Phonon I: lattice waves

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(February 18, 2019)

Abstract

A lecture note on the lattice waves in the solid is presented. In a crystal each atom are coupled with the neighboring atoms by spring constants. The collective motion of atoms leads to a well-defined traveling wave over the whole system, leading to the collective motion, so called phonon. Here the equation of motion of atoms around thermal equilibrium position will be discussed in terms of several methods, which include numerical calculation on the eigenvalue problem (based on the Mathematica) and the translation operators in the quantum mechanics. We show that all these methods lead to the same conclusion, the existence of lattice wave, phonon in the quantum mechanics. For students who just start to study the solid state physics, it may be difficult to understand the validity of the assumption that the deviation of the displacement of the atoms from the thermal equilibrium is well described by a traveling wave. We numerically solve the eigenvalue-problem of the motion of atoms in the linear chain (typically 50 - 100 atoms) using Mathematica. We will give a bit of evidence for the existence of the normal modes propagating along the linear chain.

Content

1. Introduction

Phonons are a quantum mechanical version of a special type of vibrational motion, known as normal modes in classical mechanics, in which each part of a lattice oscillates with the same frequency. These normal modes are important because, according to a well-known result in classical mechanics, any arbitrary vibrational motion of a lattice can be considered as a superposition of normal modes with various frequencies; in this sense, the normal modes are the *elementary* vibrations of the lattice. Although normal modes are wave-like phenomena in classical mechanics, they acquire certain particle-like properties when the lattice is analyzed using quantum mechanics (see wave-particle duality.) They are then known as *phonons*.

There have been many excellent textbooks on the physics of lattice waves. Typical books[1-14] which we read during the preparation of writing this lecture note, are presented in References. These books are very useful for our understanding physics.

2 Lattice waves

2.1 Overview

Consider the elastic vibrations of a crystal with one atom in the primitive cell. We want to find the frequency of an elastic wave in terms of the wavevector $\boldsymbol{k}$ and the elastic constants. When a wave propagates along the x-direction, entire planes of atoms move in phase with displacements either parallel or perpendicular to the direction of $\boldsymbol{k}$.

We can describe with a single co-ordinate u_s the displacement of the plane s from its equilibrium position.

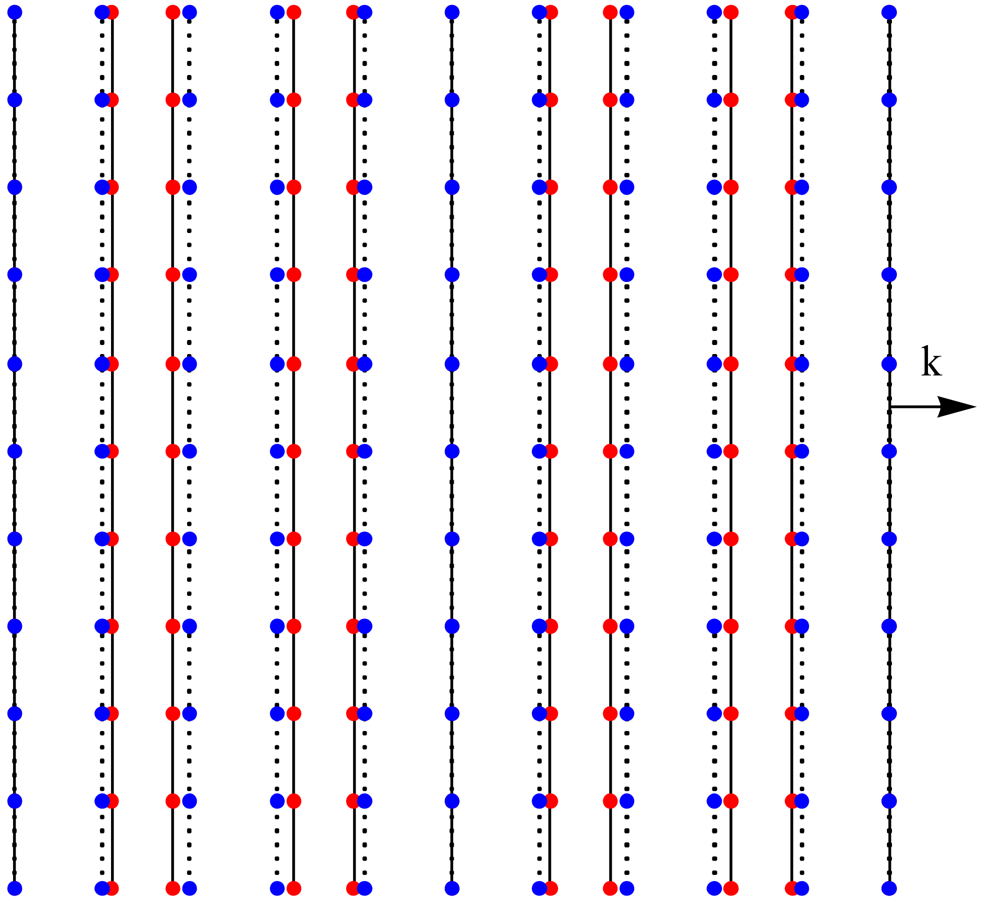


Fig.1 (a)

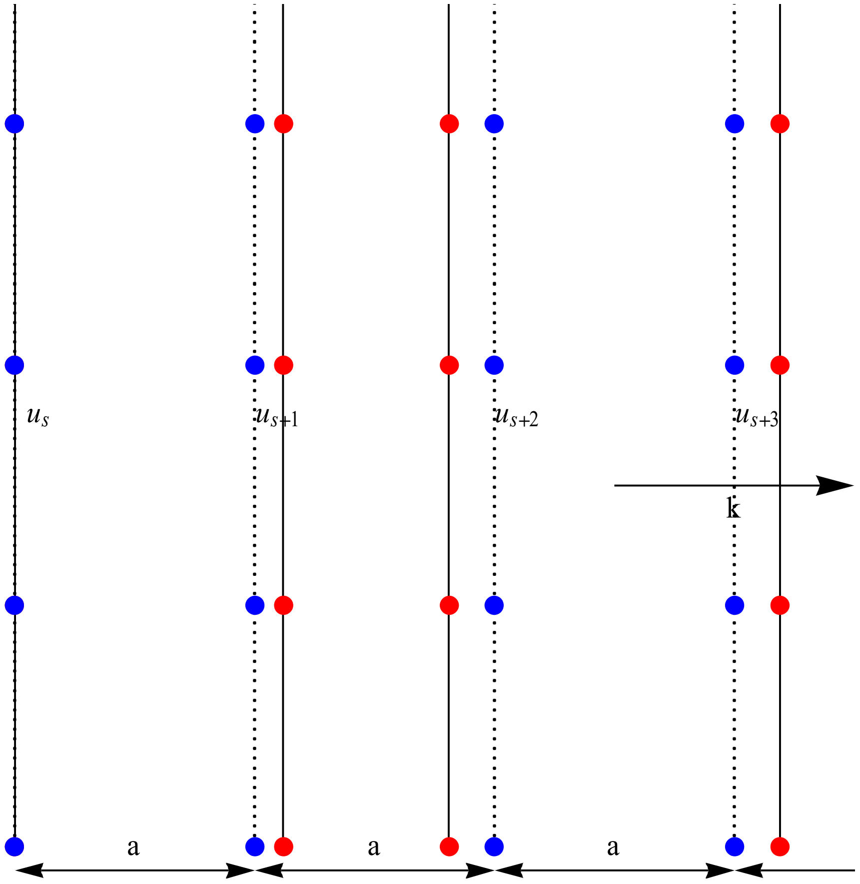


Fig.1 (b)

Fig.1(a) and (b)

Planes of atoms in thermal equilibrium (blue atoms). *a* is the nearest neighbor separation distance between planes. Planes of atoms when displaced as for a longitudinal wave (red atoms). The direction of the oscillation is parallel to that of the propagating waves. ***k*** is the wavevector. The coordinate u_s measures the displacement of the planes. Longitudinal wave. $k = n\ (2\pi/Na)$. $N = 10$. $a = 1$. $n = 4$. N is the total number of planes.

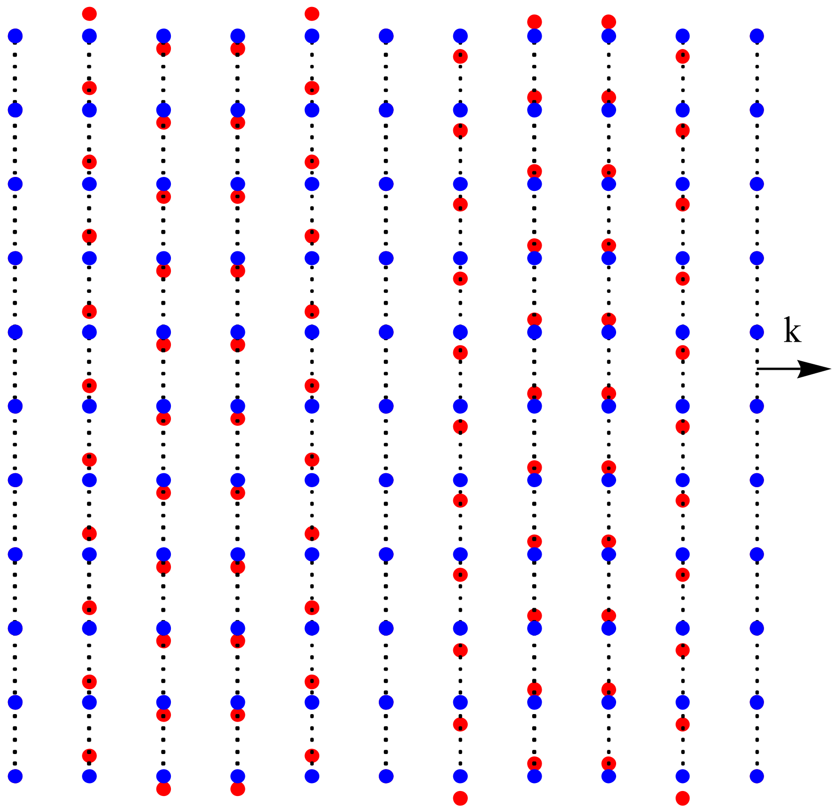


Fig.1 (c)

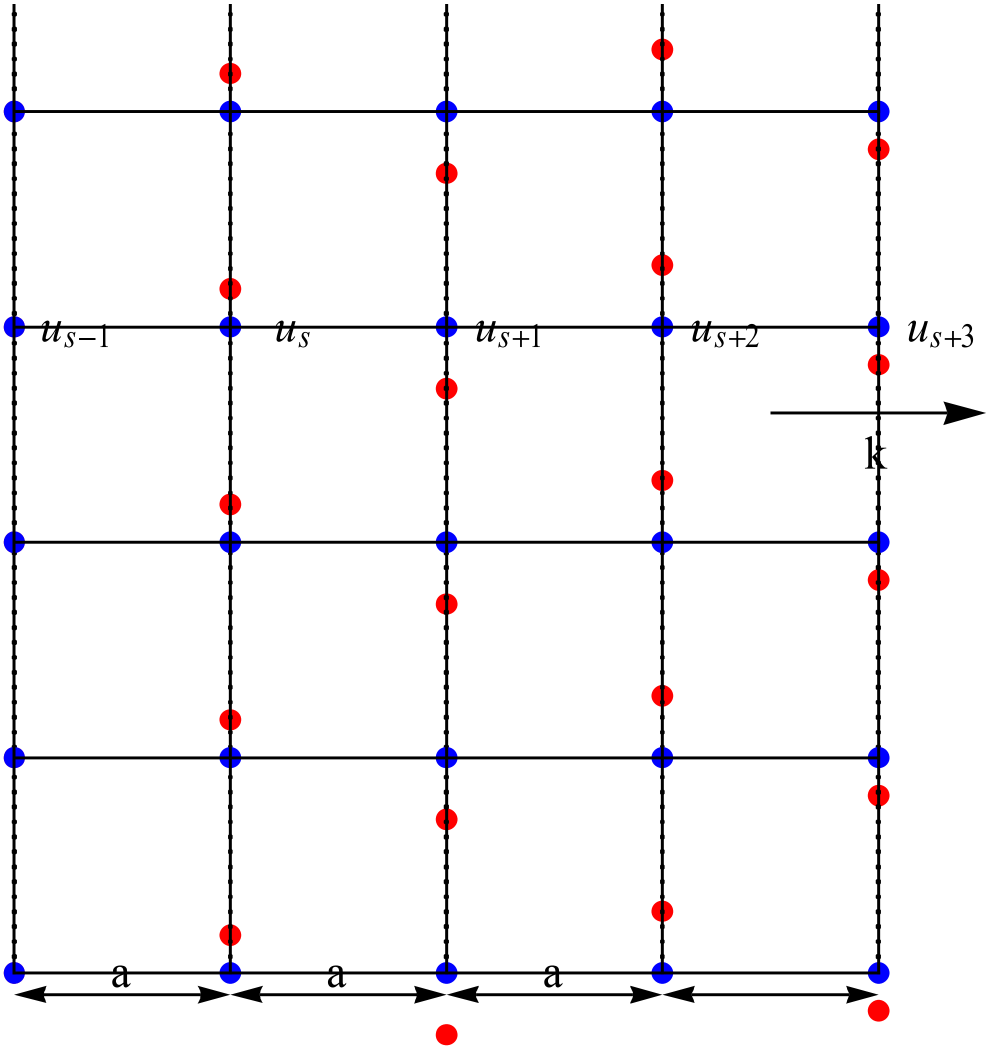


Fig.1 (d)

Fig.1(c) and (d)

Plane of atoms as displaced during passage of transverse wave (red atoms). Atoms in thermal equilibrium (blue atoms). The direction of the oscillation is perpendicular to that of the propagating waves. $k = n\ (2\pi/Na)$. $N = 10$. $a = 1$. $n = 4$.

For each wavevector there are three modes; one of longitudinal polarization, two of transverse polarization. We assume that the elastic response of the crystal is a linear function of the forces. Or the elastic energy is a quadratic function of the relative displacement of any two points in the crystal. The forces on the plane s caused by the displacement of the plane $s+p$ is proportional to the difference u_{s+p} - u_s of their displacements.

For brevity, we consider only nearest-neighbor interactions, so that $p = \pm 1$. The total force on s comes from planes $s \pm 1$.

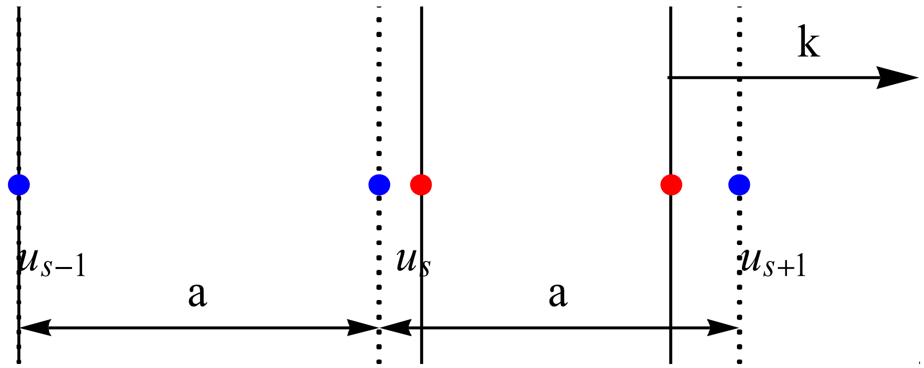


Fig.2 (a) Longitidinal wave.

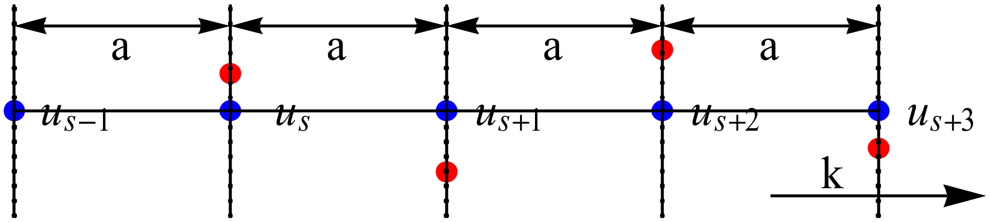


Fig.2 (b) Transverse wave.

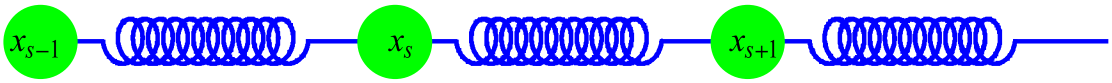
Fig.2(a) and (b)

The displacements of atoms with mass M are denoted by u_{s-1}, u_s, and u_{s+1}. The repeat distance is a in the direction of the wavevector $\boldsymbol{k}$. The direction of u_s is parallel to the direction of the wavevector $\boldsymbol{k}$ for the longitudinal wave (a) and is perpendicular to the direction of the wavevector $\boldsymbol{k}$ for the transverse wave (b).

2.2 One dimensional case: longitudinal mode

We start our discussion with the Lagrangian for the displacement of the s-th plane, given by

$$\begin{aligned} L_s &= T_s - V_s \\ &= \frac{1}{2}M\dot{u}_s{}^2 - \frac{1}{2}C[(x_{s+1} - x_s - a)^2 + (x_s - x_{s-1} - a)^2] \\ &= \tfrac{1}{2}M\dot{u}_s{}^2 - \tfrac{1}{2}C[(u_{s+1} - u_s)^2 + (u_s - u_{s-1})^2] \qquad (2.1) \end{aligned}$$



where x_s is the position of the atom at the s-th site and a is assumed to be the length of the un-stretched spring.

$$x_s = u_s + sa$$

where a is the distance between the adjacent atoms in thermal equilibrium. The Lagrange's equation for this system is derived as

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{u}_s}\right) = \frac{\partial L}{\partial u_s}, \tag{2.2}$$

or

$$\begin{aligned} M\ddot{u}_s &= -\frac{1}{2}C[2(u_{s+1} - u_s)(-1) + 2(u_s - u_{s-1})] \\ &= -C(-u_{s+1} + u_s + u_s - u_{s-1}) \\ &= C(u_{s+1} - 2u_s + u_{s-1}) \\ &= F_s \end{aligned} \tag{2.3}$$

where

$$F_s = C(u_{s+1} - 2u_s + u_{s-1})$$

is the effective force on the s-th plane (Hooke's law), C is the force constant between nearest-neighbor planes, $C_L \neq C_T$ (C_L: force constant for longitudinal wave, C_T: force constant for transverse wave). 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 the plane s is

$$M\frac{d^2u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1}), \tag{2.4}$$

where M is the mass of an atom in the s-th plane. Suppose that this equation has the traveling wave solutions of the form

$$u_s = ue^{i(ksa-\omega t)}. \tag{2.5}$$

Note that the validity of this assumption will be verified by solving directly the eigenvalue problem (see Sec. 2.5). The boundary condition is illustrated below.

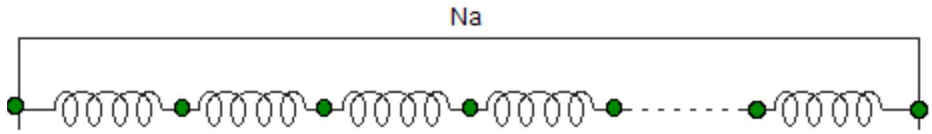


Fig.3 One-dimensional array of equal masses and springs. This is the simplest model of a vibrational band.

Alternative representation of the Born-von Karman boundary condition. The object connecting the ion on the extreme left with the spring on the extreme right is a massless rigid rod of length $L = Na$.

$$\Downarrow$$

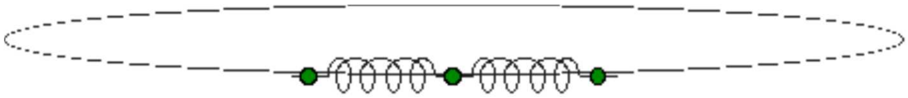


Fig.4 The Born-von Karman periodic boundary condition for the linear chain.

2.3 Born-von Karman boundary condition

The Born-von Karman or periodic boundary condition;

$$u_s = u_{s+N}, \tag{2.6}$$

$$u_s = e^{i(ksa-\omega t)}. \tag{2.7}$$

The periodic boundary condition requires that

$$e^{ikNa} = 1, \qquad \text{or} \qquad k = \frac{2\pi}{a}\frac{\ell}{N}, \tag{2.8}$$

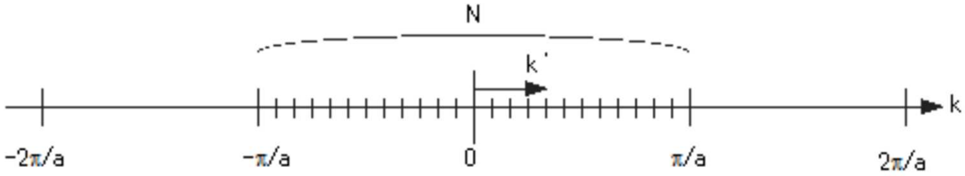


Fig.5 N modes for $-\pi/a \le k \le \pi/a$

where

$$\lambda = -\frac{N}{2}, -\frac{N}{2}+1, \ldots, \frac{N}{2}-1,\ \frac{N}{2} \tag{2.8}$$

((**Note**))

(a) 1D system.

For each k, there are only one longitudinal mode. Then we have

1xN modes = N modes

(b) 2D system.

For each $\boldsymbol{k}$, there are one longitudinal mode and one transverse mode. Then we have

2xN modes = 2N modes

(c) 3D system:

For each $\boldsymbol{k}$, there are one longitudinal mode and two transverse modes. Then we have

(1+2)N modes = 3N modes

$\Updownarrow$

N atoms: each atom has 3 freedoms 3N

$$u_s = e^{i(ksa-\omega t)},$$

$$k' = k + \frac{2\pi}{a}n \qquad (n\text{: integer}). \qquad (2.9)$$

The displacement of the n-th atom for the wave k'

$$u_s = e^{i(k'sa-\omega t)} = e^{i[(k - \frac{2\pi}{a}n)sa-\omega t]} = e^{i(ksa-\omega t)}. \qquad (2.10)$$

So the displacement u_s is the same as for the wavevector k, for any atom whatsoever. Thus the wave k' cannot be physically differentiated from the wave k.

2.4 First Brillouin zone

What range of k is physically significant for elastic waves?

$\Rightarrow$ Only those in the first Brillouin.

$$\frac{u_{s+1}}{u_s} = e^{ika}. \qquad (2.11)$$

The range $-\pi$ to π for the phase ka covers all independent values of the exponential.

$$-\pi \le ka \le \pi \qquad \text{or} \qquad -\frac{\pi}{a} \le k \le \frac{\pi}{a}. \qquad (2.12)$$

In the continuum limit (a = 0),

$$k_{\max} = \frac{\pi}{a} \to \infty. \qquad (2.13)$$

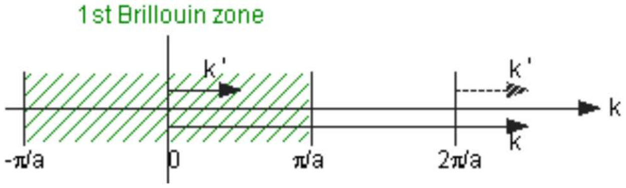


Fig.6 The relation between *k*’ and *k* = *k*’+2*π*/*a*.

Suppose that

$$k' = k + \frac{2\pi}{a} n \qquad (n\text{: integer}) \tag{2.14}$$

Then

$$\frac{u_{s+1}}{u_s} = e^{ika} = e^{i(k' + \frac{2\pi}{a} n)a} = e^{ik'a}. \tag{2.15}$$

Thus the displacement can always be described by a wavevector within the first Brillouin zone. Note that $G = \frac{2\pi}{a} n$ is a reciprocal lattice vector. Thus by subtraction of an appropriate reciprocal lattice vector from ***k***, we always obtain an equivalent wavevector in the 1st zone: ***k*** = ***k'*** + ***G***, where ***k'*** is the wavevector in the first Brillouin zone.

2.5 Normal modes

We solve the equations of motion

$$M \frac{d^2 u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1}), \tag{2.16}$$

by assuming that

$$u_s = e^{i(ksa - \omega t)}. \tag{2.17}$$

Then we have

$$\frac{d^2 u_s}{dt^2} = -\omega^2 u_s, \tag{2.18}$$

$$u_{s\pm1} = e^{\pm ika} u_s, \tag{2.19}$$

$$-\omega^2 M u_s = C\left[e^{ika} + e^{-ika} - 2\right] u_s, \tag{2.20}$$

leading to the dispersion relation

$$\omega^2 = \frac{C}{M}(2-2\cos ka) = \frac{2C}{M}(1-\cos ka) = \frac{4C}{M}\sin^2(\frac{ka}{2}), \qquad (2.21)$$

or

$$\omega = \sqrt{\frac{4C}{M}}\,|\sin(\frac{ka}{2})|. \qquad (2.22)$$

It is usual for one to assume that ω is positive. Then the wave propagates along the positive x direction for $k>0$ and along the negative x direction for $k<0$.

