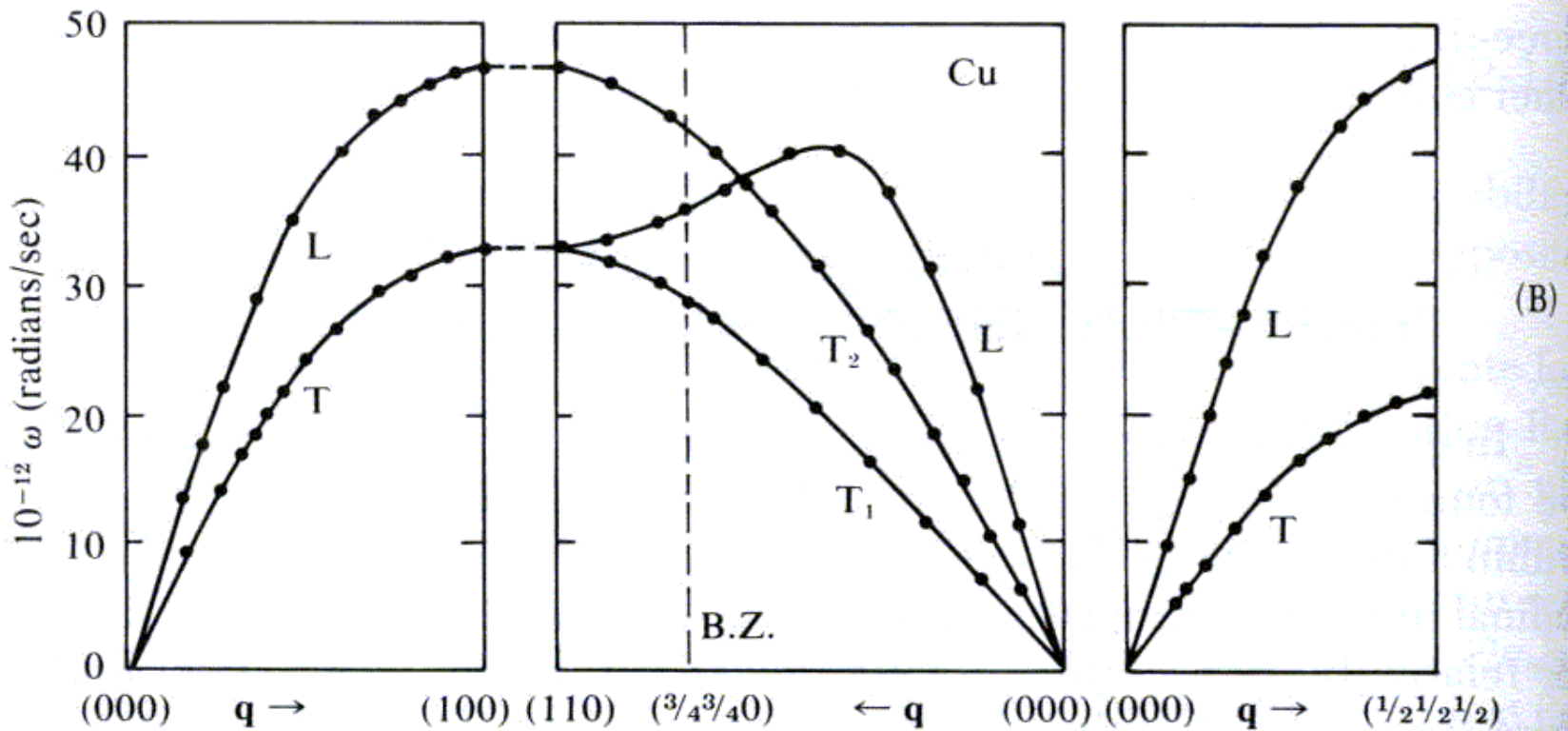
get a 3×3 determinant

is a **3rd** order equation of ω^2 , which leads to **three** solutions, i.e., 3 branches of dispersion relations.

All of these 3 dispersion relation curves pass through the origin, i.e., they are all **acoustic waves**!

Note:

- ✓ For 3D case, the dispersion is not necessarily isotropic in all directions, therefore, 2D plot can only show $\omega - q$ relation on *some specific directions*.
- ✓ To reveal the complete info. of the phonon dispersion relation, one has to adopt a **contour-like plot** for all \vec{q} points.



The phonon dispersion spectra for two metals which crystallize in the F.C.C. structure. Part (A) shows data for lead, and part (B) for copper. Angular frequency ω is plotted against the dimensionless vector $q = (\mathbf{ka}/\pi)$ measured from the center of the Brillouin zone in three principal directions. For the $[110]$ direction, the curves are extended through the Brillouin zone (B.Z.) boundary. Data for lead from Brockhouse et al., Phys. Rev. **128**, 1099 (1962). Data for copper from Svensson et al., Phys. Rev. **155**, 619 (1967), and from G. Nilsson and S. Rolandson, Phys. Rev. **B.7**, 2393 (1973). Data for both materials were obtained by inelastic scattering of monochromatic neutron beams.

II. 3D compound lattice

Consider P different atoms in a primitive cell, *each atom* corresponds to a E.O.M., therefore it contains P equations in a primitive cell:

equiv. to $3P$ *scalar* equations 

$3P \times 3P$ matrix equation

is $3P$ -rank equation of ω^2 having $3P$ roots, leading to $3P$ dispersion relations:

✓ 3 *acoustic* branches, and rest $3P - 3$ *optical* branches.

III. first Brillouin zone

\vec{q} and $\vec{q} + \vec{G}_h$ describe exactly the same vibration states, so by using all \vec{q} values within a primitive cell in reciprocal lattice, one is capable to describe all possible lattice waves.

Select a symmetric region centered at $\vec{q} = 0$, with the size of a primitive reciprocal cell — 1st Brillouin zone:

$$-\frac{b_i}{2} < q_i \leq \frac{b_i}{2}$$

IV. periodic boundary condition

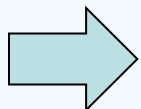
Lattice with N primitive cells, the numbers of cells along $\vec{a}_1, \vec{a}_2, \vec{a}_3$ are

$$N_1, N_2, N_3 \quad N = N_1 \cdot N_2 \cdot N_3$$

Under periodic boundary condition:

$$e^{iN_i q_i a} = 1$$

$$N_i q_i a = 2\pi l_i \quad l_i \text{ ——integer}$$


$$q_i = \frac{l_i 2\pi}{N_i a_i}$$

4.4 Vibration of 3D lattices

$$-\frac{b_i}{2} < q_i \leq \frac{b_i}{2}$$

$$-\frac{1}{2} \frac{2\pi}{a_i} < \frac{l_i 2\pi}{N_i a_i} \leq \frac{1}{2} \frac{2\pi}{a_i}$$

$$-\frac{N_i}{2} < l_i \leq \frac{N_i}{2}$$

l_i can choose N_i values, so does q_i .

Total number of \vec{q} values $N = N_1 \cdot N_2 \cdot N_3$, equals # of primitive cells in the crystal.

- ✓ A primitive cell contains P different atoms, thus there are $3P$ different vibration branches, of which 3 are acoustic branches;
- ✓ In a crystal containing N primitive cells, there are $3PN$ modes in total, of which there are $3N$ acoustic, and $3N(P-1)$ optical modes.