The boundary of the first Brillouin zone lies at $k = \pm\frac{\pi}{a}$.

$$\frac{d\omega^2}{dk} = 2\omega\frac{d\omega}{dk} = \frac{2Ca}{M}\sin ka, \qquad (2.23)$$

$$\Rightarrow \frac{d\omega}{dk} = 0 \text{ at } k = \pm\frac{\pi}{a}. \qquad (2.24)$$

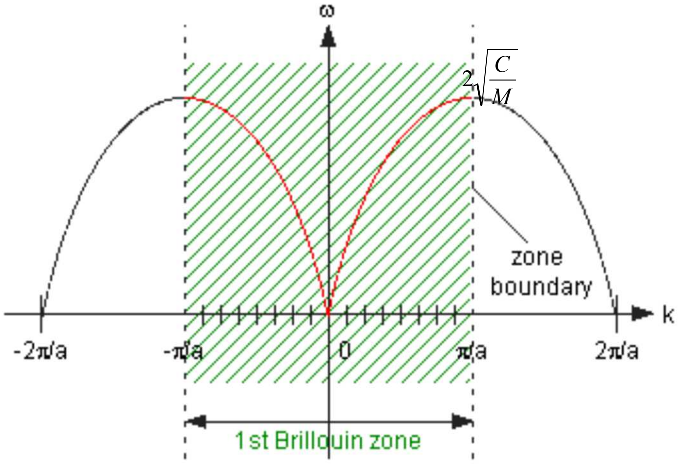


Fig.7 The dispersion curve (ω vs k) for a monatomic linear lattice with nearest neighbor interactions only. The first Brillouin zone is the segment between $-\pi/a$ and π/a. ω is linear for small k and that dω/dk vanishes at the zone boundaries ($k = \pm\pi/a$.

$$\omega^2 = \frac{4C}{M}\sin^2\left(\frac{ka}{2}\right) \quad \text{or} \quad \omega = \sqrt{\frac{4C}{M}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

(dispersion relation) (2.25)

((**Note**)) Discreteness of quantum states

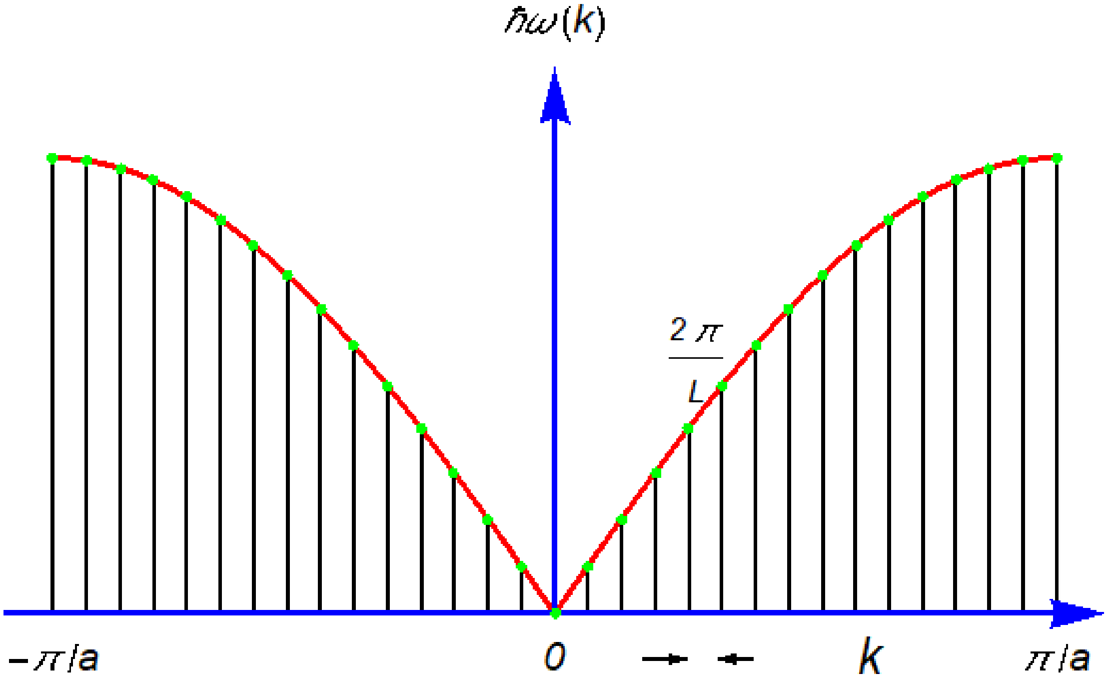


Fig.7(b) The energy dispersion of phonon. The discreteness of *k* (=*2π*/*L*) arises from the Born-Karman boundary condition. The state *k* is the same as the state *k*+*G*.

For $-\frac{\pi}{a} \le k \le \frac{\pi}{a}$, there are *N* discrete states (*k*) where the wave number is given by $k = \frac{2\pi}{L} n$. Note that $N = \frac{L}{a}$. We note that the state *k*+*G* is the same as the state *k*.

2.6 Continuum wave equation

We consider an original wave equation given by

$$M \frac{d^2 u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1}) . \qquad (2.26)$$

We assume that $u_s(x) = u(x, t)$. In the small limit of $a = \Delta x$, $sa = x$ and *s* is continuous variable. Under this assumption, *u*(*x*, *t*) can be expanded using a Taylor expansion,

$$u_{s+1}(t) = u(x + \Delta x, t) = u(x,t) + \frac{\Delta x}{1!} \frac{\partial u(x,t)}{\partial x} + \frac{(\Delta x)^2}{2!} \frac{\partial^2 u(x,t)}{\partial x^2} + O(\Delta x)^3 , \quad (2.27)$$

Then the original wave equation can be rewritten as

$$M\frac{\partial^2 u(x,t)}{\partial t^2} = C[u(x,t) + \frac{\Delta x}{1!}\frac{\partial u(x,t)}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 u(x,t)}{\partial x^2}$$
$$- 2u(x,t) + u(x,t) - \frac{\Delta x}{1!}\frac{\partial u(x,t)}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 u(x,t)}{\partial x^2}] \qquad (2.28)$$

or

$$M\frac{\partial^2 u(x,t)}{\partial t^2} = C(\Delta x)^2 \frac{\partial^2 u(x,t)}{\partial x^2}], \qquad \text{(wave equation)} \qquad (2.29)$$

or

$$\frac{\partial^2 u(x,t)}{\partial t^2} = \frac{C}{M}(\Delta x)^2 \frac{\partial^2 u(x,t)}{\partial x^2} = \frac{C}{M}a^2 \frac{\partial^2 u(x,t)}{\partial x^2} = v^2 \frac{\partial^2 u(x,t)}{\partial x^2}, \qquad (2.30)$$

which is the continuum elastic wave equation with the velocity of sound given by

$$v = \sqrt{\frac{C}{M}}a. \qquad (2.31)$$

((Note)) Units

[C]=N/m. [M]=N s^2/m. [a] = m. [v] = m/s

The solution of Eq.(2.30) is given by

$$u(x,t) = f(x - vt),$$

where *f* is an arbitrary function.

3. Eigenvalue-problem; solution using Mathematica

We solve the eigenvalue-problem given by

$$\omega^2 u_s = K(-u_{s+1} + 2u_s - u_{s-1}), \qquad (3.1)$$

where $s = 1, 2, \ldots, N$, $K = C/M$. These equations can be expressed using a matrix M (for example, N x N) and column matrix (1xN);

$$M\boldsymbol{U} = \omega^2\boldsymbol{U}. \qquad (3.2)$$

Here ω^2 is the eigenvalue. The number of eigenvalues is N. For example, the matrix M and the column matrix $\boldsymbol{U}$ for $N = 12$ (for example), are given by

$$M=\begin{pmatrix} 2K & -K & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -K & 2K & -K & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -K & 2K & -K & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -K & 2K & -K & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -K & 2K & -K & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -K & 2K & -K & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -K & 2K & -K & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -K & 2K & -K & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -K & 2K & -K & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -K & 2K & -K & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -K & 2K & -K \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -K & 2K \end{pmatrix}, \tag{3.3}$$

and

$$\boldsymbol{U}=\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \\ u_{10} \\ u_{11} \\ u_{12} \end{pmatrix}, \text{ for each eigenvalue.} \tag{3.4}$$

Using the Mathematica (program called Eigenvalues), we can calculate the dispersion relation of ω_k vs $k = (\pi/a)\ (n/N)$ with $N = 1, 2, 3,\ldots, N\text{-}1, N$. For simplicity, here we choose $N = 100$. For comparison we also make a plot of the solution given by $\omega = \sqrt{4C/M}\,|\sin(ka/2)|$. We find that there is a good agreement between these two curves. $K = C/M$.

((**Mathematica-1**))

Phonon dispersion relation for one atom in the unit cell.

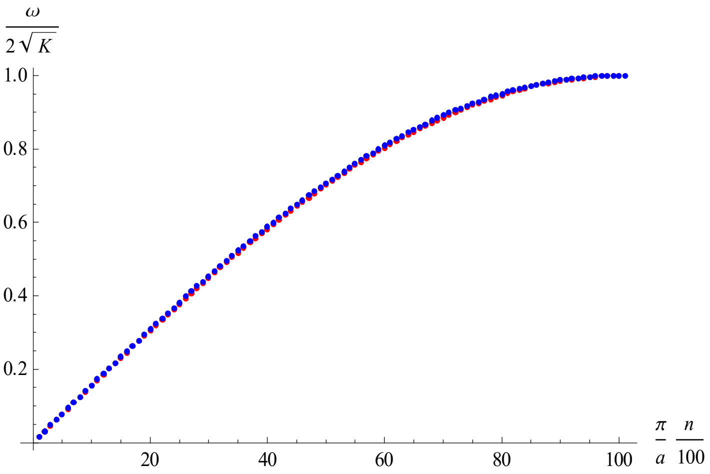


Fig.8 The dispersion relation with red (from Mathematica calculation) and blue ($\omega = \sqrt{4K}\sin(ka/2)$ with $K = C/M$). The x axis is $k = (\pi/a)(n/N)$ with $n = 1, 2, \ldots, N$ (= 100). The y axis is $\omega/(2\sqrt{K})$. The agreement between these two results are excellent.

((**Mathematica-2**))

Here we use the Mathematica program (Eigensystem) to obtain the eigenvalues and the corresponding eigenfunction ***U***. For each eigenvalue, we can calculate the deviation (u_s) of the position of the atom from the equilibrium position, as a function of the equilibrium position $x_s = s\,a$, where $s = 1, 2, 3, \ldots, N$. Here we consider the eigenvalue problem (N = 50). We show the plot of $\boldsymbol{U}_n = (u_1, u_2, u_3, \ldots, u_N)$ as a function of the location ($x_s = s\,a$), where $n = 1, 2, \ldots, N$. $\|\mathbf{u}\| = 1$. We find that the wavelength λ_n is given by $\lambda_n = 2Na/n$. The corresponding wavenumber q_n is equal to $k_n = (2\pi/\lambda_n) = (\pi/a)(n/N)$. The deviation u_s is well described by the form $\sin[\pi s(n/N)] = \sin[k_n(sa)]$ ($\approx e^{ik_n sa}$).

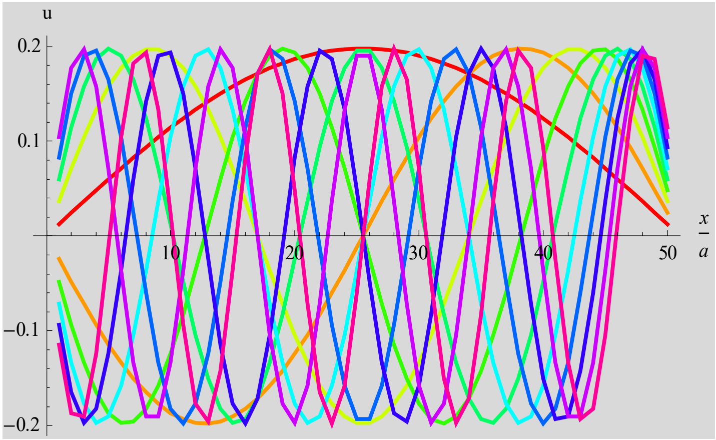
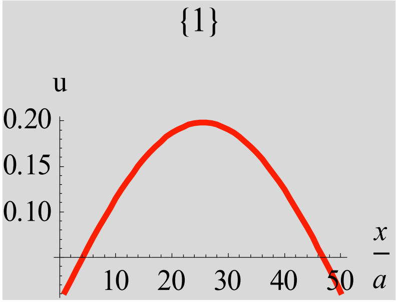


Fig.9 Plot of $\boldsymbol{u} = (u_1, u_2, u_3, \ldots, u_{50})$ as a function of $x_s = s\,a$ for the eigenvalues ω_i (i = 1, 2, 3, …, 10). $\omega_1 < \omega_2 < \ldots < \omega_{10}$. Note that $\boldsymbol{u}$ is normalized ($\|\mathbf{u}\| = 1$). $N = 50$.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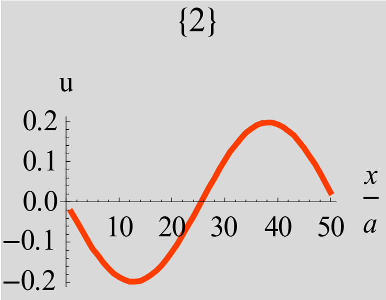
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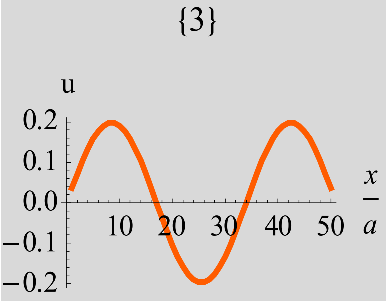
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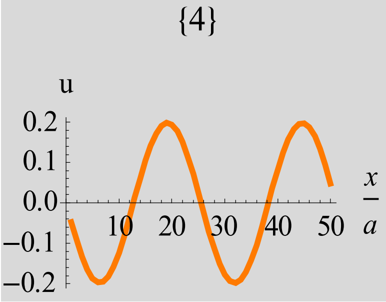
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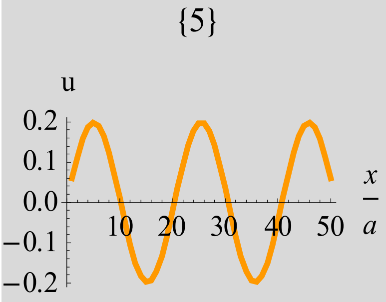
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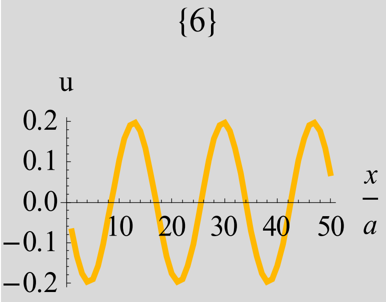
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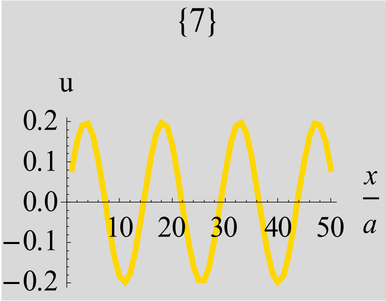
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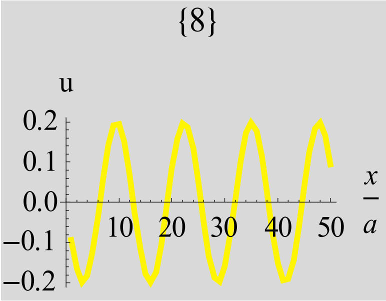
{8}
u
0.2
0.1
0.0
−0.1
−0.2
10
20
30
40
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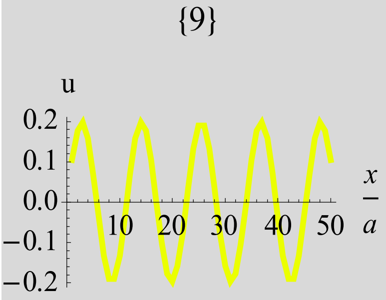
x/a


{9}
u
0.2
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x/a

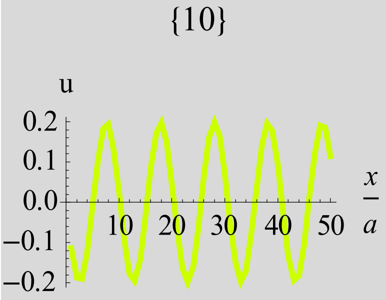

{10}
u
0.2
0.1
0.0
−0.1
−0.2
10
20
30
40
50
x/a

Fig.10 Plot of $u = (u_1, u_2, u_3, \ldots, u_{50})$ as a function of $x_s = s\, a$ for the eigenvalues ω_i (i = 1, 2, 3, …, 10). $\omega_1 < \omega_2 < \ldots < \omega_{10}$. The wavenumber $k_n = (\pi/Na)n$. The value of n is denoted in each figure.

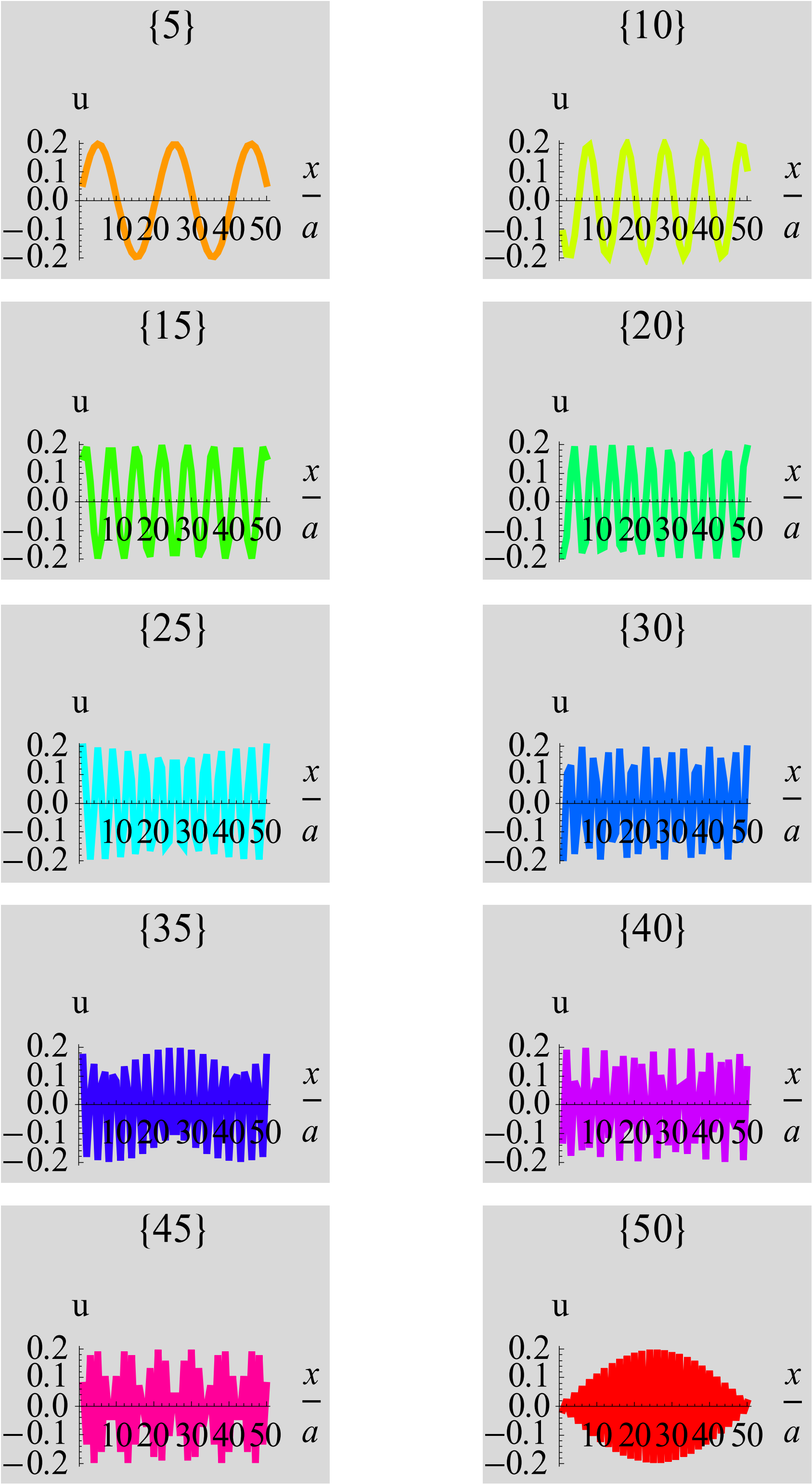


Fig.11 Plot of $u = (u_1, u_2, u_3, \ldots, u_{50})$ as a function of $x_s = s\,a$ for the eigenvalues ω_n (n = 5, 10, 15, 20, 25, 30, 35, 40, 45, 50). $\omega_5<\omega_{10}<\ldots<\omega_{50}$. $\|u\|=1$. N = 50. The wavenumber $k_n = (\pi/Na)n$. The value of n is denoted in each figure.

((**Note**))
The eigenvalue problems for several simple systems (chains of 2 atoms, 3 atoms, 4 atoms, and 5 atoms) is discussed in detail in my web site,

http://bingweb.binghamton.edu/~suzuki/pdffiles/Oscillation_and_Waves_Note.pdf

4. First Brillouin zone and group velocity

4.1 Definition of the group velocity

The transmission velocity of a wave pocket is the group velocity

$$\boldsymbol{v}_g = \frac{\partial\omega}{\partial\boldsymbol{k}} = \nabla_{\boldsymbol{k}}\omega(\boldsymbol{k}). \tag{4.1}$$

This is the velocity of energy propagation in the medium.

$$v_g = \frac{\partial\omega}{\partial k} = \sqrt{\frac{Ca^2}{M}}\cos\left(\frac{1}{2}ka\right), \tag{4.2}$$

$$v_g = 0 \text{ at } k = \frac{\pi}{a}$$

The wave is a standing wave: zero net transmission velocity for a standing wave. Note that the phase velocity is defined by $v_p = \omega/k$.

Long wavelength limit
When $ka \ll 1$,

$$1-\cos ka = 1-\left[1-\frac{1}{2!}(ka)^2\right] \cong \frac{1}{2}(ka)^2. \tag{4.3}$$

Then

$$\omega^2 = \frac{2C}{M}\frac{1}{2}k^2a^2 = \frac{C}{M}k^2a^2 \quad \text{or} \quad \omega = \sqrt{\frac{Ca^2}{M}}k, \tag{4.4}$$

$$v_g = \frac{\partial\omega}{\partial k} = \sqrt{\frac{C}{M}}a = v_0 \quad \text{at} \quad ka = 0. \tag{4.5}$$

The velocity of sound is independent of frequency in this limit. Thus $\omega = vk$, exactly as in the continuum theory of elastic waves --- in the continuum limit a = 0 and thus ka = 0.

4.2 The physical meaning of the first Brillouin zone

We discuss the physical meaning of the first Brillouin zone. To this end, we consider the case of u_s with

$$k = k_0 = \frac{\pi}{3a} \text{ and } k = k_0 + G = \frac{\pi}{3a} + \frac{2\pi}{a} = \frac{7\pi}{3a}.$$

(i) $k = k_0 = \dfrac{\pi}{3a}$.

At $t = 0$, we have $u_s = ue^{i(ksa-\omega t)}$ at $t = 0$. We make a plot of

$$\mathrm{Re}[u_s] = \mathrm{Re}[e^{i(\frac{\pi}{3}s-\omega t)}] = \cos\left(\frac{\pi}{3}s\right),$$

as a function of s, where $s = 0, 1, 2, 3, \ldots$, where $u = 1$ in Fig.17.

(ii) $k = k_0 + G = \dfrac{\pi}{3a} + \dfrac{2\pi}{a} = \dfrac{7}{3a}\pi$

We also make a plot of $\mathrm{Re}[u_s] = \mathrm{Re}[e^{i\left(\frac{7\pi}{3}s\right)}] = \cos\left(\frac{7\pi}{3}s\right)$ at $t = 0$ in Fig.17.

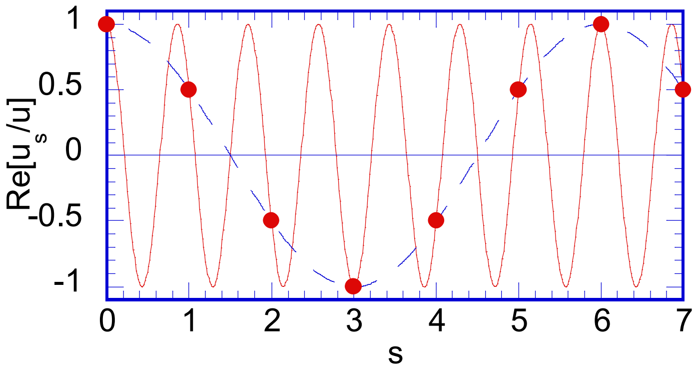


Fig.12(a) Plot of $\mathrm{Re}[e^{i(ksa-\omega t)}]$ at $t = 0$ for k = $k_0 + G = 7\pi/3$ (the red solid line) and $k = k_0 = \pi/3a$ (the dotted blue line).

As shown in Fig.12, the wave represents by the solid curve ($k = 7\pi/3a$) conveys no information not give by the dashed curve ($k = \pi/3a$). Because the wave displacement is defined only at lattice points, the propagation of a large wavenumber ($k_0 + G$) lying outside the first Brillouin zone is identical to a short wavenumber k_0 lying inside the first Brillouin zone. In a continuum, the amplitudes would have a value everywhere, as represented by the continuous lines, so that both wavenumbers would be distinguishable.

((**Example**))

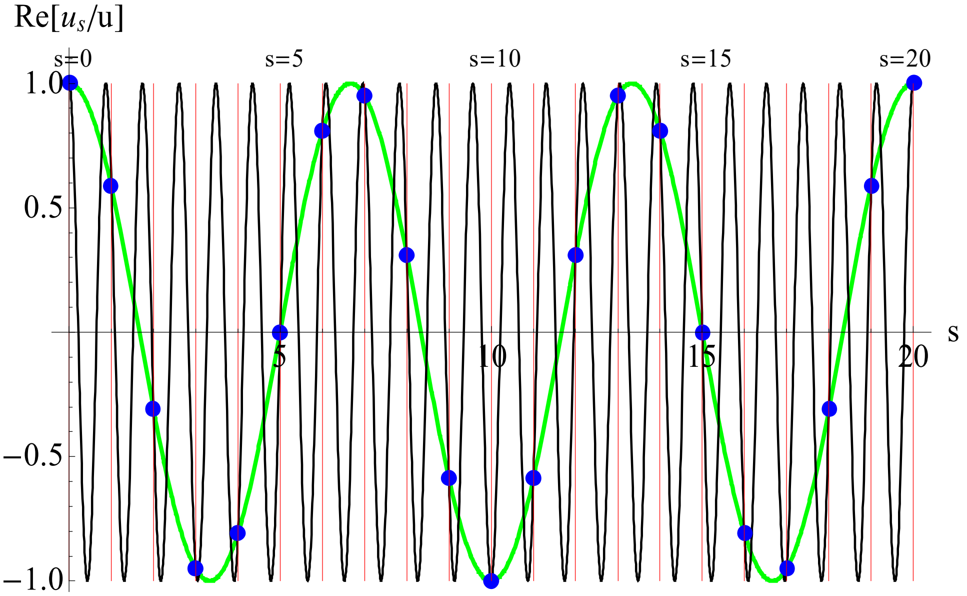


Fig.12(b) Identity of long and short waves on a lattice. $N = 20$. $a = 1$. $k = 3\pi/(10a)$. $G = 2\pi/a$. $k' = k + G = 23\pi/(10a)$. Re[$u_s/u(0)$] for $k = 3\pi/(10a)$ (green line). Re[$u_s/u(0)$] for $k = 23\pi/(10a)$ (black line). These two lines intersect each other at the integers s (s = 1, ,2, 3,......., 20).

4.3 Standing wave

At the zone boundary $k = \pm\pi/a$, the group velocity is equal to zero, implying that no energy is propagated. The amplitude Re[u_s] at time t is described

$$\mathrm{Re}[u_s] = \mathrm{Re}\left[ue^{i(ksa-\omega t)}\right] = \mathrm{Re}\left[u(-1)^s e^{-i\omega t}\right] = u(-1)^s \cos\omega t \qquad (4.1)$$

The alternate atoms oscillate in opposite phases, because $(-1)^s = -1$ for odd integers s and $(-1)^s = 1$ for even integers s. Note that the wave is a standing wave. A standing wave is an example of wave motion with zero group velocity. The wave moves neither to the right nor to the left. This situation is equivalent to Bragg reflections of x-ray.

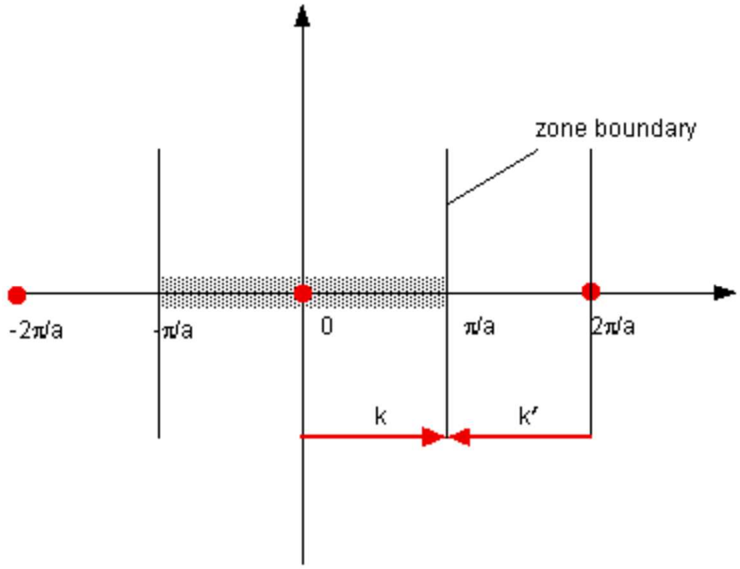


Fig.13 The condition for the Bragg reflection in the reciprocal lattice. $k - k' = 2\pi / a$ (or $k = \pi / a$ and $k' = -\pi / a$)

The Bragg reflection arises when $k = \pm \pi / a$. Even if we excite only the state $k = \pi/a$. we should obtain $k = -\pi/a$ through the Bragg reflection. The superposition of these two wave leads to a standing wave,

$$\begin{aligned} \frac{1}{\sqrt{2}}\left[e^{i(ksa-\omega t)} \pm e^{i(k'sa-\omega t)}\right] &= \frac{1}{\sqrt{2}} e^{-i\omega t}\left[e^{is\pi} \pm e^{-is\pi}\right] \\ &= \frac{1}{\sqrt{2}} e^{-i\omega t}\begin{Bmatrix} 2\cos s\pi \\ 2i\sin s\pi \end{Bmatrix} = \sqrt{2} e^{-i\omega t}\begin{Bmatrix} \cos s\pi \\ i\sin s\pi \end{Bmatrix} \end{aligned} \tag{4.6}$$

This implies that the wave cannot propagate in a lattice, but through successive reflections back and forth, a standing wave is set up.

4.4 General property of the group velocity

There are two main features of the phonon dispersion relation;

(i) $E = \hbar\omega_k$ is an even function of k; $\hbar\omega_{-k} = \hbar\omega_k$ or $E_{-k} = E_k$, where $\hbar$ is the Dirac's constant ($\hbar = h/2\pi$) and h is the Planck's constant. This is related to the fact that the equations of motion are invariant with respect to the time reversal.

(ii) Periodicity in $E_{k+G} = E_k$ with G [= $(2\pi/a)$ times integer] is the reciprocal lattice.

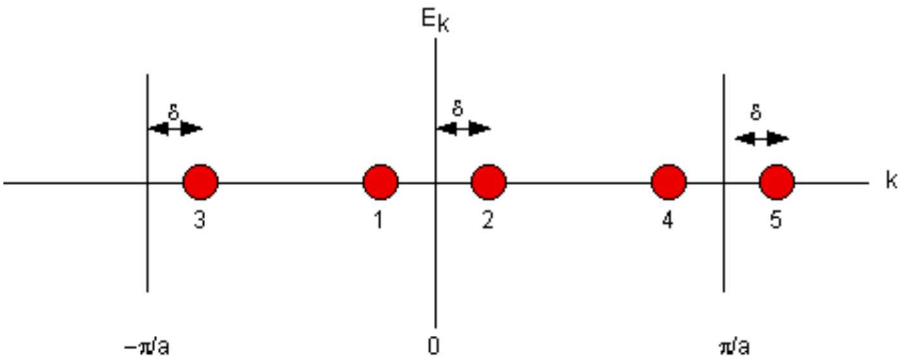


Fig.14 Values of k in the first Brillouin zone related by the symmetrical relation ($E_{k+G} = E_k$ and $E_{-k} = E_k$). $k = \pm\pi/a$ is the boundary of the first Brillouin zone ($|k| \leq \pi/a$).

We now consider the value of the group velocity at the Brillouin zone boundary. From the condition, $E_k = E_{-k}$, we have $E(3) = E(4)$. From the condition, $E_k = E_{k+G}$, we have $E(3) = E(5)$. Therefore, we have $E(4) = E(5)$. On taking $\delta \rightarrow 0$, the group velocity at the boundary of Brillouin zone is defined as $[E(5) - E(4)]/2\delta$, which reduces to zero ($dE_k/dk \rightarrow 0$).

((**Note**))

It follows that from the condition ($E_k = E_{-k}$), we have $E(1) = E(2)$. On taking $\delta \rightarrow 0$, the group velocity defined by $[E(2) - E(1)]/2\delta$ reduces to zero ($dE_k/dk \rightarrow 0$). On applying the periodicity condition $E_k = E_{k+G}$ this result can immediately be extended as follows. $dE_k/dk \rightarrow 0$ at $k = 0$, $\pm 2\pi/a$, $\pm 4\pi/a$,….. This prediction (only from the symmetry consideration) that the group velocity is equal to *zero* at $k = 0$, may be inconsistent with the result derived from the linear chain model above described. In the linear chain model, it is predicted that there is a discontinuous jump in the group velocity at $k = 0$, from $-v_0$ ($v_0 = a\sqrt{C/M}$) at $k = 0^-$ to $-v_0$ at $k = 0^+$. We note that this motion at $k = 0$ is a translation of the crystal as a whole and it is therefore not property of a vibration.

5. Determination of force constants

5.1 The system with the nearest neighbor interaction

We can make a statement about the range of the forces from the observed dispersion relation for ω. The generalization of the dispersion relation to p nearest planes is found to be

$$\omega_k^2 = \frac{2}{M} \sum_{p>0} [1 - \cos(pka)] C_p , \tag{5.1}$$

$$M \int_{-\pi/a}^{\pi/a} dk \omega_k^2 \cos(rka) = 2 \sum_{p>0} C_p \int_{-\pi/a}^{\pi/a} dk [1 - \cos(pka)] \cos(rka) . \tag{5.2}$$

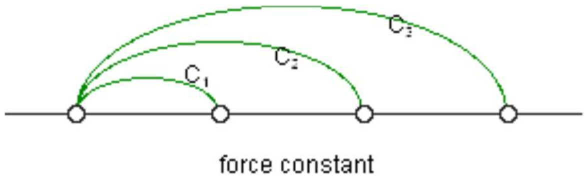


Fig.15 Linear chain having the nearest-neighbor coupling (C_1), the second nearest-neighbor coupling (C_2), and the third nearest-neighbor coupling (C_3), and the

Here

$$\int_{-\pi/a}^{\pi/a} dk \cos(rka) = \left[\frac{\sin(rka)}{ra} \right]_{-\pi/a}^{\pi/a} = 0 , \tag{5.3}$$

and

$$\begin{aligned} \int_{-\pi/a}^{\pi/a} dk \cos(pka)\cos(rka) &= \int_{-\pi/a}^{\pi/a} dk \frac{1}{2} \left[\cos\{(p+r)ka\} + \cos\{(p-r)ka\} \right] \\ &= \frac{1}{2} \int_{-\pi/a}^{\pi/a} dk \cos[(p-r)ka] = \begin{cases} \dfrac{1}{2}\dfrac{2\pi}{a} & \text{for } p = r \\ 0 & \text{otherwise} \end{cases} , \end{aligned} \tag{5.4}$$

Thus

$$M \int_{-\pi/a}^{\pi/a} dk \omega_k^2 \cos(rka) = -2\pi \frac{C_r}{a} , \tag{5.5}$$

or

$$C_p = -\frac{Ma}{2\pi} \int_{-\pi/a}^{\pi/a} dk \omega_k^2 \cos(pka) , \tag{5.6}$$

gives the force constant at range *pa*, for a structure with a monatomic basis.

5.2 System with long-ranged interactions

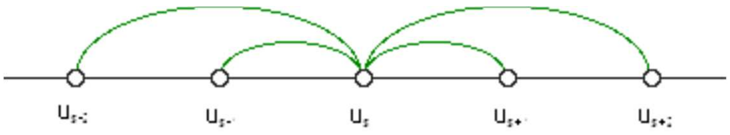


Fig.16 Linear chain with the nearest-neighbor and the next nearest-neighbor interactions.

Here we assume that there are the second-, third,…nearest neighbor interactions in the system in addition to the nearest neighbor-interaction. Then the Lagrangian L is given by

$$\begin{aligned} L &= T - V \\ &= \sum_{s} \frac{1}{2} M \dot{u}_s{}^2 - \sum_{s} \sum_{p=1}^{\infty} \frac{1}{2} C_p \{(u_s - u_{s+p})^2 + (u_s - u_{s-p})^2\} \end{aligned}$$

(5.7)

The Lagrange equation is

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{u}_s}\right) = \frac{\partial L}{\partial u_s},$$

(5.8)

or

$$M\ddot{u}_s = \sum_{p} C_p (u_{s+p} - 2u_s + u_{s-p})$$

(5.9)

Here we assume a traveling wave given by $u_s = ue^{i(ksa-\omega t)}$. Then we have

$$-M\omega^2 u_s = \sum_{p=1}^{\infty} C_p \left(e^{ipka} - 2 + e^{-ipka}\right) u_s$$

(5.1-)

or

$$-M\omega^2 = \sum_{p=1}^{\infty} C_p \left(e^{ipka} - 2 + e^{-ipka}\right), \qquad (5.11)$$

or

$$\omega^2 = \frac{2}{M} \sum_{p=1}^{\infty} C_p (1 - \cos pka) = \frac{2C_1}{M}[1 - \cos(ka)] + \frac{2C_2}{M}[1 - \cos(2ka)] + \ldots,$$

(5.12)

which includes the higher harmonics terms through long-range spring constants. The value of C_p can be determined experimentally from the phonon dispersion relation.

6A.. Vibration of square lattice[4]

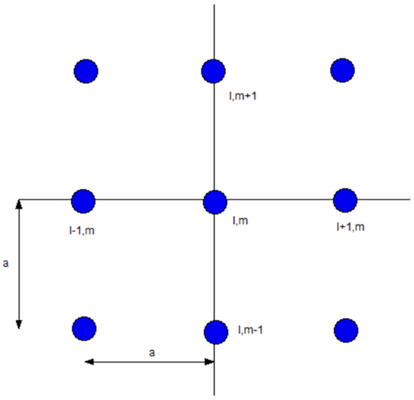


Fig.17 Square array of lattice constant a. The displacements are normal to the plane of the lattice.

We consider transverse vibrations of a planar lattice of rows and columns of identical atoms, and let $\boldsymbol{u}(l, m)$ denote the displacement normal to the plane of the lattice of the atom in the l-th column and m-th row. The mass of each atom is M, and C is the force constant for nearest neighbor atoms.

The equation of motion is expressed by

$$\begin{aligned} M\frac{d^2\boldsymbol{u}(l,m)}{dt^2} &= C\{[\boldsymbol{u}(l+1,m)+\boldsymbol{u}(l-1,m)-2\boldsymbol{u}(l,m)] \\ &\quad +[\boldsymbol{u}(l,m+1)+\boldsymbol{u}(l,m-1)-2u(l,m)] \end{aligned} \tag{6.1}$$

We assume that the solution of $\boldsymbol{u}(l, m)$ is given by

$$\boldsymbol{u}(l,m)=\boldsymbol{u}(0)\exp[i(lk_xa+mk_ya-\omega t), \tag{6.2}$$

where a is the spacing between nearest-neighbor atoms. The equation of motion is satisfied only if

$$\omega=\sqrt{\frac{2C}{M}}\sqrt{2-\cos(k_xa)-\cos(k_ya)}\,, \tag{6.3}$$

where the first Brillouin zone is

$$-\frac{\pi}{a}\le k_x\le\frac{\pi}{a}\ \text{and}\ -\frac{\pi}{a}\le k_x\le\frac{\pi}{a}\,. \tag{6.4}$$

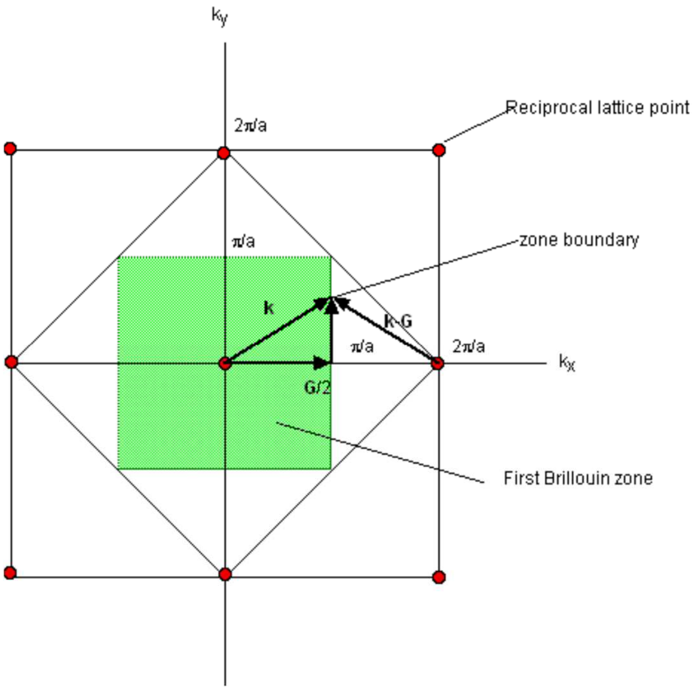


Fig.18a Brillouin zone of the two-dimensional square lattice with a lattice constant *a*. Bragg reflections occur at the zone boundary of the first Brillouin zone.

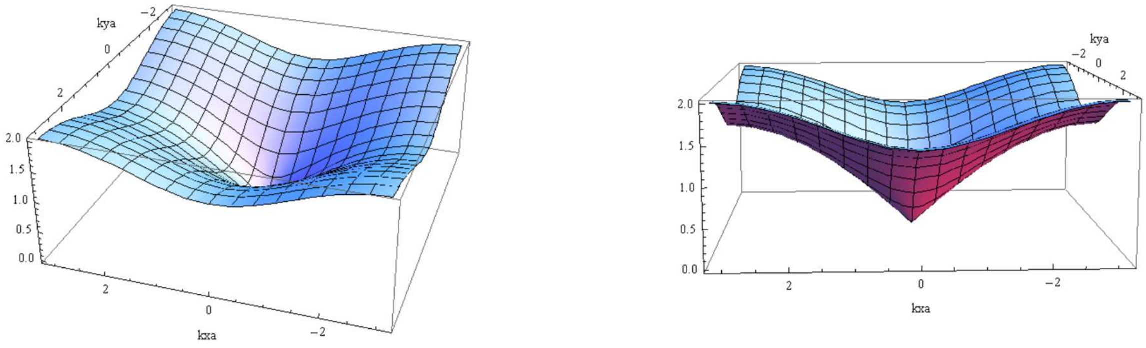


Fig.18b Three-dimensional plot of the dispersion relation (of the 2D square lattice. The height (ω) is plotted as a function k_xa vs k_ya (in the 2D wavevector-plane).

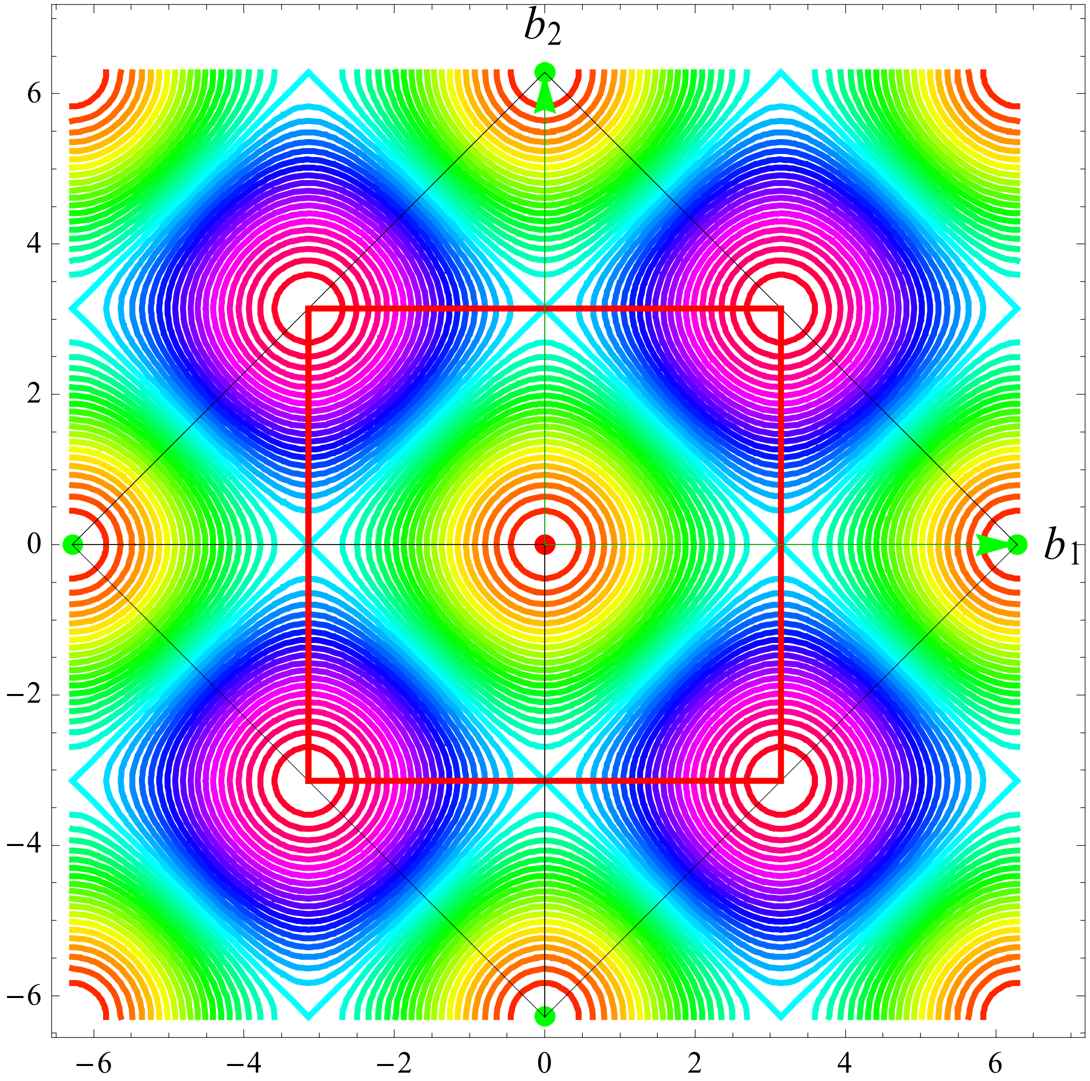


Fig.18c Contour plot of constant energy in the reciprocal lattice plane. The first Brillouin zone is shown by the red solid line. The energy of the point (the corner of the first Brillouin zone) is higher than that of the point (the middle of the zone boundary).

6B. Two-dimensional triangular lattice (supplement)

Problem 5-10 (H. Myer, Introductory Solid State Physics, Taylor & Francis, 1990. London, U.K.).

Consider the following two-dimensional close-packed lattice and its unit cell:

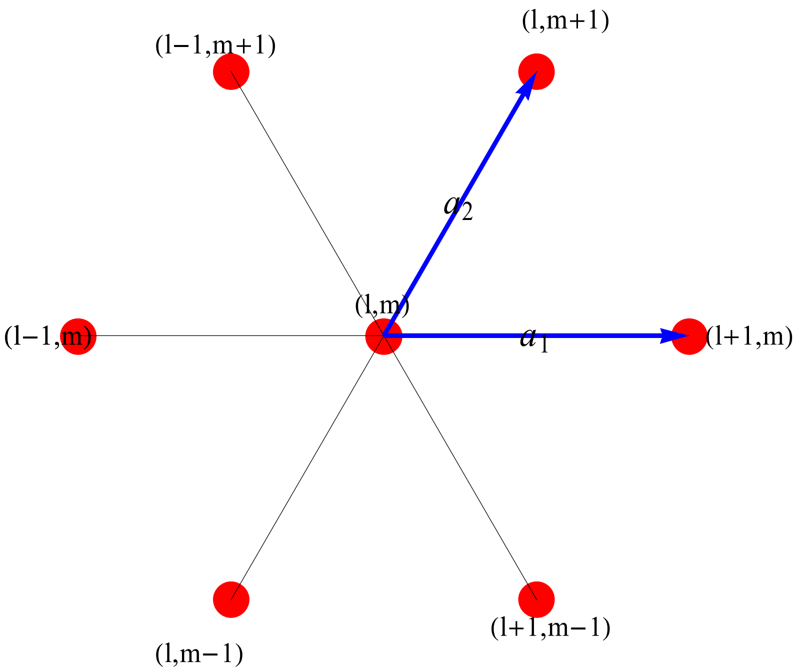


Fig.19a Real space for the 2D triangular lattice.

Primitive cell vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are shown. Determine the first Brillouin zone appropriate to this lattice. Arrange that the reciprocal lattice vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ are correctly oriented. Then, using the nearest-neighbor approximation for a vibrating net of point masses, determine the dispersion equation [let the central mass points have coordinates ($l\boldsymbol{a}_1$, $m\boldsymbol{a}_2$)]. Calculate the frequency at two-non-equivalent symmetry points on the zone boundary.

((**Solution**))
The primitive lattice vectors:

$$\boldsymbol{a}_1 = a(\cos(0°), \sin(0°)) = a(1,0), \qquad \boldsymbol{a}_2 = a(\cos(60°), \sin(60°)) = a(\frac{1}{2}, \frac{\sqrt{3}}{2}).$$

The reciprocal lattice vectors;

$$\boldsymbol{b}_1 = \frac{4\pi}{\sqrt{3}a}((\cos(-30°), \sin(-30°)) = \frac{4\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{2}, -\frac{1}{2}),$$

$$\boldsymbol{b}_2 = \frac{4\pi}{\sqrt{3}a}((\cos(90°), \sin(90°)) = \frac{4\pi}{\sqrt{3}a}(0,1)$$

We set up the equation of the motion for the atom at the center. There are nearest neighbor interactions from atoms surrounding the atom at the center.

$$M\frac{d^2}{dt^2}\boldsymbol{u}(l,m) = C[\boldsymbol{u}(l+1,m) + \boldsymbol{u}(l,m+1) + \boldsymbol{u}(l-1,m+1) + \boldsymbol{u}(l-1,m)$$

$$+\boldsymbol{u}(l,m-1)+\boldsymbol{u}(l+1,m-1)-6\boldsymbol{u}(l,m) \tag{6.5}$$

where M is the mass of atom, C is the spring constant, and $\boldsymbol{u}(l,m)$ is the displacement vector for the atom at the position ($l\boldsymbol{a}_1$, $m\boldsymbol{a}_2$). We assume the solution of the form as

$$\boldsymbol{u}(l,m)=\boldsymbol{u}(0)\exp[i\boldsymbol{k}\cdot(l\boldsymbol{a}_1+m\boldsymbol{a}_2)-\omega t].$$

with

$$\boldsymbol{u}(l\pm 1,m)\ =\exp(\pm i\boldsymbol{k}\cdot\boldsymbol{a}_1)\boldsymbol{u}_{l,m},$$

$$\boldsymbol{u}(l,m\pm 1)=\exp(\pm i\boldsymbol{k}\cdot\boldsymbol{a}_2)\boldsymbol{u}_{l,m}.$$

Substituting these into Eq.(1), we get

$$\begin{aligned}-M\omega^2\boldsymbol{u}(l,m)=C[&\exp(i\boldsymbol{k}\cdot\boldsymbol{a}_1)+\exp(i\boldsymbol{k}\cdot\boldsymbol{a}_2)+\exp[i(-\boldsymbol{k}\cdot\boldsymbol{a}_1+\boldsymbol{k}\cdot\boldsymbol{a}_2)\\ &+\exp(-i\boldsymbol{k}\cdot\boldsymbol{a}_1)+\exp(-i\boldsymbol{k}\cdot\boldsymbol{a}_2)+\exp[i(\boldsymbol{k}\cdot\boldsymbol{a}_1-\boldsymbol{k}\cdot\boldsymbol{a}_2)-6]\boldsymbol{u}(l,m)\end{aligned}$$

Then we have the dispersion relation of ω vs $\boldsymbol{k}$ as

$$\frac{M\omega^2}{2C}=[3-\cos(\boldsymbol{k}\cdot\boldsymbol{a}_1)-\cos(\boldsymbol{k}\cdot\boldsymbol{a}_2)-\cos(\boldsymbol{k}\cdot\boldsymbol{a}_1-\boldsymbol{k}\cdot\boldsymbol{a}_2)]$$

where

$$\boldsymbol{k}=k_x\boldsymbol{e}_x+k_y\boldsymbol{e}_y$$

The Brillouin zone for the triangular lattice is shown below.

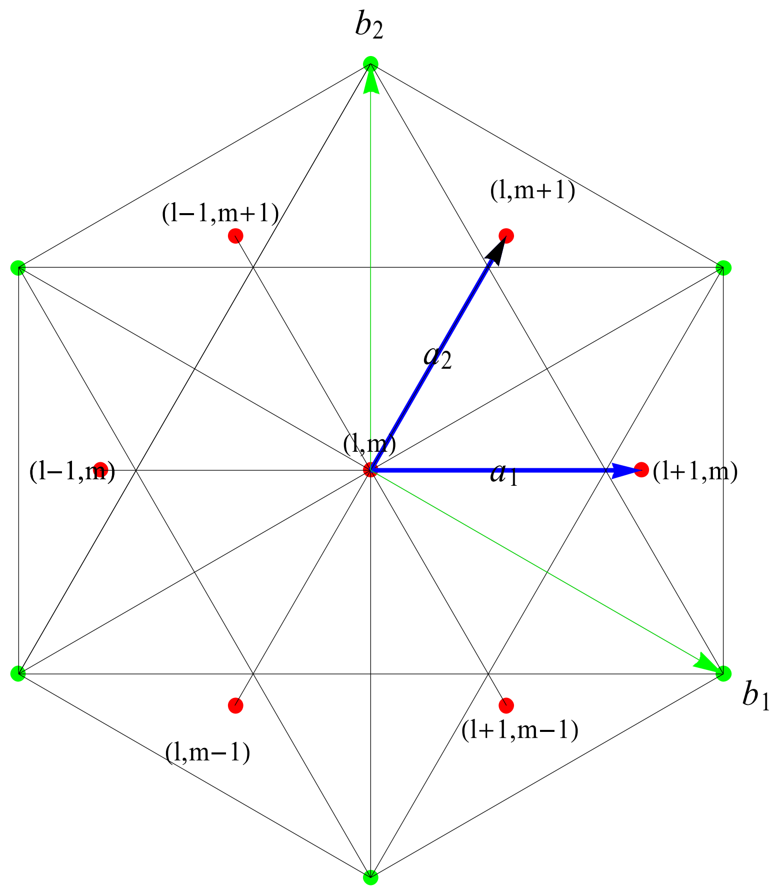


Fig.19b Relation between the real space (lattice vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$) and the reciprocal lattice ($\boldsymbol{b}_1$ and $\boldsymbol{b}_2$). The magnitude of $\boldsymbol{a}_1$ and $\boldsymbol{b}_1$ are chosen appropriately.

(a) At the middle of a Brillouin zone (zone boundary)

$$\boldsymbol{k} = \frac{\boldsymbol{b}_1 + \boldsymbol{b}_2}{2}.$$

$$\boldsymbol{k}\cdot\boldsymbol{a}_1 = \frac{1}{2}\boldsymbol{a}_1\cdot\boldsymbol{b}_1 = \pi, \qquad \boldsymbol{k}\cdot\boldsymbol{a}_2 = \frac{1}{2}\boldsymbol{a}_2\cdot\boldsymbol{b}_2 = \pi.$$

Then we get

$$\frac{M\omega^2}{2C} = 3 - \cos(\pi) - \cos(\pi) - \cos(\pi - \pi) = 4$$

or

$$\omega^2 = \frac{8C}{M}$$

(b) At the corner of a Brillouin zone.

$$\boldsymbol{k} = \frac{\boldsymbol{b}_1 + 2\boldsymbol{b}_2}{3}$$

$$\boldsymbol{k}\cdot\boldsymbol{a}_1 = \frac{1}{3}\boldsymbol{a}_1\cdot\boldsymbol{b}_1 = \frac{2\pi}{3}, \qquad \boldsymbol{k}\cdot\boldsymbol{a}_2 = \frac{2}{3}\boldsymbol{a}_2\cdot\boldsymbol{b}_2 = \frac{4\pi}{3}$$

Then we get

$$\frac{M\omega^2}{2C} = 3 - \cos(\frac{2\pi}{3}) - \cos(\frac{4\pi}{3}) - \cos(-\frac{2\pi}{3}) = \frac{9}{2}$$

or

$$\omega^2 = \frac{9C}{M}$$

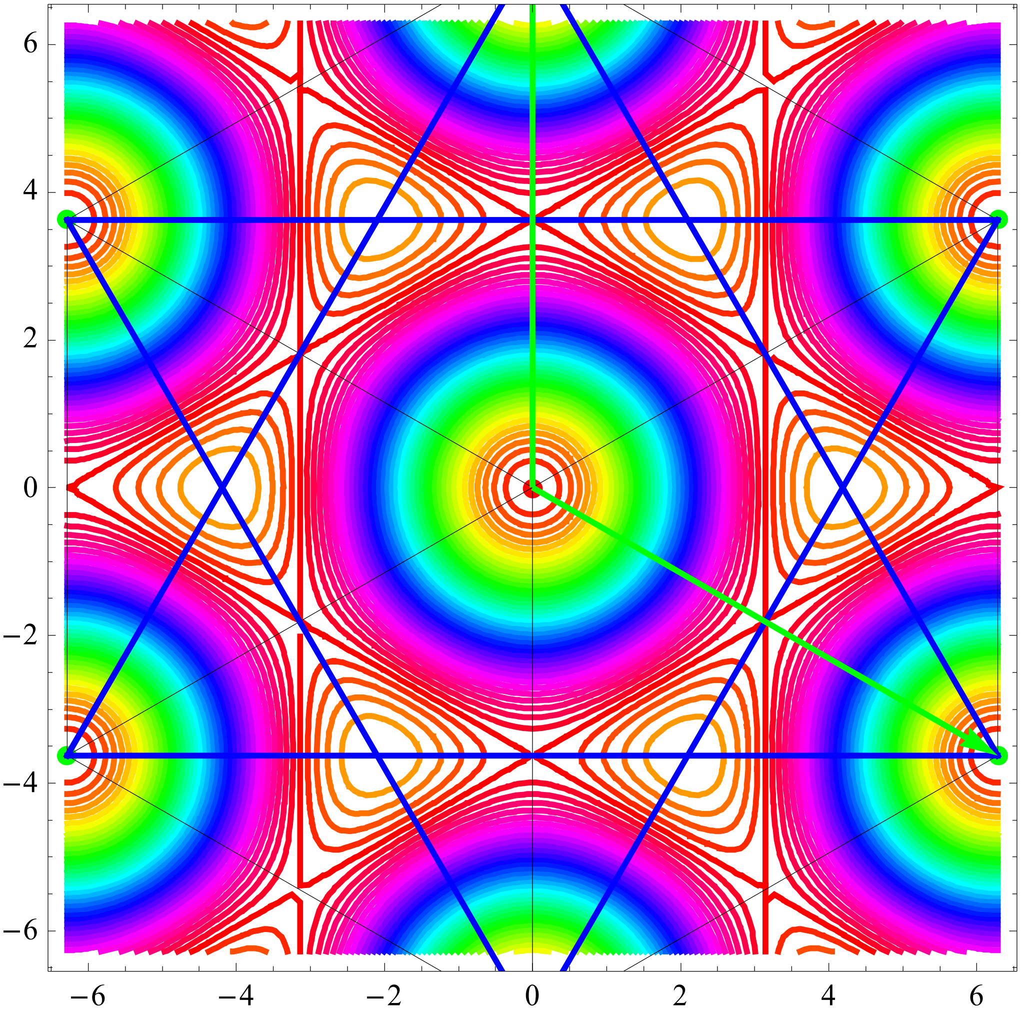


Fig.19c Contour plot of constant energy in the reciprocal lattice plane. The first Brillouin zone is shown by the blue solid line. The energy of the point K (the corner of the first Brillouin zone) is higher than that of the point M (the middle of the zone boundary).

((Note))
The Brillouin zone for the 2D triangular lattice is shown below.

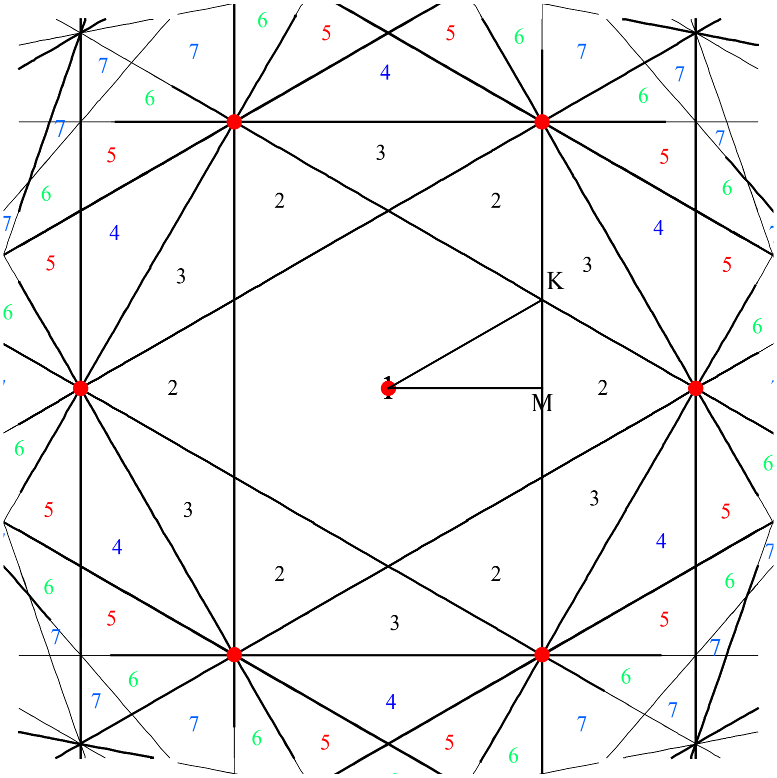


Fig.19d Reciprocal lattice. Brillouin zone. M (the zone boundary) and K (the corner). The numbers are related to the number of Brillouin zone.

7. Two atoms per primitive basis

We consider a cubic crystal where atoms of mass M_1 lie on one set of planes and atoms of mass M_2 lie on planes interleaved between those of the first set.

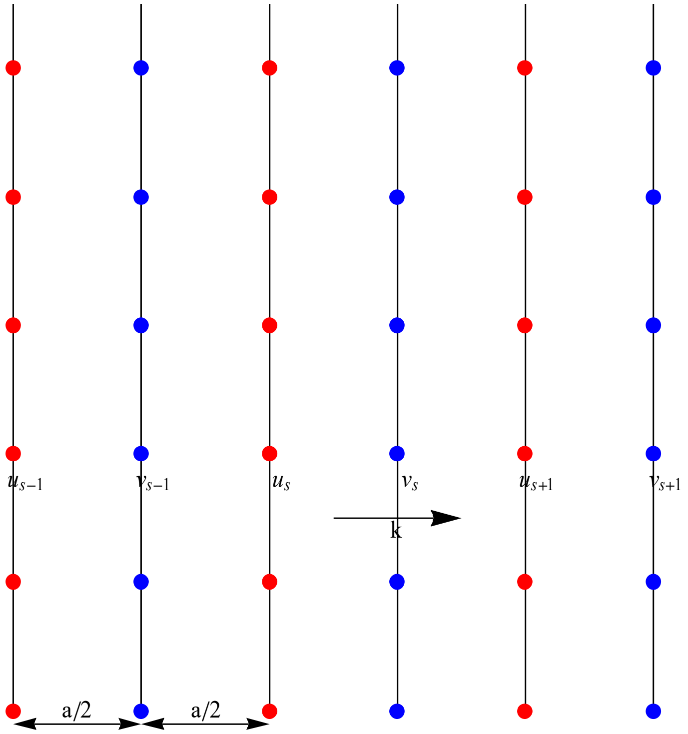


Fig.20(a)

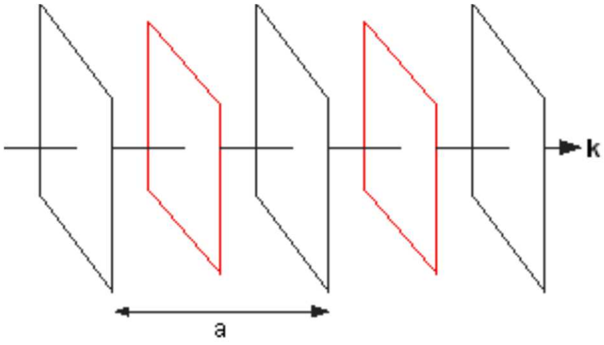


Fig.20(b)

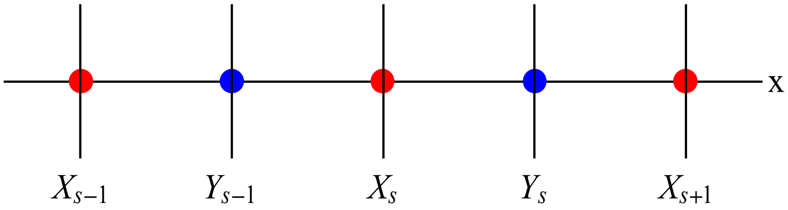


Fig.20(c)

Fig.20 (a), (b) Diatomic linear chain, There are two atoms with masses M_1 and M_2 per unit cell (lattice constant a). (b) The plane of atoms stacked alternatively (lattice constant a).

The Lagrangian of the system is given by

$$L = \frac{1}{2}M_1\dot{X}_s{}^2 + \frac{1}{2}M_2\dot{Y}_s{}^2 + \ldots$$
$$-\frac{1}{2}C[(X_{s+1} - Y_s - \frac{a}{2})^2 + (Y_s - X_s - \frac{a}{2})^2 + \left(X_s - Y_{s-1} - \frac{a}{2})^2\right] + \cdots.$$

or

$$L = \frac{1}{2}M_1\dot{u}_s{}^2 + \frac{1}{2}M_2\dot{v}_s{}^2 + \ldots$$
$$-\frac{1}{2}C[(u_{s+1} - v_s)^2 + (v_s - u_s)^2 + (u_s - v_{s-1})^2] + \cdots.$$

(7.1)

Note that the coordinates of the positions of the atom with mass M_1 and atom with mass M_2 are described by

$$X_s = sa + u_s, \quad Y_s = sa + \frac{a}{2} + v_s.$$

or

$$Y_s - X_s - \frac{a}{2} = (sa + \frac{a}{2} + v_s) - (sa + u_s) - \frac{a}{2} = v_s - u_s.$$

The Lagrange's equations are as follows.

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{u}_s} = \frac{\partial L}{\partial u_s}$$

(7.2)

or

$$M_1\ddot{u}_s = -\frac{1}{2}C[-2(v_s - u_s) + 2(u_s - v_{s-1}),$$

(7.3)

or

$$M_1\ddot{u}_s = -C(-v_s + 2u_s - v_{s-1}) = C(v_s + v_{s-1} - 2u_s).$$

(7.4)

Similarly

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{v}_s} = \frac{\partial L}{\partial v_s},$$

(7.5)

$$M_2 \ddot{v}_s = -\frac{1}{2}C[-2(u_{s+1} - v_s) + 2(v_s - u_s)] = C(u_{s+1} - 2v_s + u_s)$$

(7.6)

Let *a* denote the repeat distance of the lattice in the direction normal to the lattice plane. Equation of motion is given by

$$\begin{cases} M_1 \dfrac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s) \\ M_2 \dfrac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s) \end{cases}, \tag{7.7}$$

Here we assume that each plane interacts only with its nearest-neighbor and that the force constants are identical between all pairs of nearest-neighbor planes. Suppose that u_s and v_s have the forms of

$$\begin{cases} u_s = ue^{i(ska-\omega t)} \\ v_s = ve^{i(ska-\omega t)} \end{cases}. \tag{7.8}$$

Then

$$\begin{aligned} -\omega^2 M_1 u &= Cv(1 + e^{-ika}) - 2Cu \\ -\omega^2 M_2 v &= Cu(e^{ika} + 1) - 2Cv \end{aligned}. \tag{7.9}$$

When the determinant of the coefficients of *u* and *v* vanishes, the homogeneous linear equations have a non-trivial solution.

$$\begin{vmatrix} 2C - M_1\omega^2 & -C(1 + e^{-ika}) \\ -C(1 + e^{ika}) & 2C - M_2\omega^2 \end{vmatrix} = 0, \tag{7.10}$$

or

$$M_1 M_2 \omega^4 - 2C(M_1 + M_2)\omega^2 + 2C^2(1 - \cos ka) = 0\,.$$

(7.11)

Suppose that $\alpha = M_2/M_1$. $y = \sqrt{\frac{M_1}{4C}}\omega$, $x = ka$. Thus Eq.(7.11) can be rewritten as

$$8\alpha y^4 - 4y^2(1 + \alpha) + 1 - \cos x = 0$$

The dispersion relation (y vs x) depends only on the ratio α. We make a plot of y as a function of x by using the ContourPlot, where the ratio α is changed as a parameter.

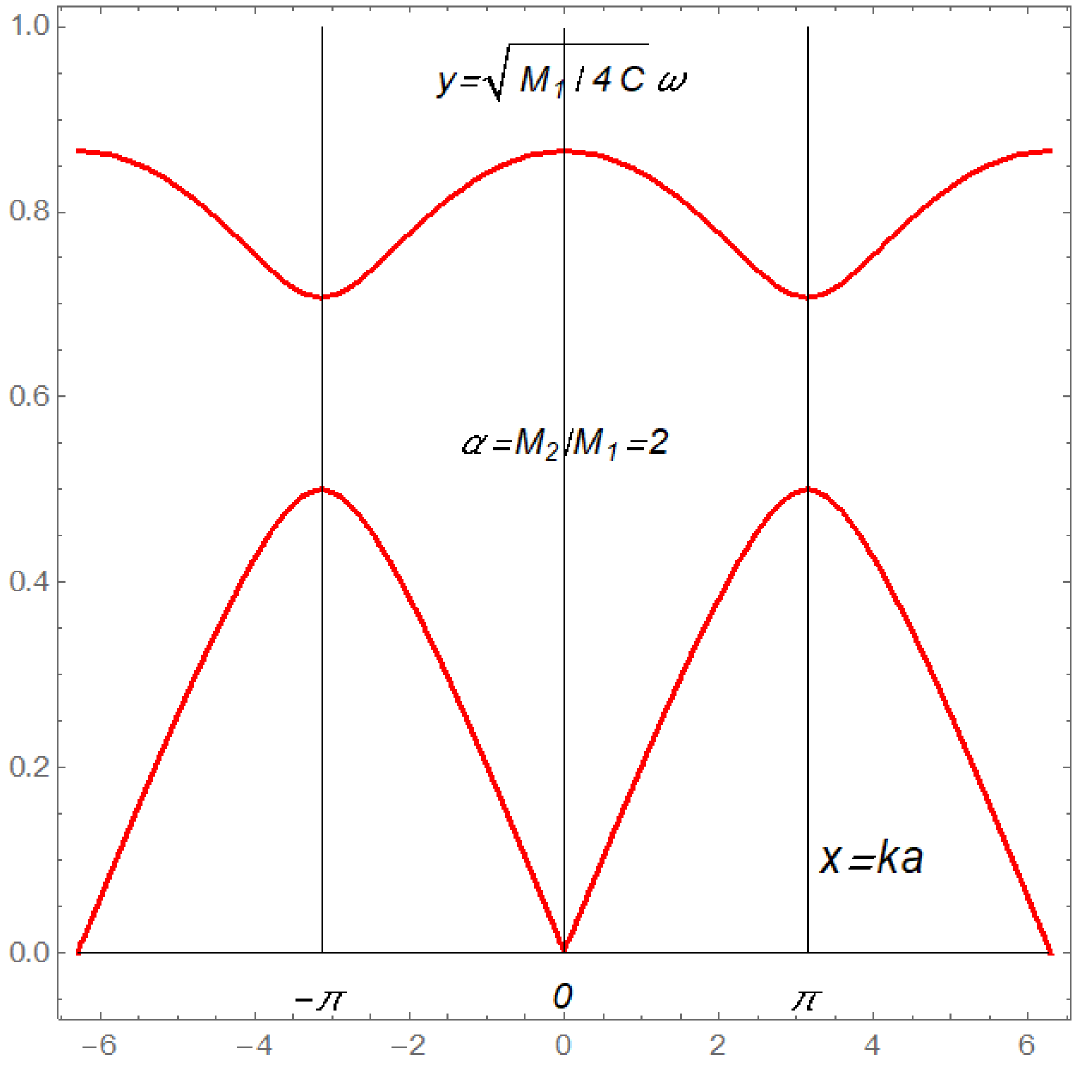


Fig.21(a) The energy dispersion of y vs x with $\alpha = 2$, where $\alpha = M_2/M_1$. $y = \sqrt{\frac{M_1}{4C}}\omega$. $x = ka$.

((**Note-2**))

If we look for solutions in the gap with ω real, then ***k*** will be complex, so that the wave is damped in space.

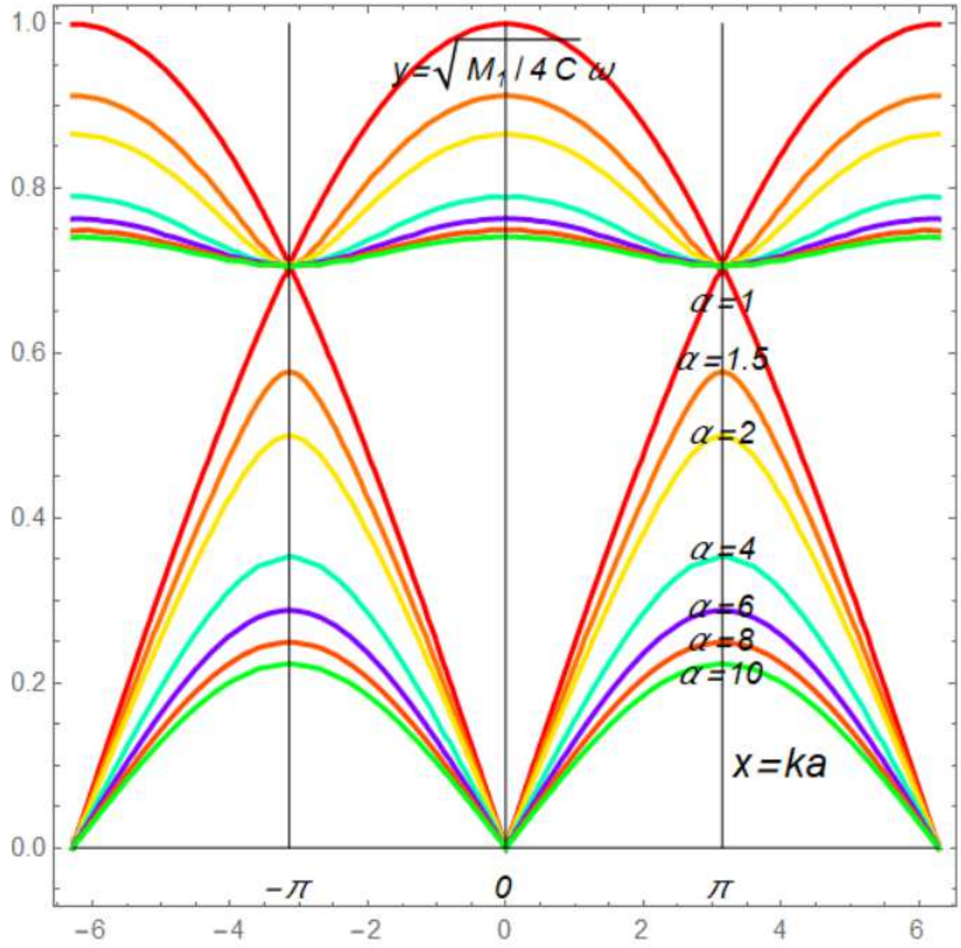


Fig.21(b) The dispersion curve of the diatomic linear chain with two atoms in a unit cell. The ratio $\alpha = M_2/M_1$ is varied as a parameter between 2, 3, 4, … and 10.

((**Note-2**)) **Group velocity and optical velocity for the acoustic phonon and optical phonon in the case of diatomic system (Ibach and Luth, problem 5-4)**

Here we discuss the group-velocity as a function of the wavenumber k in the case of $\alpha = 5$.

Suppose that $a = M_2/M_1$. $y = \sqrt{\frac{M_1}{4C}}\omega$, $x = ka$. Thus Eq.(7.11) can be rewritten as

$$8ay^4 - 4y^2(1+a) + 1 - \cos x = 0$$

We use $\alpha = 5$.

(a) Phonon dispersion relation

We make a plot of y vs x below.

y vs x: $y = \sqrt{\frac{M_1}{4C}}\omega.$, $x = ka$

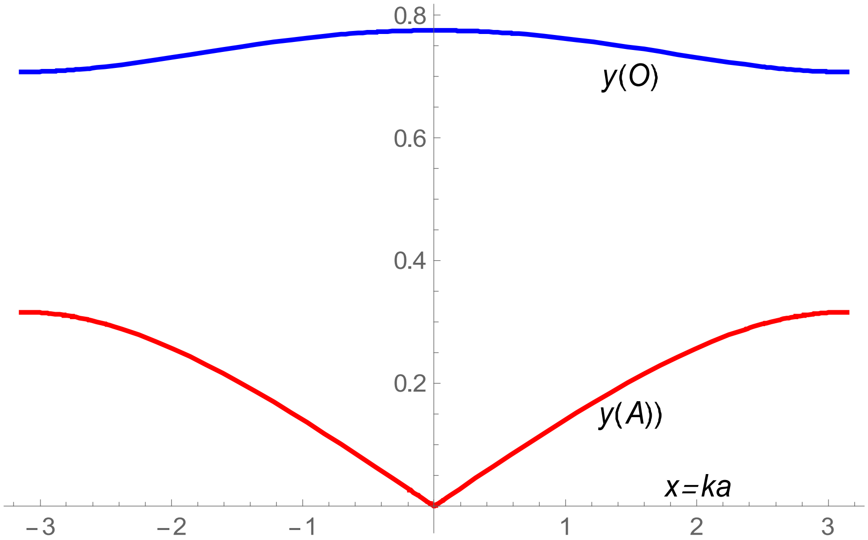


Fig. Phonon dispersion: y(O): optical phonon. y(A): acoustic phonon. $\alpha = 5$.
$y = \sqrt{\frac{M_1}{4C}}\omega.$, $x = ka$.

(b) Group velocity for acoustic and optical branches

The group velocity $v_g = \frac{\partial\omega}{\partial k}$ is related to $\frac{\partial y}{\partial x}$ as

$$\frac{\partial y}{\partial x} = \frac{1}{a}\sqrt{\frac{M_1}{4C}}\frac{\partial\omega}{\partial k} = \frac{1}{a}\sqrt{\frac{M_1}{4C}}v_g$$

and

$$\frac{\partial y}{\partial x} = \frac{\sin x}{8(1+\alpha)y - 32\alpha y^3}$$

The plot of the group velocity can be obtained with the use of Mathematica.

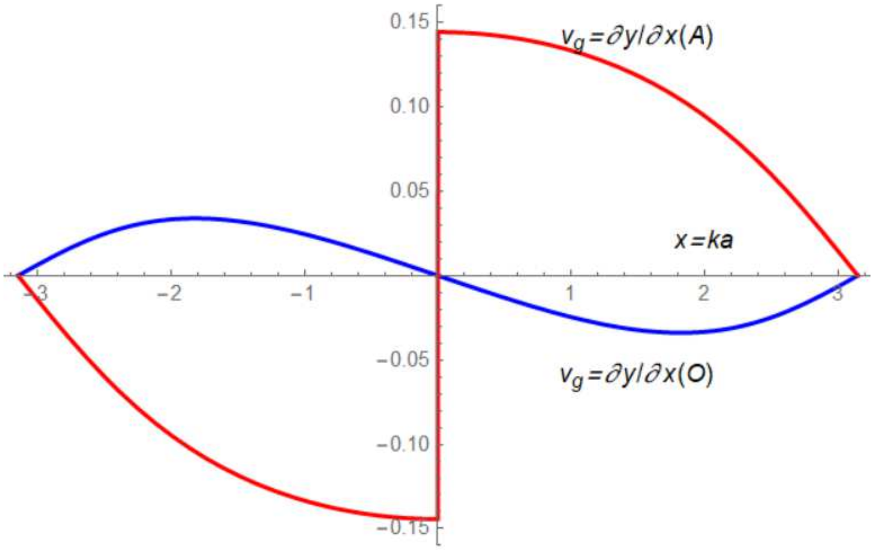


Fig. Group velocity: $\frac{\partial y}{\partial x}$(O): optical phonon. $\frac{\partial y}{\partial x}$ (A): acoustic phonon. $\frac{\partial y}{\partial x} = \frac{1}{a}\sqrt{\frac{M_1}{4C}}\frac{\partial \omega}{\partial k} = \frac{1}{a}\sqrt{\frac{M_1}{4C}}v_g$. $\alpha = 5$.

(c) Phase velocity for acoustic and optical branches

The phase velocity $\frac{\omega}{k}$ is related to y/x

$$\frac{y}{x} = \frac{1}{a}\sqrt{\frac{M_1}{4C}}\frac{\omega}{k}$$

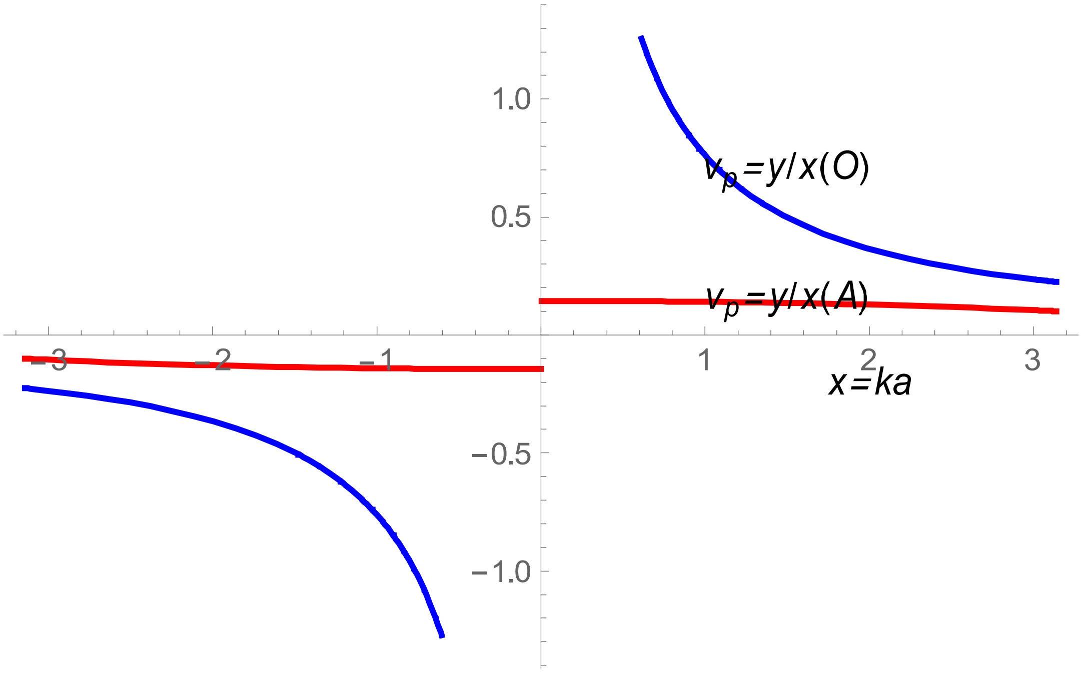


Fig. Phase velocity: $\frac{y}{x}$(O) for optical phonon. $\frac{y}{x}$ (A) for acoustic phonon. $\alpha = 5$.

$$\frac{y}{x} = \frac{1}{a}\sqrt{\frac{M_1}{4C}}\frac{\omega}{k} = \frac{1}{a}\sqrt{\frac{M_1}{4C}}v_p. \qquad v_p = \frac{\omega}{k}$$

((**Note-3**)) Link
Phonon dispersion relation in the Brillouin zone (Wolfram Demonstrations Project)
Phonon modes in one dimensional crystal with two atoms.
http://demonstrations.wolfram.com/PhononDispersionRelationInBrillouinZone/

We examine this equation in the limiting cases

(i) $ka \ll 1$
(ii) $ka = \pm\pi$ at the zone boundary

(i) $ka \ll 1$

$$1 - \cos ka \approx \frac{1}{2}k^2a^2$$

$$M_1M_2\omega^4 - 2C(M_1 + M_2)\omega^2 + C^2k^2a^2 = 0, \qquad (7.12)$$

or

$$\begin{aligned}\omega^2 &= \frac{C(M_1+M_2)\pm\sqrt{C^2(M_1+M_2)^2-M_1M_2C^2k^2a^2}}{M_1M_2}\\ &= \frac{C(M_1+M_2)}{M_1M_2}\left[1\pm\sqrt{1-\frac{M_1M_2C^2k^2a^2}{C^2(M_1+M_2)^2}}\right] \quad . \qquad (7.13)\\ &\approx \frac{C(M_1+M_2)}{M_1M_2}\left[1\pm\left\{1-\frac{M_1M_2C^2k^2a^2}{2C^2(M_1+M_2)^2}\right\}\right]\end{aligned}$$

Then we have the two roots for *ka* « 1

$$\omega^2 = 2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)$$ (optical

branch), (7.14)

$$\omega^2 = \frac{C}{2(M_1+M_2)}k^2a^2 \qquad \text{(acoustic branch).} \qquad (7.15)$$

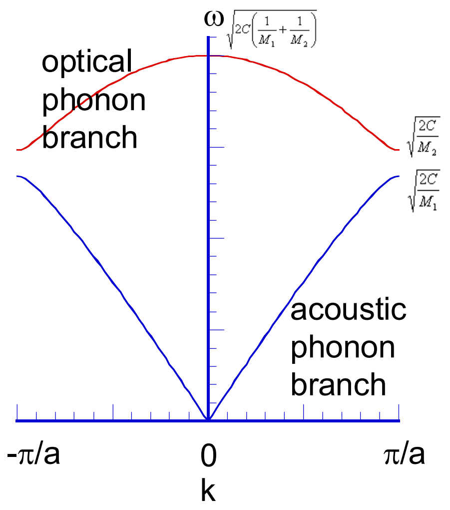
(*) The extent of the first Brillouin zone is $-\frac{\pi}{a}\le k\le\frac{\pi}{a}$.

(ii) $ka=\pm\pi$

$$\begin{aligned}&M_1M_2\omega^4-2C(M_1+M_2)\omega^2+4C=0\\ &\left(M_1\omega^2-2C\right)\left(M_2\omega^2-2C\right)=0\end{aligned} \qquad (7.16)$$

or

$$\omega^2=\frac{2C}{M_1}; \qquad \omega^2=\frac{2C}{M_2}. \qquad (7.17)$$



for $M_1 > M_2$

Fig.22 The dispersion curve (ω vs k) for a diatomic linear chain with nearest neighbor atoms interacting with interaction C only. The masses of the atoms are M_1 and M_2; The first Brillouin zone is the segment between $-\pi/a$ and π/a. There is an acoustic mode (lower branch) and an optical mode (upper branch).

We consider the particle displacement in LA and LO branches. For the optical branch at k = 0, we have

$$-\omega^2 M_1 u = 2Cv - 2Cu$$

or

$$\frac{u}{v} = \frac{2C}{2C - M_1\omega^2} = \frac{2C}{2C - M_1 2C\left(\frac{1}{M_1} + \frac{1}{M_2}\right)} = -\frac{M_2}{M_1} \qquad \text{: out-of-phase} \qquad (7.18a)$$

We also note that the velocity of the center of mass defined by

$$v_{CM} = \frac{M_1 u + M_2 v}{M_1 + M_2}. \qquad (7.18b)$$

is equal to zero.

For the acoustical branch at $k = 0$, we have

$$-\omega^2 M_1 u = 2Cv - 2Cu. \qquad (7.19)$$

Since $\omega^2 = 0$, then we have

$$u = v. \qquad : \text{in-phase}$$

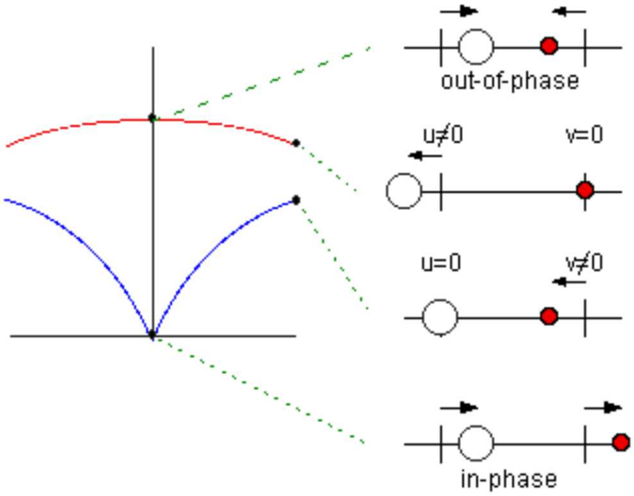


Fig.23 Nature of the vibration in the acoustical and optical branch of a vibrational spectrum.

$$u_s = ue^{i(ska-\omega t)}, \ v_s = ve^{i(ska-\omega t)}. \qquad (7.20)$$

Acoustical waves in a diatomic linear lattice ($k = \frac{\pi}{2a}$)

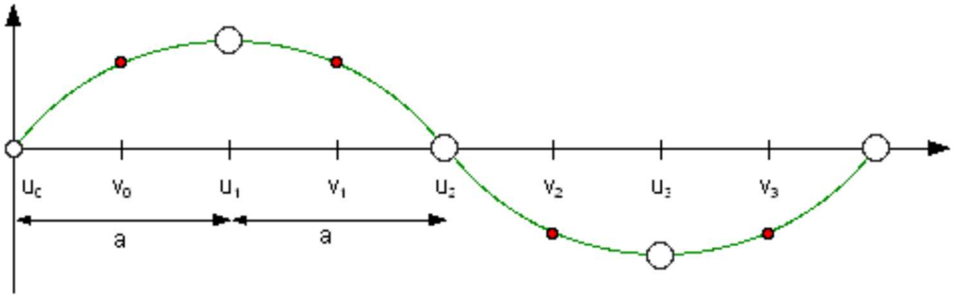


Fig.24 Transverse acoustic waves in a diatomic linear lattice.

$$u\cos(ska) = v\cos(ska). \qquad (7.21)$$

Optical waves in a diatomic linear lattice ($k = \frac{\pi}{2a}$)

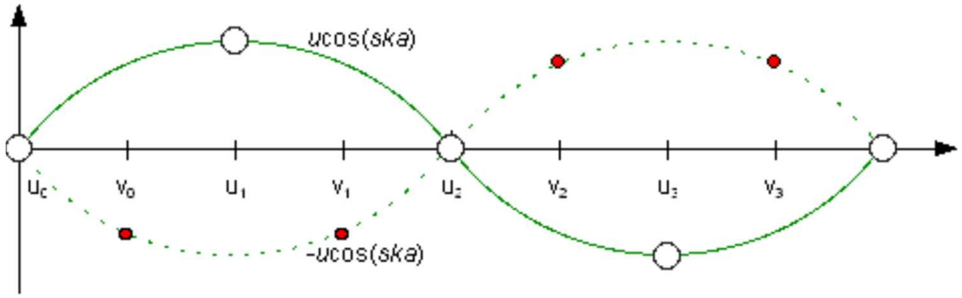


Fig.25 Transverse optical waves in a diatomic linear lattice. Figure represents a snapshot of the wave motion.

$$v_c \equiv \frac{M_1 u + M_2 v}{M_1 + M_2} = 0 \quad \Rightarrow \text{The velocity of center of mass does not move.}$$

The atoms vibrate against each other, but their center of mass is fixed. If the two atoms carry opposite charges, we may excite a motion of this type with the electric field of a light wave.

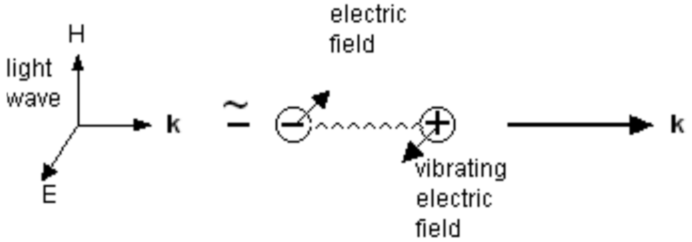


Fig.26 Origin of the name of optical mode

So that the branch is called the optical branch. The atoms (and their center of mass) move together, as in long wavelength acoustical vibrations, whence the term acoustical branch.

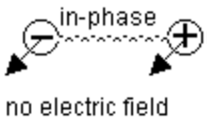


Fig.27 Origin of the name of acoustic mode

This is a frequency gap at $k_{\max} = \pm\frac{\pi}{a}$ of the first Brillouin zone.

((**Example**)) Change of the unit cell size from 2a to a when M_2 become equal to M_1.

E. Hanamura (Problems in Solid State Physics, in Japanese) Problem 3-1.

We consider a one-dimensional chain, where two kinds of atoms with different masses M_1 and M_2 are alternatively arranged. The size of unit cell is 2a, where a is the nearest neighbor distance between two different atoms. There are 2N atoms. N atoms of the mass M_1, and N

atoms of the mass M_2. There is only the nearest neighbor interaction between these two atoms. We consider the limit that that M_1 becomes equal to M_2 ($M_1 = M_2 = M$). In this case, there are $2N$ atoms of the mass M. The nearest neighbor distance is a.
Discuss the dispersion relation of these systems.

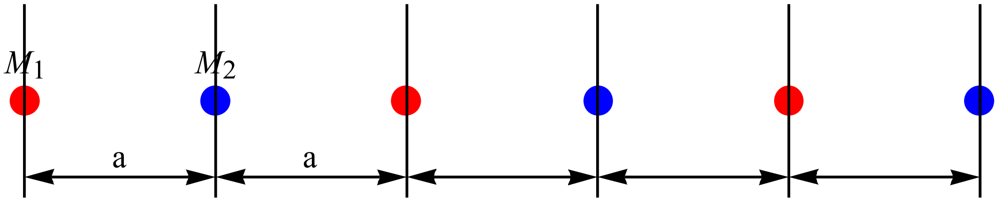


Fig.28 $M_2 \neq M_1$. The size of unit cell is $2a$. There are N unit cells in the system. $L = 2aN$.

First we consider the case (only the longitudinal wave) where M_1 is not equal to M_2. The size of unit cell is $2a$. The Brillouin zone is in the range $|k| < \frac{\pi}{2a}$. The total number of atoms are $2N$, leading to the $2N$ modes; 1 acoustic branch (N modes) and 1 optical branch (N mode). The size of the system is $L = 2Na$.

$$u_s = u\exp[i(s2ak - \omega t\}]$$
$$v_s = v\exp[i\{s(2a+1)k - \omega t\}]$$

We use the periodic boundary condition;

$$u_{N+s} = u_s, \qquad v_{N+s} = v_s$$

or

$$\exp[\,i(2Nak\,)] = 1\,.$$

or

$$2Nak = 2\pi n, \qquad \text{or} \qquad k = \frac{2\pi n}{2Na} = \frac{\pi}{a}\frac{n}{N},$$

There are N modes for each branch (1 optical and 1 acoustic branches). We choose

$$|k| < \frac{\pi}{2a}.$$

where $k = 0$, $\pm\pi/(aN)$, $\pm 2\pi/(aN)$. The dispersion relation is given by

$$M_1 M_2 \omega^4 - 2C(M_1 + M_2)\omega^2 + 4C^2 \sin^2(ka) = 0$$

For $k = \pm \frac{\pi}{2a}$,

$$M_1 M_2 \omega^4 - 2C(M_1 + M_2)\omega^2 + 4C^2 = 0.$$

or

$$(M_1\omega^2 - 2C)((M_2\omega^2 - 2C) = 0$$

or

$$\omega = \sqrt{\frac{2C}{M_1}} \qquad \omega = \sqrt{\frac{2C}{M_2}}.$$

In the limit of $M_1 = M_2 = M$, these are equal ($\omega = \sqrt{\frac{2C}{M}}$).

For $k = 0$,

$$M_1 M_2 \omega^4 - 2C(M_1 + M_2)\omega^2 = 0$$

or

$$\omega = 0, \qquad \omega = \sqrt{\frac{2C(M_1 + M_2)}{M_1 M_2}}$$

In the limit of $M_1 = M_2 = M$, the latter is equal to ($\omega = \sqrt{\frac{4C}{M}}$).

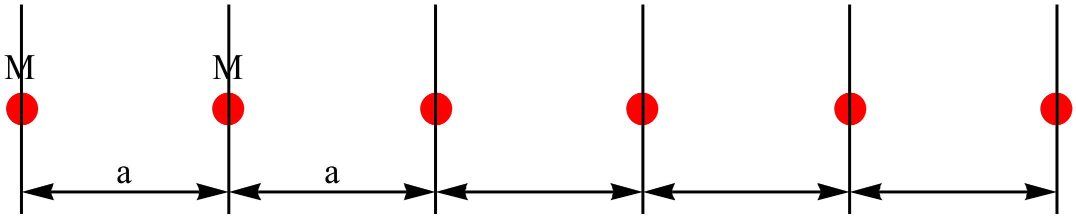


Fig.29 $M_1 = M_2$. The size of unit cell is a. There are $2N$ cells in the system. $L = 2Na$.

Now we consider the case (only the longitudinal wave) where $M_1 = M_2 = M$. The size of unit cell is a. The Brillouin zone is in the range $|k|<\pi/a$. The total number of atoms are $2N$, leading to the $2N$ modes; 1 acoustic branch ($2N$ modes). No optical mode exists. The size of the system is $L = 2Na$.

$$u_s = u\exp[i(sak-\omega t)]$$

We use the periodic boundary condition;

$$u_{2N+s} = u_s,$$

or

$$\exp[i(2Nak)] = 1.$$

or

$$2Nak = 2\pi n, \qquad \text{or} \qquad k = \frac{2\pi n}{2Na} = \frac{2\pi}{a}\frac{n}{2N},$$

where $n = -N, -N+1, \ldots\ldots, N-1, N$. There are $2N$ modes for 1 acoustic branch,

$$|k| < \frac{\pi}{a}.$$

The dispersion relation is given by

$$\omega = 2\sqrt{\frac{C}{M}}\left|\sin(\frac{ak}{2})\right|.$$

In the zone boundary, $|k| = \frac{\pi}{a}$, we have

$$\omega = 2\sqrt{\frac{C}{M}}$$

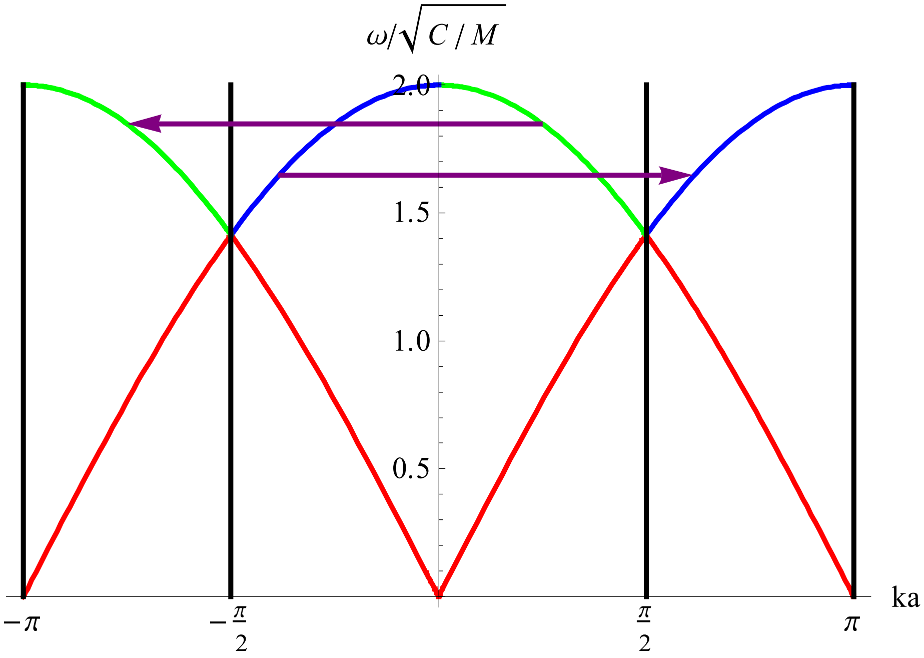


Fig.30 The dispersion relation for $M_1 = M_2$. When M_2 is slightly larger than M_1, the dispersion relation consists of the optical branch (N modes) and the acoustic branch (N modes) for the first Brillouin zone ($|k| < \frac{\pi}{2a}$). The extended zone scheme for the optical branch and acoustic brance (for $M_2 \approx M_1$) is shown in this Fig.. When $M_1 = M_2$, ω at $k = \pm\frac{\pi}{2a}$ for the optical branch becomes equal to that for the acoustic branch. The size of the Brillouin zone becomes twice larger. Correspondingly, a part of the optical branch (denoted by green line) shifts to the acoustic branch by $-\pi/a$, while a part of the optical branch (denoted by blue line) shifts to the acoustic branch by π/a.

F. The folding effect

We use the above examples to explain the folding effect of the first Brillouin zone.

(i) Suppose that there are one kinds of mass (the mass M_1 denoted by red circles). Here we have a chain with the total size $L = 2Na$, where $2N$ is the number of unit cell and a is the lattice constant. When we consider the lattice vibration in this system (only in the case of longitudinal waves).

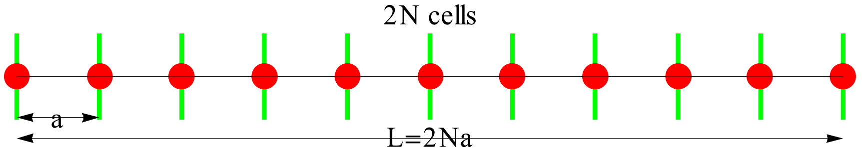


Fig.31

Then we have one longitudinal acoustic branch with $2N$ modes in the first Brillouin zone ($|k(a)|<\pi$), since the lattice constant is a. The total number of modes is $2N$.

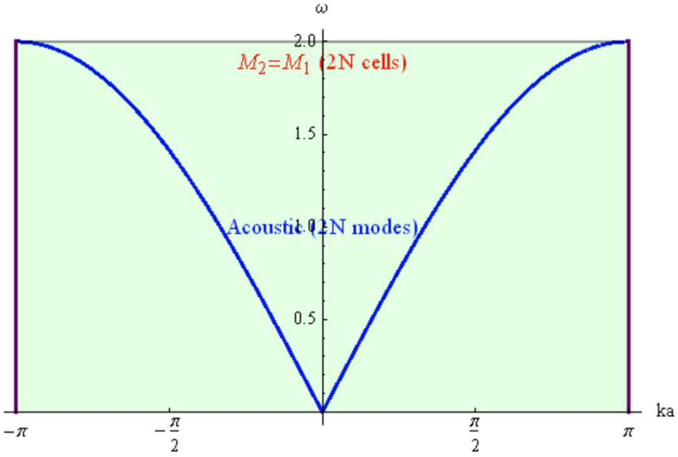


Fig.32

(ii) Suppose that there are two kinds of masses (the mass M_1 (= M) denoted by red circles and M_2 ($M_2 \neq M_1$) denoted by blue circles). Here we have a chain with the total size $L = 2Na$, where $2N$ is the number of unit cell and $2a$ is the lattice constant. When we consider the lattice vibration in this system (only in the case of longitudinal waves).

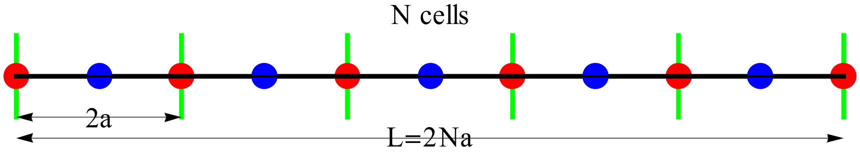


Fig.33

Then we have one longitudinal acoustic branch with N modes, and one optical branch with N modes. in the first Brillouin zone ($|k(2a)|<\pi$, or , $|ka|<\pi/2$), since the lattice constant is $2a$. The total number of modes is $2N$. When M_1 becomes different from M_2, the lattice constant changes from a to $2a$. Correspondingly, the size of the Brillouin zone suddenly reduces from the region of $|ka|<\pi$ to the region of $|ka|<\pi/2$. As a result, at the zone boundary ($|ka|=\pi/2$), there occurs the folding effect of the acoustic branch. A part of the acoustic branch ($|ka|>\pi/2$) becomes the optical branches in the new first Brillouin zone ($|ka|<\pi/2$).

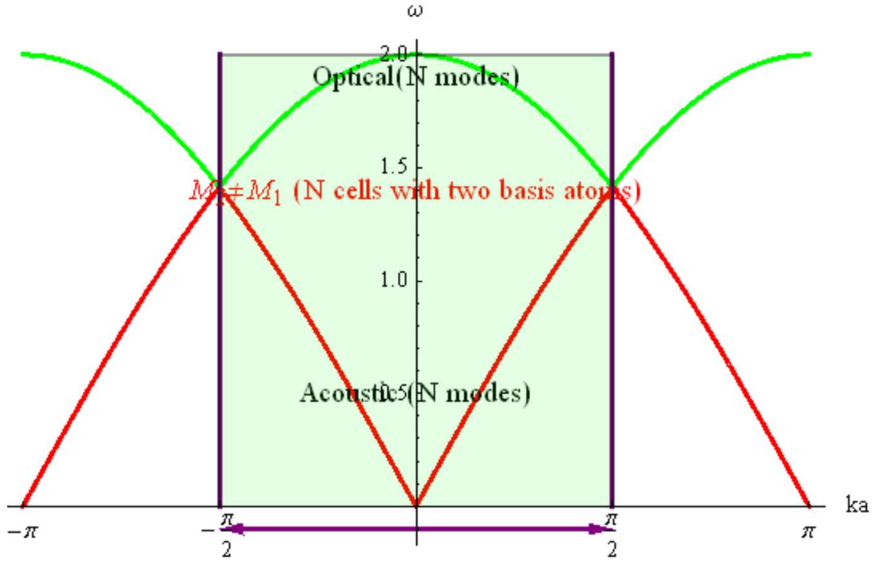


Fig.34

8. The number of modes; degree of freedom

8.1 Three-dimensional case (prediction)

We consider the degree of freedom for *N* atoms in the linear lattice chain. There are *N* atoms (each unit cell has one atom). Each atom has three degrees of freedom. One for each of the *x*, *y*, *z* directions. Then we have 3*N* degree of freedoms. This indicates that there are 3*N* modes in the system. This implies that the number of allowed *k* values in a single branch is just *N* for each Brillouin zone; 2*N* transverse acoustic (TA) modes and *N* longitudinal acoustic (LA) mode.

2 TA mode (2*N* states)
1 LA mode (*N* states)

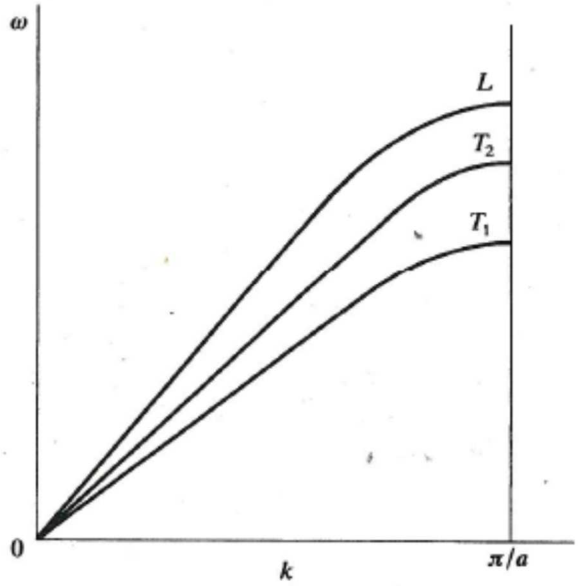


Fig.35 Longitudinal and transverse acoustic modes. The transverse modes may be degenerate as in the cubic structures

8.2 Three-dimensional case

We consider the lattice waves in the 3D system. The displacement vector $\boldsymbol{u}_s$ is given by

$$\boldsymbol{u}_s \sim e^{i\boldsymbol{k}\cdot\boldsymbol{R}_n}, \tag{7.1}$$

where $\boldsymbol{R}_n$ is the position vector of the atom located in the equilibrium positions of the lattice.

$$\boldsymbol{R}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3, \tag{7.2}$$

$\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and $\boldsymbol{a}_3$ are the primitive lattice vectors along the x, y, and z directions. From the boundary condition, we have

$$e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_n + N_1\boldsymbol{a}_1)} = e^{i\boldsymbol{k}\cdot\boldsymbol{R}_n}, \qquad \text{or} \qquad e^{ik_x N_1 a_1} = 1, \tag{7.3}$$

leading to the selected values of wavenumber k_x

$$k_x = \frac{2\pi}{N_1 a_1} l_1 = \frac{2\pi}{N_1 a} l_1 \qquad \text{for } a_1 = a_2 = a_3 = a. \tag{7.4}$$

Similarly, we have

$$k_y = \frac{2\pi}{N_2 a_2} l_2 = \frac{2\pi}{N_2 a} l_2, \qquad \text{and} \qquad k_z = \frac{2\pi}{N_3 a_3} l_3 = \frac{2\pi}{N_3 a} l_3 \tag{7.5}$$

Here l_1, l_2, and l_3 are integers given by

$$l_1 = -\frac{N_1}{2}, -\frac{N_1}{2} + 1, \ldots, \frac{N_1}{2} - 1, \frac{N_1}{2}, \tag{7.6}$$

$$l_2 = -\frac{N_2}{2}, -\frac{N_2}{2} + 1, \ldots, \frac{N_2}{2} - 1, \frac{N_2}{2},$$

$$l_3 = -\frac{N_3}{2}, -\frac{N_3}{2} + 1, \ldots, \frac{N_3}{2} - 1, \frac{N_3}{2}.$$

This means that there are N ($=N_1N_2N_3$) modes, where N is the number of unit cells in the system.

Each mode has 3 degrees of freedom (1 longitudinal mode and 2 transverse modes). Then the total number of modes is $3 \times N = 3N$.

(a)

In the case of one atom per unit cell, we have $3N$ degree of freedom, with N longitudinal acoustic mode and transverse acoustic mode $2N$

(b)

We consider the number of degrees of freedom of the atoms. With p atoms in the primitive cell and N primitive cells, there are pN atoms. Each atom has three degrees of freedom, one for each of the x, y, z directions, making a total of $3pN$ degrees of freedom for the crystal. The number of allowed k values in a single branch is just N for one Brillouin zone. Thus, the one LA and two TA branches have a total of $3N$ modes. The remaining $(3p - 3) \times N$ degrees of freedom are accommodated by the optical branches.

3 acoustical branches; $3N$ states
  1 longitudinal acoustical (LA) mode
  2 transverse acoustical (TA) mode

$3p$ - 3 optical branches; $N(3p-3)$ states
  (p - 1) longitudinal optical (LO) mode
  2(p - 1) transverse optical (TO) mode

The number of the total states is $3pN$

For $p = 2$, for example, we have 1 LA, 1 LO modes, and 2 TA and 2 TO modes.

9. Classical Model

9.1 Theory of the transverse wave in a string

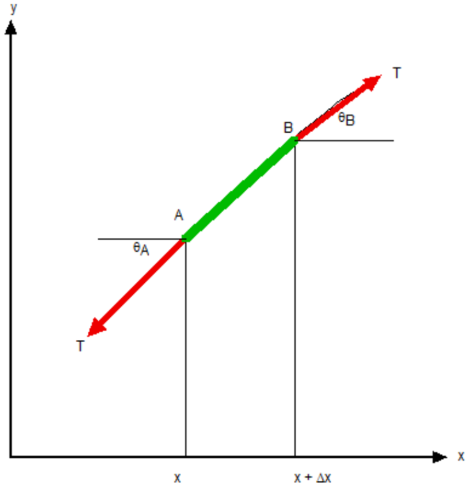


Fig.36 Oscillation of one-dimensional continuum

Suppose that a traveling wave is propagating along a string that is under a tension T_s. Let us consider one small element of length Δx. The ends of the element make small angle θ_A and θ_B with the x axis. The net force acting on the element along the y-axis is

$$\begin{aligned}\sum F_y &= T\sin\theta_B - T\sin\theta_A \\ &= T(\sin\theta_B - \sin\theta_A) \approx T(\tan\theta_B - \tan\theta_A)\end{aligned}, \tag{9.1}$$

or

$$F_y = T[\left(\frac{\partial y}{\partial x}\right)_B - \left(\frac{\partial y}{\partial x}\right)_A]. \tag{9.2}$$

We now apply the Newton's second law to the element, with the mass of the element given by $m = \mu\Delta x$,

$$F_y = ma_y = \mu\Delta x\frac{\partial^2 y}{\partial t^2}. \tag{9.3}$$

Then we have

$$\begin{aligned}\mu\Delta x\frac{\partial^2 y}{\partial t^2} &= T_s[\left(\frac{\partial y}{\partial x}\right)_B - \left(\frac{\partial y}{\partial x}\right)_A] \\ \frac{\mu}{T_s}\frac{\partial^2 y}{\partial t^2} &= \frac{\left(\frac{\partial y}{\partial x}\right)_B - \left(\frac{\partial y}{\partial x}\right)_A}{\Delta x} = \frac{\partial^2 y}{\partial x^2}\end{aligned}, \tag{9.4}$$

which leads to a wave equation given by

$$\frac{\partial^2 y}{\partial x^2} = \frac{\mu}{T_s}\frac{\partial^2 y}{\partial t^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}, \tag{9.5}$$

where v is the velocity of the sound,

$$v = \sqrt{\frac{T_s}{\mu}}. \tag{9.6}$$

Here we use the Taylor expansion,

$$\left(\frac{\partial y}{\partial x}\right)_B - \left(\frac{\partial y}{\partial x}\right)_A = \left(\frac{\partial y}{\partial x}\right)_{x+\Delta x} - \left(\frac{\partial y}{\partial x}\right)_x = \Delta x \frac{\partial}{\partial x}\left(\frac{\partial y}{\partial x}\right) = \Delta x \frac{\partial^2 y}{\partial x^2}. \tag{9.6}$$

9.2 Energy density of the elastic wave

When the length of element changes to Δx to $\Delta x\sqrt{1+\left(\frac{\partial y}{\partial x}\right)^2}$, the work done in the system (= W_c) of the conserved system is given by

$$-T_s\Delta x\sqrt{1+\left(\frac{\partial y}{\partial x}\right)^2} + T_s d\Delta = -T_s d\Delta[1+\frac{1}{2}\left(\frac{\partial y}{\partial x}\right)^2 - 1] = -\frac{T_s}{2}\Delta x\left(\frac{\partial y}{\partial x}\right)^2. \tag{9.7}$$

Since the potential energy ΔU is related to W_c by $\Delta U = -W_c$, the potential energy ΔU is given by

$$\Delta U = \frac{T_s}{2}\Delta x\left(\frac{\partial y}{\partial x}\right)^2. \tag{9.8}$$

The kinetic energy contribution ΔK is given by

$$\Delta K = \mu\Delta x\frac{1}{2}\left(\frac{\partial y}{\partial t}\right)^2. \tag{9.9}$$

Then the energy density is given by

$$\Delta E = \Delta K + \Delta U = \Delta x[\frac{T_s}{2}\left(\frac{\partial y}{\partial x}\right)^2 + \frac{\mu}{2}\left(\frac{\partial y}{\partial t}\right)^2]. \tag{9.10}$$

10. Quantum mechanical approach: phonon

10.1 Annihilation and creation operators[1,3]

We assume $\boldsymbol{U} = (u_1, u_2,$ $, u_N)$ for the eigenvalue $\omega = \omega_k$. The displacement $u(x)$ is expressed using a Dirac delta function,

$$u(x) = \sum_l u_l \delta(x - la)$$

, (10.1)

with $L = Na$.

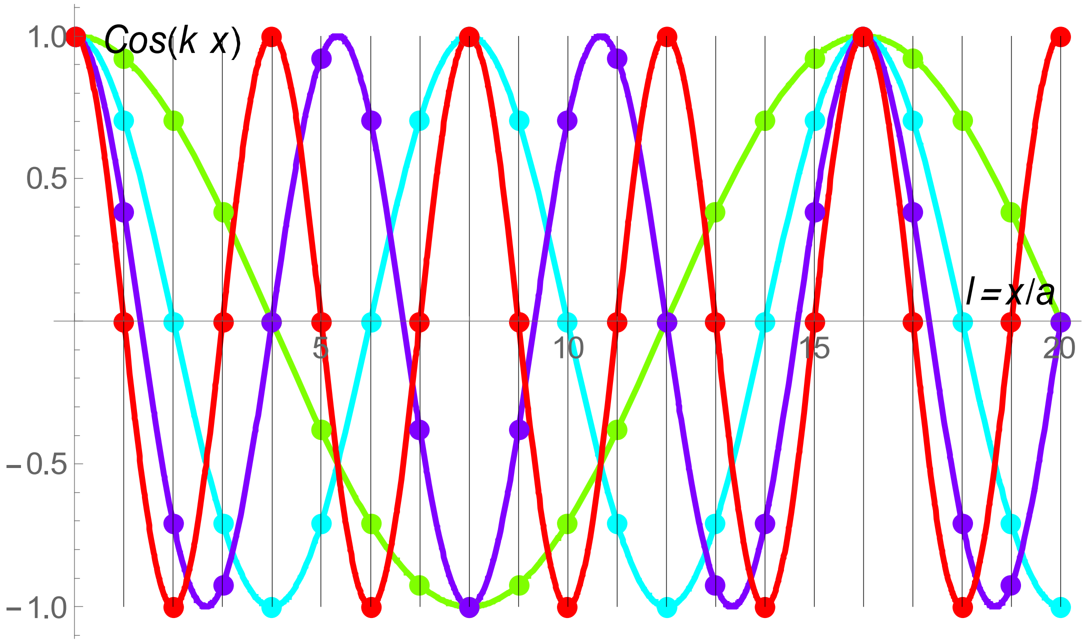


Fig.37 Plot of $u(x) = \sum_l e^{ilka}\delta(x - la)$ with the wavenumber k being changed as a parameter. $l = x/a$ (integers). $u(x)$ is equal to $\cos(kla) = \cos(kx)$ at $x = la$.

The Fourier transform of $u(x)$ is given by

$$U_k = \frac{1}{\sqrt{N}} \int dx u(x) e^{-ikx} = \frac{1}{\sqrt{N}} \sum_s u_s e^{-iksa}. \tag{10.2}$$

The inverse Fourier transform of U_k is

$$\frac{1}{\sqrt{N}} \sum_k e^{iksa} U_k = \frac{1}{\sqrt{N}} \sum_k \frac{1}{\sqrt{N}} \sum_{s'} u_s{}' e^{-iks'a} e^{iksa}$$

$$= \frac{1}{N} \sum_{s'} u_s{}' \sum_k e^{ika(s-s')}$$

$$= \frac{N}{N}\sum_{l'} u_{l}'\delta_{l,l'}$$
$$= u_s$$

(10.3)

or

$$u_l = \frac{1}{\sqrt{N}}\sum_k e^{ikla}U_k$$

(10.4)

The Lagrangian of the system is given by

$$\begin{aligned} L &= T - V \\ &= \sum_l [\frac{M}{2}\dot{u}_l{}^2 - \frac{1}{2}C(u_{l+1} - u_l)^2] \end{aligned}$$

(10.5)

We use the notation

$$u_l = \frac{1}{\sqrt{N}}\sum_k e^{ikla}U_k$$

. (10.6)

Since u_l is real, it is required that

$$U_{-k} = U_k^{\ *}. \qquad (10.7)$$

Using these relations, we have

$$\begin{aligned} \sum_l \dot{u}_l{}^2 &= \frac{1}{N}\sum_k\sum_{k'}\sum_l \dot{U}_k\dot{U}_{k'}e^{i(k+k')la} \\ &= \sum_k\sum_{k'}\dot{U}_k\dot{U}_{k'}\delta_{k',-k} \\ &= \sum_k \dot{U}_k\dot{U}_{-k} \end{aligned}$$

(10.8)

Here we use

$$\sum_{s=1}^{N} e^{i(k+k')sa} = N\delta_{k',-k} \, . \tag{10.9}$$

Similarly

$$\begin{aligned} C\sum_{l}(u_{l+1}-u_{l})^{2} &= 2C\sum_{k} U_{k}U_{-k}(1-\cos ka) \\ &= \sum_{k} M\omega_{k}{}^{2}U_{k}U_{-k} \end{aligned} \tag{10.10}$$

where

$$\omega_{k}{}^{2} = \frac{2C}{M}(1-\cos ka) = \frac{4C}{M}\sin^{2}\frac{ka}{2} \tag{10.11}$$

or

$$\omega_{k} = \sqrt{\frac{4C}{M}}\left|\sin\frac{ka}{2}\right|$$

(the dispersion relation)

Then the Lagrangian *L* can be rewritten as

$$L = \sum_{k}\left(\frac{M}{2}\dot{U}_{k}\dot{U}_{-k} - \frac{M\omega_{k}{}^{2}}{2}U_{k}U_{-k}\right) \tag{10.12}$$

The linear momentum P_k conjugate to U_k is defined by

$$P_{k} = \frac{\partial L}{\partial \dot{U}_{k}} = M\dot{U}_{-k}, \tag{10.13}$$

Then Hamiltonian *H* is obtained as

$$H = \sum_{k} P_{k}\dot{U}_{k} - L$$

$$= \sum_k \left(\frac{1}{2M} P_k P_{-k} + \frac{1}{2} M \omega_k{}^2 U_k U_{-k}\right)$$

(10.14)

Note that we define the Fourier transform of the linear momentum by

$$p_l = \frac{1}{\sqrt{N}} \sum_k e^{-ikla} P_k$$

$$P_k = \frac{1}{\sqrt{N}} \sum_k e^{ikla} p_s$$

(10.15)

with

$$P_{-k} = P_k^* = P_k^+, \qquad U_{-k} = U_k^* = U_k^+ \qquad \text{(definition)}$$

(10.16)

Let us work it out by the operator technique, starting from the commutation relations,

$$[u_l, p_{l'}] = i\hbar \delta_{l,l'}$$

(10.17)

Then the commutation relation is preserved in $[U_k, P_{k'}] = i\hbar\delta_{k,k'}$, since

$$\begin{aligned} [U_k, P_{k'}] &= \left[\frac{1}{\sqrt{N}} \sum_l e^{-ikla} u_l \, , \frac{1}{\sqrt{N}} \sum_{l'} e^{ik'l'a} p_{l'}\right] \\ &= \frac{1}{N} \sum_l \sum_{l'} e^{-ikla} [u_l, p_{l'}] e^{ik'l'a} \\ &= \frac{i\hbar}{N} \sum_l \sum_{l'} e^{-ikla} e^{ik'l'a} \delta_{l,l'} \\ &= \frac{i\hbar}{N} \sum_l e^{-i(k-k')la} \\ &= i\hbar \delta_{k,k'} \end{aligned}$$

(10.18)

Thus our new displacements and momenta are canonically conjugate, and non-commuting, if they are of the same wavenumber; otherwise they are dynamically independent operators. The Hamiltonian is rewritten as

$$H = \sum_k \left(\frac{1}{2M} {P_k}^+ P_k + \frac{1}{2} M {\omega_k}^2 {U_k}^+ U_k\right)$$

(10.19)

The final step is the introduction of annihilation and creation operators defined by

$$a_k{}^+ = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{M\omega_k}{\hbar}} U_k{}^+ - \frac{1}{\sqrt{M\hbar\omega_k}} iP_k\right)$$

$$a_k = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{M\omega_k}{\hbar}} U_k + \frac{1}{\sqrt{M\hbar\omega_k}} iP_k{}^+\right)$$

(10.20)

where a_k and $a_k{}^+$ act to destroy, and create a phonon of wavenumber, k and energy $\hbar\omega_k$, respectively. One can get the expressions for P_k and U_k from the above equations for a_k and $a_k{}^+$

$$P_k = i\sqrt{\frac{M\hbar\omega_k}{2}}(a_k{}^+ - a_{-k}),$$

(10.21)

$$U_k = \sqrt{\frac{\hbar}{2M\omega_k}}(a_k + a_{-k}{}^+)$$

. (10.22)

The annihilation and creation operators satisfy the commutation

$$\left[a_k, a_{k'}^+\right] = \delta_{k,k'},$$ (10.23)

$$\left[a_k, a_{k'}\right] = \left[a_k^+, a_{k'}^+\right] = 0,$$ (10.24)

The transformed Hamiltonian is

$$H = \sum_k \hbar\omega_k\left(a_k{}^+ a_k + \frac{1}{2}\right) = \sum_k \hbar\omega_k\left(N_k + \frac{1}{2}\right)$$

(10.25)

where $N_k = a_k^+ a_k$. So that each phonon may be regarded as possessing an energy $\hbar\omega_k$. The total Hamiltonian is the sum of the Hamiltonian of independent linear oscillators of angular frequency ω_k. The excitations correspond to waves travelling to right or left round the ring of atoms, with angular frequency ω_k and wavenumber k. The eigenstates of the Hamiltonian can be written in the form

$$|n_1, n_1, \dots, n_k, \dots.\rangle$$

corresponding to there being n_k quanta in the k-th mode. Various properties of the operators and eigenstates of the Hamiltonian are seen in the **Appendix A**.

11. Crystal momentum

A phonon of $\boldsymbol{k}$ will interact with particles such as photons, neutrons, and electrons as if it had a momentum $\hbar\boldsymbol{k}$. However, a phonon does not carry physical momentum. The physical momentum of a crystal is given by

$$\begin{aligned} P_k &= \frac{\partial L}{\partial \dot{U}_k} \\ &= M\dot{U}_{-k} \\ &= \frac{M}{\sqrt{N}} \sum_s \dot{u}_s e^{iska} \end{aligned}$$

(12.1)

where

$$U_k = \frac{1}{\sqrt{N}} \int dx u(x) e^{-ikx} = \frac{1}{\sqrt{N}} \sum_s u_s e^{-iksa}. \tag{12.2}$$

We assume that $\dot{u}_s$ is independent of s; $\dot{u}_s = \dot{u}$. Then the momentum P_k is evaluated as

$$\begin{aligned} P_k &= \frac{M}{\sqrt{N}} \dot{u} \sum_s e^{iska} \\ &= \frac{M}{\sqrt{N}} \dot{u}\left[1 + e^{ika} + e^{2ika} + \dots + e^{ika(N-1)}\right] \\ &= M\sqrt{N}\dot{u}\delta_{k,0}, \end{aligned}$$

(12.3)

where $k = \dfrac{2\pi r}{Na}$ (r = 0, ±1, ±2,…, ±N/2). The mode k = 0 represents a uniform translation of the crystal as a whole. Such a translation does carry momentum. For most practical purpose, a phonon acts as if its momentum were $\hbar\boldsymbol{k}$, sometimes called the crystal momentum.

((Note-1)) H.P.Myers, Introductory Solid State Physics (Taylor & Francis, 1990).

A discrete vibrational state or mode has a well defined wave vector k and an application of de Broglie's principle implies a linear momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$. However, the only true mechanical momentum that can arise is a rigid motion of the whole specimen. The vibrational modes transport energy, but they are completely described by the relative motion of the individual atoms, whose average displacement is zero; they cannot therefore contain a net momentum and the quantity $\hbar\boldsymbol{k}$ is not to be identified with the conventional linear momentum.

((Mote-2)) S.H. Simon, The Oxford Solid State Basis (Oxford, 2013).

The wavevector of a phonon is defined only modulo the reciprocal lattice. In other words, $\boldsymbol{k}$ is the same as $\boldsymbol{k} + \boldsymbol{G}$, where $\boldsymbol{G}$ is the reciprocal lattice. In other words, $\boldsymbol{k}$ is the same as $\boldsymbol{k} + \boldsymbol{G}$. Now we are supposed to think of these phonons as particles - and we lie to think of these particles as having energy $\hbar\omega$ and momentum $\hbar\boldsymbol{k}$. But we cannot define a phonon's momentum this way because physically it is the same phonon whether we describe it as $\hbar\boldsymbol{k}$ or $\hbar(\boldsymbol{k} + \boldsymbol{G})$. We thus instead define a concept as the crystal momentum which is the momentum modulo the reciprocal lattice – or equivalently we agree that we must always describe within the first Brillouin zone. In an elastic collision of two (or more) phonons, the total energy and crystal momentum are conserved.

12. Propagation of phonon

12.1 Introduction ((Feynman))

We consider a simpler example to illustrate the generality of the motion: a particle in a periodic potential. $V(x) = 1 - \cos(Gx)$ with $G = \dfrac{2\pi}{a}$ (reciprocal lattice) for the one-dimensional chain with a lattice constant a. The minima are at $x=ma$, where m is any integer. The symmetry of the problem is the discrete translation $x = la \rightarrow (l+1)a$. The approximate states, $|l\rangle$, which are Gaussians centered around the classical minima, break the symmetry and are converted to each other by $T_x(a)$, the operator that translates $x = la \rightarrow (l+1)a$

$$T_x(a)|l\rangle = |l+1\rangle.$$

However, adjacent classical minima are connected by a nonzero tunneling amplitude of the type we just calculated and the Hamiltonian H has off-diagonal amplitudes between $|l\rangle$ and. (There are also solutions describing tunneling to next-nearest-neighbor minima, but these have roughly double the action as the nearest-neighbor tunneling process and lead to an off-diagonal matrix element that is roughly the square of the one due to nearest-neighbor tunneling.) Suppose the one-dimensional world were finite and forms a closed ring of size *N,* so that there were *N* degenerate classical minima. These would evolve into *N* nondegenerate levels due to the mixing due to tunneling.

The content of this topics can be found in the Feynman's lecture on physics.

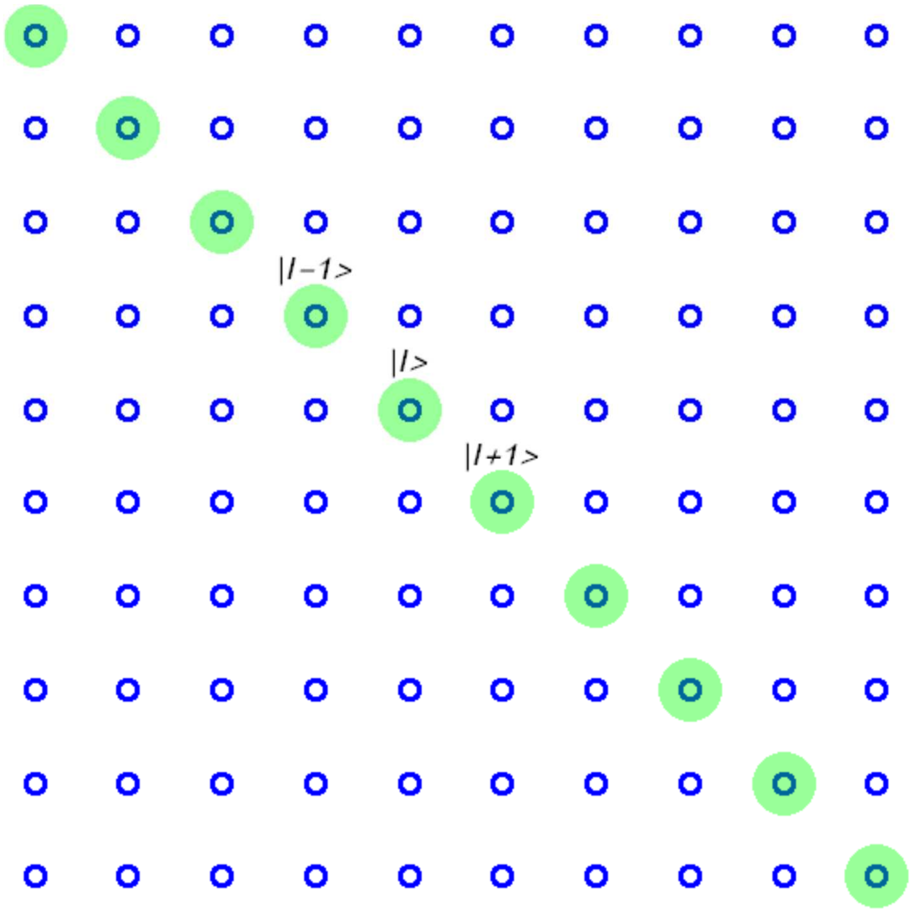


Fig.38 The base states of an electron in a one-dimensional crystal.

12.2. Quantum state $|\theta_k\rangle$: simultaneous eigenket of H and $T_x(a)$

We consider a periodic lattice with a lattice constant a. The translation operator $T_x(a)$ commutes with the Hamiltonian H,

$$[T_x(a), H] = 0.$$

Thus we have a simultaneous eigenket of $T_x(a)$ and H.

$$H|\theta\rangle = E|\theta\rangle, \qquad T_x(a)|\theta\rangle = \lambda|\theta\rangle,$$

The operator $T_x(a)$ is unitary (a; lattice constant) and hence its eigenvalues need not be real. Let us suppose that the potential barrier between the lattice points is infinitely high. Let $|l\rangle$ be the state localized in the lattice cell l, i.e.

$$\langle x|l\rangle \neq 0 \qquad \text{only if } x \approx la.$$

The state $|l\rangle$ is not an eigenstate of the translation $T_x(a)$

$$T_x(a)|l\rangle = |l+1\rangle,$$

We assume that

$$|\theta\rangle = \sum_{l=-\infty}^{\infty} e^{il\theta}|l\rangle$$

where θ is a real parameter and

$$-\pi \leq \theta \leq \pi \, .$$

Thus we have

$$\begin{aligned} T_x(a)|\theta\rangle &= \sum_{l=-\infty}^{\infty} e^{il\theta}T_x(a)|l\rangle \\ &= \sum_{l=-\infty}^{\infty} e^{il\theta}|l+1\rangle \\ &= \sum_{l=-\infty}^{\infty} e^{i(l-1)\theta}|l\rangle \\ &= e^{-i\theta}\sum_{l=-\infty}^{\infty} e^{il\theta}|l\rangle \\ &= e^{-i\theta}\sum_{l=-\infty}^{\infty} e^{il\theta}|l\rangle \\ &= e^{-i\theta}|\theta\rangle \end{aligned}$$

which satisfies the Bloch condition (as will be described). Thus $|\theta\rangle$ is the eigenstate of $T_x(a)$ with the eigenvalue $e^{-i\theta}$. Using the relation

$$T_x(a)|l\rangle = |l+1\rangle$$

We have

$$[T_x(a)]^2|l\rangle = |l+2\rangle$$

……

$$[T_x(a)]^N|l\rangle = |l+N\rangle = |l\rangle$$

Using the periodic boundary (Born-von Karman) condition, we have

$$e^{-iN\theta} = 1$$

or

$$N\theta = 2\pi s$$

with s (integer). Thus we have

$$\theta = \frac{2\pi s}{N} = \frac{2\pi s}{Na} a = ka$$

where k is the wave number and defined by

$$k = \frac{2\pi}{Na} s$$

$$(s = 0, 1, 2, \quad , N\text{-}1),$$

or

$$-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}, \qquad \Delta k = \frac{2\pi}{Na}$$

N is the total number of atoms in the 1D chain. Hereafter, we use $|\theta_k\rangle$ instead of $|\theta\rangle$,

$$|\theta_k\rangle = \sum_{l=-\infty}^{\infty} e^{ilka} |l\rangle \tag{11.1}$$

where k is a wavenumber (there are N states with different k).

12.3. Energy eigenvalue of *H* (quantum mechanical approach)

The quantum mechanics of phonon has been extensively discussed in standard text book of solid state physics (such as Kittel and Ziman). The Lagrangian L for the one-dimensional chain is given by

$$L = T - V$$

$$= \sum_l [\frac{M}{2}\dot{u}_l{}^2 - \frac{1}{2}C(u_{l+1} - u_l)^2]$$

$$= L(\dot{u}_1, \dot{u}_2, \dots, \dot{u}_{N-1}, u_1, u_2, \dots, u_{N-1}\ ).$$

(11.2)

The linear momentum conjugate to u_l, is given by

$$p_l = \frac{\partial L}{\partial \dot{u}_l} = M\dot{u}_l$$

(11.3)

Then the Hamiltonian H can be derived as

$$H = \sum_l p_l \dot{u}_l - L$$

$$= \sum_l M\dot{u}_l{}^2 - \sum_l [\frac{M}{2}\dot{u}_l{}^2 - \frac{1}{2}C(u_{l+1} - u_l)^2]$$

$$= \sum_l [\frac{M}{2}\dot{u}_l{}^2 + \frac{1}{2}C(u_{l+1} - u_l)^2]$$

(11.4)

or

$$H = \sum_l [\frac{p_l{}^2}{2M} + \frac{1}{2}C(u_l - u_{l+1})^2].$$

We note that

$$T_x{}^+(a) p_l T_x(a) = p_l$$

$$T_x{}^+(a) p_l{}^2 T_x(a) = p_l{}^2$$

$$T_x{}^+(a) u_l T_x(a) = u_{l+1}$$

$$T_x{}^+(a)(u_{l+1} - u_l) T_x(a) = (u_{l+2} - u_{l+1})$$

$$T_x{}^+(a)(u_{l+1} - u_l)^2 T_x(a) = (u_{l+2} - u_{l+1})^2$$

where $T_x{}^+(a)$ is the Hermitian conjugate of $T_x(a)$. Such relations lead to the commutation relation,

$$[H, T_x(a)] = 0.$$

$|\theta\rangle$ is the simulutaneous eigenket of H and $T_x(a)$;

$$T_x(a)|\theta_k\rangle = e^{-i\theta_k}|\theta_k\rangle, \qquad H|\theta_k\rangle = E_k|\theta_k\rangle$$

We will show that $|\theta_k\rangle$ is the eigenket of H with the energy eigenvalue E_k.

12.4. Simultaneous eigenket of H and $T_x(a)$

We discuss the possibility that

$$|\theta_k\rangle = \frac{1}{\sqrt{N}}\sum_{l=0}^{N} e^{ilka}|l\rangle$$

is the energy eigenstate of H with the energy eigenvalue,

$$E_k = \hbar\omega_k = \hbar\sqrt{\frac{4C}{M}}\left|\sin\frac{ka}{2}\right|$$

We now consider the eigenvalue problem,

$$H|\theta_k\rangle = \frac{1}{\sqrt{N}}\sum_{l=-\infty}^{\infty} e^{ilka}H|l\rangle$$

Because all lattice cells are exactly alike we must have

$$H|l\rangle = E|l\rangle$$

or

$$E = \langle l|H|l\rangle$$

for any $|l\rangle$. Then we have

$$\begin{aligned} H|\theta_k\rangle &= \frac{1}{\sqrt{N}}\sum_{l,n_k} e^{ilka}H|l\rangle \\ &= E\frac{1}{\sqrt{N}}\sum_{l,} e^{ilka}|\, l\rangle \\ &= E|\theta_k\rangle. \end{aligned}$$

or

$$E = \langle \Theta_k | H | \Theta_k \rangle$$

In other word, $|\Theta_k\rangle$ is the eigenket of H with the energy eigenvalue E. We note that

$$\begin{aligned}
\langle l' | \Theta_k \rangle &= \frac{1}{\sqrt{N}} \sum_{l=1}^{N} e^{ilka} \langle l' | l \rangle \\
&= \tfrac{1}{\sqrt{N}} e^{il'ka}.
\end{aligned}$$

12.5 Bloch condition

The $|x\rangle$-representation of $|\Theta_k\rangle$

$$\langle x | \Theta_k \rangle = \frac{1}{\sqrt{N}} \sum_{l=0}^{N} e^{ilka} \langle x | l \rangle$$

where $\langle x | l \rangle$ is the wave function which is localized at $x = la$. We prove that this wave function is of the Bloch form.

$$\begin{aligned}
\langle x - a | \Theta_k \rangle &= \langle x |\, T_x(a) | \Theta_k \rangle \\
&= \frac{1}{\sqrt{N}} \sum_{l=0}^{N} e^{ilka} \, \langle x |\, T_x(a) | l \rangle \\
&= \frac{1}{\sqrt{N}} \sum_{l=0}^{N} e^{ilka} \, \langle x | l + 1 \rangle \\
&= e^{-ika} \frac{1}{\sqrt{N}} \sum_{l=0}^{N} e^{i(l+1)ka} \, \langle x | l + 1 \rangle \\
&= e^{-ika} \langle x | \Theta_k \rangle
\end{aligned}$$

which is exactly the Bloch condition.

12.6 Diagonal matrix element

The diagonal matrix element of the Hamiltonian is given by

$$\begin{aligned}
E &= \langle \Theta_k | H | \Theta_k \rangle \\
&= \frac{1}{N} \sum_{l,l'} \langle l | H | l' \rangle e^{ik(l'-l)a} \\
&= \frac{1}{N} \sum_{l,l'} \langle l | H | l \rangle \delta_{l,l'} e^{ik(l'-l)a} \\
&= \frac{1}{N} \sum_{l} \langle l | H | l \rangle
\end{aligned}$$

which leads to E,

12.7 The form of wave function

$$H|l\rangle = \hbar\omega(n+\frac{1}{2})|l\rangle$$

The wave function of the simple harmonics which is localized at $x = la$,

$$\langle x|l\rangle = 2^{-\frac{n}{2}}\pi^{-\frac{1}{4}}(n!)^{-\frac{1}{2}}e^{-\frac{z^2}{2}}H_n(z)$$

with

$$z = \sqrt{\frac{m\omega}{\hbar}}(x-la)$$

$$E_n = \hbar\omega(n+\frac{1}{2})$$

Hermite polynomial:

$$H_n(z) = (-1)^n e^{z^2}\frac{d^n}{dz^n}e^{-z^2}$$

We make a plot of

$$Re[\langle x|\theta_k\rangle] = Re[\sum_{l=1}^{N} e^{ikla}\langle x|l\rangle]$$
$$= \sum_{l=1}^{N}\cos((kla)\langle x|l\rangle]$$

as a function of *x*, where

$$\langle x|l\rangle = 2^{-\frac{n}{2}}\pi^{-\frac{1}{4}}(n!)^{-\frac{1}{2}}e^{-\frac{z^2}{2}}H_n(z)$$

with

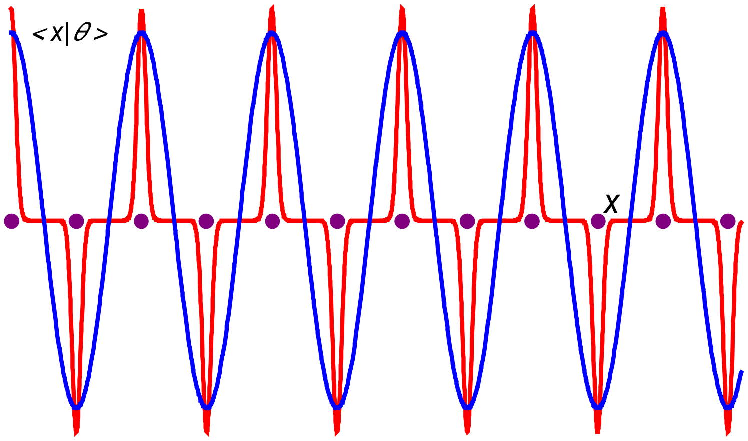
$$z = \sqrt{\frac{m\omega}{\hbar}}(x-la)$$

For *n* = 0 (the ground state of the simple harmonics).

$$\langle x|l\rangle = \pi^{-\frac{1}{4}}\exp[-\frac{m\omega}{2\hbar}(x-la)^2]$$

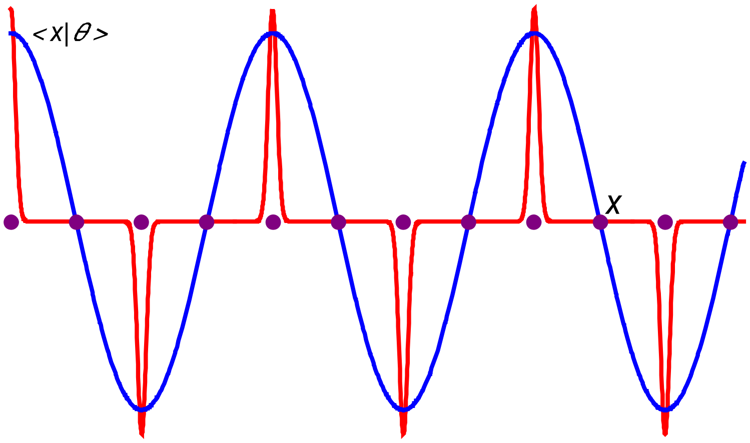
which is the Gaussian form (which is localized at $x = la$).

(a) $k = \frac{\pi}{a}$

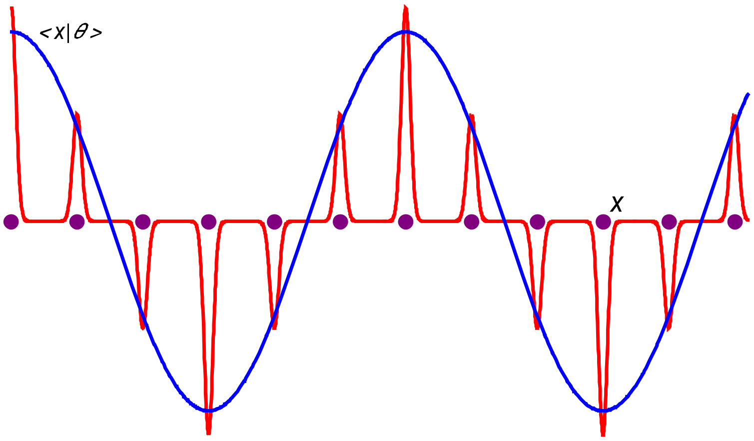


The position of atoms is denoted by purple

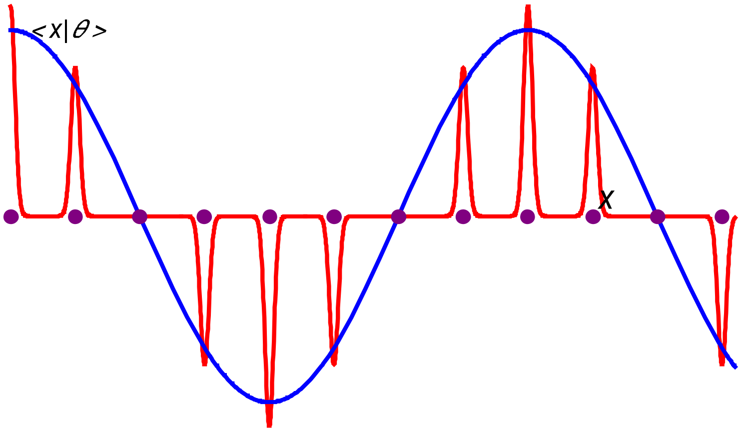
(b) $k = \frac{\pi}{2a}$



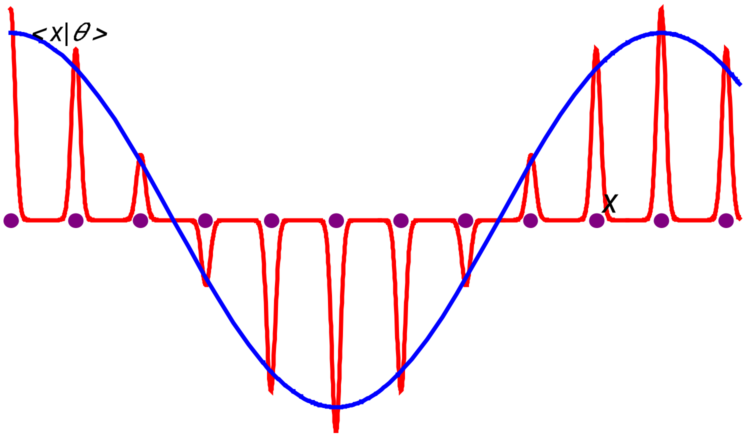
(c) $k = \frac{\pi}{3a}$



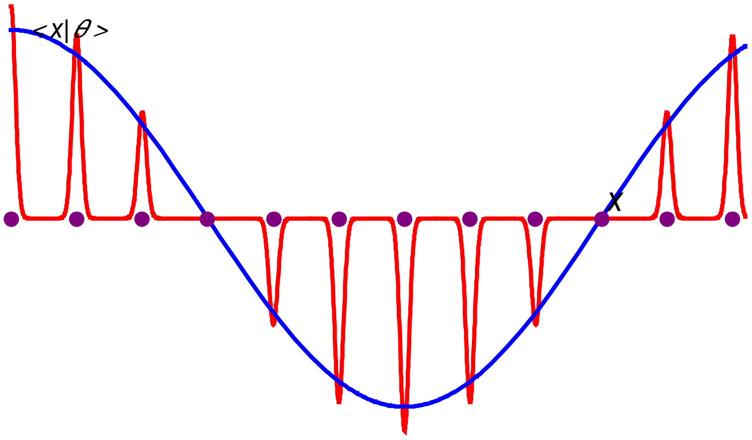
(d) $k = \frac{\pi}{4a}$



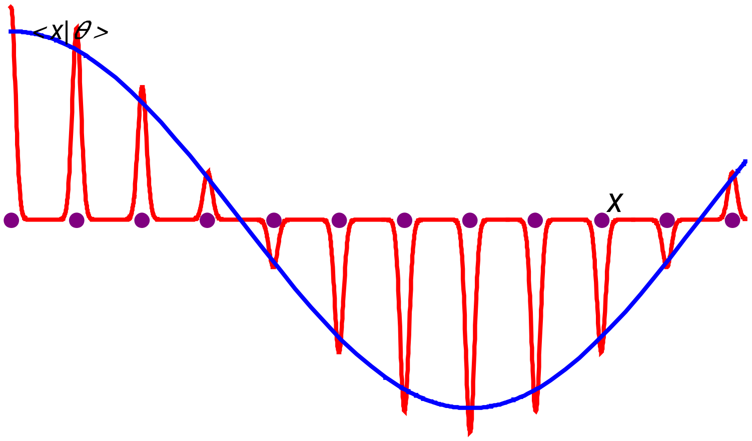
(e) $k = \frac{\pi}{5a}$



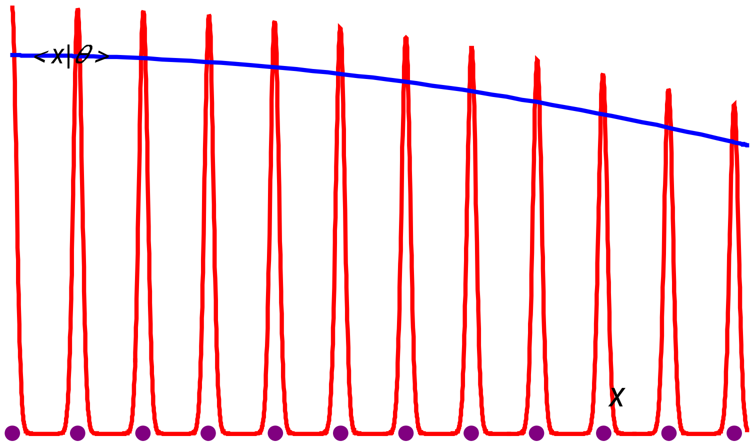
(f) $k = \frac{\pi}{6a}$



(g) $k = \frac{\pi}{7a}$



(h) $k = \frac{\pi}{50a}$



13 Semi-classical approach

13.1 Simple case

The energy of a lattice vibration is quantized. The quantum of energy is called a phonon. Elastic waves in crystals are made up of phonons. Thermal vibrations in crystals are thermally excited phonons. The energy of an elastic mode of angular frequency ω_k is

$$\varepsilon_k = \left(\langle n_k \rangle + \frac{1}{2} \right) \hbar\omega_k , \tag{13+.1}$$

when the mode is excited to quantum number $\langle n_k \rangle$, where the mode is occupied by n photons. The term $\frac{1}{2}\hbar\omega$ is the zero pint energy of the mode. We consider the wave of the mode k with the amplitude.

$$u = u_k \cos(\omega_k t - kx) , \tag{13.2}$$

where u is the displacement of a volume element from its equilibrium positions at x in the crystal.

$$u_k = u_0 \cos(\omega t - kx) = u_0 (\cos\omega t \cos kx + \sin\omega t \sin kx) . \tag{13.3}$$

The energy in the mode is

$$\varepsilon_k = [\langle K \rangle + \langle P \rangle] = 2\langle K \rangle \qquad (\because \langle K \rangle = \langle P \rangle) \tag{13.4}$$

when it is averaged over time.

$$K = \frac{1}{2}\rho\left(\frac{\partial u}{\partial t}\right)^2, \tag{13.5}$$

$$\frac{\partial u}{\partial t} = u_0\omega_k\left[-\sin\omega_k t\cos kx + \cos\omega_k t\sin kx\right], \tag{13.6}$$

where ρ is the mass density.

$$\begin{aligned}\int KdV = \frac{1}{2}\rho u_0^2\omega_k^2\int_V dV[-\sin^2\omega_k t\cos^2 kx + \cos^2\omega_k t\sin^2 kx \\ -2\sin\omega_k t\cos\omega_k t\sin kx\cos kx]\end{aligned}. \tag{13.7}$$

Note that

$$dV = Adx$$

where A is the total area in the y-z plane (the x axis is normal to this plane), and the total volume V is given by $V = AL = ANa$. Here we have

$$\begin{cases} x = 0 \sim Na(=L) \\ k = \dfrac{\pi}{a\left(\dfrac{N}{2}\right)}\ell = \dfrac{2\pi}{aN}\ell \quad \left(\ell = 0, \pm1, \cdots, \pm\dfrac{N}{2}\right), \end{cases} \tag{13.8}$$

from the boundary condition: cos(kNA) = 1 ⇒ $kNa = 2\pi\ell$). Then we obtain

$$\int_0^{Na} dx\cos^2 kx = \int_0^{Na} dx\frac{1}{2}(1+\cos 2kx) = \frac{1}{2}Na + [k\sin 2kx]_0^{Na} = \frac{1}{2}Na\,. \tag{13.9}$$

$$(\because 2kNa = 2\left(\frac{2\pi}{aN}\ell\right)Na = 4\pi\ell).$$

Similarly, we have

$$\int_0^{Na} dx\sin^2 kx = \frac{1}{2}Na\,, \qquad \int_0^{Na} dx\sin kx\cos kx = 0\,. \tag{13.10}$$

Then we have

$$\int KdV = \int KAdx = \frac{V}{4}\rho u_0^2\omega^2(\sin^2\omega t + \cos^2\omega t) = \frac{V}{4}\rho u_0^2\omega^2\,. \tag{13.11}$$

The time average kinetic energy is

$$\langle K \rangle = \frac{V}{4}\rho u_0^2 \omega^2 \frac{1}{T}\int_0^T dt = \frac{V}{4}\rho u_0^2 \omega^2 . \tag{13.12}$$

Since $\langle K \rangle = \frac{1}{2}\varepsilon$, we have

$$\frac{V}{4}\rho u_0^2 \omega_k^2 = \frac{1}{2}\varepsilon = \frac{1}{2}\left(\langle n_k \rangle + \frac{1}{2}\right)\hbar\omega_k , \tag{13.13}$$

or

$$u_0^2 = \frac{2\hbar\left(\langle n_k \rangle + \frac{1}{2}\right)}{\rho V \omega_k} \Rightarrow u_{eff} = \frac{1}{\sqrt{2}} u_0 . \tag{13.15}$$

Since $\rho V = NM$,

$$u_0^2 = \frac{2\hbar\left(\langle n_k \rangle + \frac{1}{2}\right)}{NM\omega_k} . \tag{13.16}$$

This relates the displacement in a given mode to the phonon occupancy n of the mode. An optical mode with ω close to zero is called a soft mode.

13.2 General case

The Lagrangian L is given by

$$\begin{aligned} L &= T - V \\ &= \sum_s \left[\frac{M}{2}\dot{u}_s{}^2 - \frac{1}{2}C(u_{s+1} - u_s)^2\right] \\ &= L(\dot{u}_1, \dot{u}_2 \ldots . \dot{u}_{N-1}, u_1, u_2 \ldots . u_{N-1}) \end{aligned} \tag{13.17}$$

The linear momentum conjugate to us, is given by

$$p_s = \frac{\partial L}{\partial \dot{u}_s} = M\dot{u}_s \tag{13.18}$$

Then the Hamiltonian H can be derived as

$$\begin{aligned} H &= \sum_s p_s \dot{u}_s - L \\ &= \sum_s M\dot{u}_s{}^2 - \sum_s [\frac{M}{2}\dot{u}_s{}^2 - \frac{1}{2}C(u_{s+1} - u_s)^2] \\ &= \sum_s \frac{M}{2}\dot{u}_s{}^2 + \frac{1}{2}\sum_s C(u_{s+1} - u_s)^2 \end{aligned}$$

. (13.19)

Now we calculate the total energy for the case of

$$u_s = u\cos(ska - \omega t). \tag{13.20}$$

$$\dot{u}_s = u(-1)(-\omega)\sin(ska - \omega t)$$

or

$$\begin{aligned} E &= \frac{1}{4}Mu^2\omega^2\sum_s[1-\cos 2(\omega t - ska)] \\ &+ \frac{1}{2}Cu^2(1-\cos ka)\sum_s\left[1-\cos 2(\omega t - ska - \frac{1}{2}ka)\right] \end{aligned}, \tag{13.21}$$

with $\rho = \frac{NM}{V}$ (mass density), $V = Na$. The dispersion relation is given by

$$\omega^2 = \frac{2C}{M}(1-\cos ka). \tag{13.22}$$

Then the total energy is

$$E = \frac{1}{4}Mu^2\omega^2\left\{\sum_s[1-\cos 2(\omega t - ska)] + \sum_s\left[1-\cos 2(\omega t - ska - \frac{1}{2}ka)\right]\right\}. \tag{13.23}$$

The time-average is

$$\begin{aligned} \langle E\rangle &= \frac{1}{T}\int_0^T E dt = \frac{1}{2}Mu^2\omega^2\sum_s 1 = \frac{1}{2}Mu^2\omega^2 N \\ &= \frac{1}{2}\rho V u^2\omega^2 \end{aligned}, \tag{13.24}$$

where

$$T = \frac{2\pi}{\omega}, \;\; \rho = \frac{NM}{V} = \frac{NM}{Na}, \;\; NM = \rho V .$$

In general, we use

$$u_s = \sum_k u_k \cos(ska - \omega t) . \qquad (13.25)$$

Then we have

$$\langle E \rangle = \frac{1}{2} \rho V \sum_k u_k^2 \omega_k^2 . \qquad (13.26)$$

This energy is compared with the result derived from the quantum mechanics.

$$\frac{1}{2} \rho V \sum_k u_k^2 \omega_k^2 = \sum_k \hbar \omega_k \left(\langle \hat{n}_k \rangle + \frac{1}{2} \right).$$

or

(13.27)

$$\frac{1}{2} \rho V u_k^2 \omega_k^2 = \hbar \omega_k \left(\langle \hat{n}_k \rangle + \frac{1}{2} \right), \qquad (13.28)$$

or

$$u_k^2 = \frac{2\hbar \left(\langle \hat{n}_k \rangle + \frac{1}{2} \right)}{\rho V \omega_k} = \frac{2\hbar \left(\langle \hat{n}_k \rangle + \frac{1}{2} \right)}{NM \omega_k}, \qquad (13.29)$$

where $\rho V = NM$. Here we define the effective amplitude as

$$u_k^{eff} = \frac{1}{\sqrt{2}} u_k , \qquad (13.30)$$

where

$$\left(u_k^{eff} \right)^2 = \frac{\hbar \left(\langle \hat{n}_k \rangle + \frac{1}{2} \right)}{NM \omega_k} . \qquad (13.31)$$

14. Conclusion

We have shown that the well-defined lattice waves propagate over the crystal, forming a so-called phonon as a quantization of the lattice waves. Phonon has the dual characters of wave and particle, which is essential to the quantum mechanics. Phonon is one of bosons, obeying the Bose-Einstein statistics. Phonons will be seen to play an important role in any phenomena for which the energy of importance is comparable to $\hbar\omega$, the energy of the phonon in question. In the BCS (Bardeen-Cooper-Schrieffer) model for the superconductivity, a specific interaction between electrons can lead to an energy gap separated from excited states by a energy gap. The formation of Cooper pairs is due to the electron-phonon interaction. The first electron interacts with the lattice and deforms it; the second electron sees the deformed lattice. Thus the second electron interacts with the first electron through the lattice deformation.

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APPENDIX-I

A Simple harmonics (1D) in quantum mechanics

(a) Annihilation and creation operator

The commutation relation

$$[\hat{x}, \hat{p}] = i\hbar \ . \tag{A.1}$$

The Hamiltonian of the simple harmonics is

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega_0^2}{2}\hat{x}^2 . \tag{A.2}$$

The eigenvalue-problem of the simple harmonics

$$\hat{H}|n\rangle = \varepsilon_n |n\rangle , \tag{A.3}$$

with

$$\varepsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega_0 , \tag{A.4}$$

where $n = 0, 1, 2, 3, \ldots.$

In the $\{|x\rangle\}$ representation, the wave function of the simple harmonics can be described as

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega_0^2}{2}x^2\right)\langle x|n\rangle = \varepsilon_n \langle x|n\rangle . \tag{A.5}$$

Here we introduce the creation operator and annihilation operators given by

$$\hat{a} = \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_0}{\hbar}}\hat{x} + \frac{i\hat{p}}{\sqrt{m\hbar\omega_0}}\right), \tag{A.6}$$

$$\hat{a}^+ = \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_0}{\hbar}}\hat{x} - \frac{i\hat{p}}{\sqrt{m\hbar\omega_0}}\right), \tag{A.7}$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}} \tag{A.8}$$

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\left(\hat{a} + \hat{a}^+\right) = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\hat{a} + \hat{a}^+\right), \tag{A.9}$$

$$\hat{p} = \frac{1}{\sqrt{2}\beta}\frac{m\omega_0}{i}\left(\hat{a} - \hat{a}^+\right) = \frac{1}{i}\sqrt{\frac{m\hbar\omega_0}{2}}\left(\hat{a} - \hat{a}^+\right), \tag{A.10}$$

$$[\hat{x}, \hat{p}] = \frac{1}{\left(\sqrt{2}\beta\right)^2}\frac{m\omega_0}{i}\left[\hat{a} + \hat{a}^+, \hat{a} - \hat{a}^+\right] = -\frac{\hbar}{i}\left[\hat{a}, \hat{a}^+\right], \tag{A.11}$$

or

$$\left[\hat{a}, \hat{a}^+\right] = \hat{1} \tag{A.12}$$

$$\hat{a}^+\hat{a} = \frac{\beta^2}{2}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) = \frac{\beta^2}{2}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega_0^2} - i\frac{1}{m\omega_0}[\hat{p}, \hat{x}]\right) \tag{A.13}$$

or

$$\hat{a}^{+}\hat{a} = \frac{1}{\hbar\omega_0}\left(\hat{H} - \frac{1}{2}\hbar\omega_0\right) \qquad \text{(A.14)}$$

or

$$\hat{H} = \hbar\omega_0\left(\hat{N} + \frac{1}{2}\right), \qquad \text{(A.15)}$$

where

$$\hat{N} = \hat{a}^{+}\hat{a}. \qquad \text{(A.16)}$$

The operator $\hat{N}$ is Hermitian since

$$\hat{N}^{+} = \left(\hat{a}^{+}\hat{a}\right)^{+} = \hat{a}^{+}\hat{a} = \hat{N}. \qquad \text{(A.17)}$$

The eigenvectors of $\hat{H}$ are those of $\hat{N}$, and vice versa since $[\hat{H},\hat{N}]=0$,

$$[\hat{N},\hat{a}] = \left[\hat{a}^{+}\hat{a},\hat{a}\right] = \hat{a}^{+}\hat{a}\hat{a} - \hat{a}\hat{a}^{+}\hat{a} = \left[\hat{a}^{+},\hat{a}\right]\hat{a} = -\hat{a}, \qquad \text{(A.18)}$$

$$[\hat{N},\hat{a}^{+}] = \left[\hat{a}^{+}\hat{a},\hat{a}^{+}\right] = \hat{a}^{+}\hat{a}\hat{a}^{+} - \hat{a}^{+}\hat{a}^{+}\hat{a} = \hat{a}^{+}\left[\hat{a},\hat{a}^{+}\right] = \hat{a}^{+}. \qquad \text{(A.19)}$$

Thus we have the relations

$$[\hat{N},\hat{a}] = -\hat{a}, \qquad \text{(A20)}$$

and

$$[\hat{N},\hat{a}^{+}] = \hat{a}^{+}, \qquad \text{(A.21)}$$

$$\hat{N}|n\rangle = \hbar\omega_0\left(n + \frac{1}{2}\right)|n\rangle. \qquad \text{(A.22)}$$

From the relation $[\hat{N},\hat{a}]|n\rangle = -\hat{a}|n\rangle$,

$$(\hat{N}\hat{a} - \hat{a}\hat{N})|n\rangle = -\hat{a}|n\rangle, \qquad \text{(A.23)}$$

or

$$\hat{N}(\hat{a}|n\rangle) = (n-1)\hat{a}|n\rangle. \qquad \text{(A.24)}$$

$\hat{a}|n\rangle$ is the eigenket of $\hat{N}$ with the eigenvalue (*n*-1).

$$\hat{a}|n\rangle \approx |n-1\rangle. \qquad \text{(A.25)}$$

From the relation

$$[\hat{N},\hat{a}^{+}]|n\rangle = \hat{a}^{+}|n\rangle, \qquad \text{(A.26)}$$

$$(\hat{N}\hat{a} - \hat{a}\hat{N})|n\rangle = -\hat{a}|n\rangle, \qquad \text{(A.27)}$$

or

$$\hat{N}(\hat{a}^{+}|n\rangle) = (n+1)\hat{a}^{+}|n\rangle. \qquad \text{(A.28)}$$

$\hat{a}^{+}|n\rangle$ is the eigenket of $\hat{N}$ with the eigenvalue (*n*+1).

$$\hat{a}^{+}|n\rangle \approx |n+1\rangle \qquad \text{(A.29)}$$

Now we need to show that *n* should be either zero or positive integers: *n* = 0, 1, 2, 3,…. We note that

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle = n\langle n|n\rangle \geq 0, \qquad \text{(A.30)}$$

$$\langle n|\hat{a}\hat{a}^{+}|n\rangle = \langle n|\hat{a}^{+}\hat{a}+1|n\rangle = (n+1)\langle n|n\rangle \geq 0 . \tag{A.31}$$

The norm of a ket vector is non-negative and the vanishing of the norm is a necessary and sufficient condition for the vanishing of the ket vector. In other words, $n \geq 0$. If $n = 0$, $\hat{a}|n\rangle = 0$. If $n \neq 0$, $\hat{a}|n\rangle$ is a nonzero ket vector of norm $n\langle n|n\rangle$.

If $n>0$, one successively forms the set of eigenkets,

$\hat{a}|n\rangle, \hat{a}^{2}|n\rangle, \hat{a}^{3}|n\rangle, \ldots . \hat{a}^{p}|n\rangle,$, belonging to the eigenvalues, n-1, n-2, n-3,….., n-p,

This set is certainly limited since the eigenvalues of $\hat{N}$ have a lower limit of zero. In other words, the eigenket $\hat{a}^{p}|n\rangle \approx |n-p\rangle$, or n-p = 0. Thus n should be a positive integer.

Similarly, one successively forms the set of eigenkets,

$\hat{a}^{+}|n\rangle, \hat{a}^{+2}|n\rangle, \hat{a}^{+3}|n\rangle, \ldots . \hat{a}^{+p}|n\rangle$, belonging to the eigenvalues, n+1, n+2, n+3,….., n+p,

Thus the eigenvalues are either zero or positive integers: n = 0, 1, 2, 3, 4, .

The properties of $\hat{a}^{+}$ and $\hat{a}$

1. $$\hat{a}|0\rangle = 0 , \tag{A.32}$$

   since $\langle 0|\hat{a}^{+}\hat{a}|0\rangle = 0$.

2. $$\hat{a}^{+}|n\rangle = \sqrt{n+1}|n+1\rangle , \tag{A.33}$$

   $$[\hat{N}, \hat{a}^{+}]|n\rangle = \hat{a}^{+}|n\rangle , \tag{A.34}$$

   $$\hat{N}\hat{a}^{+}|n\rangle = \hat{a}^{+}\hat{N}|n\rangle + \hat{a}^{+}|n\rangle = (n+1)\hat{a}^{+}|n\rangle . \tag{A.35}$$

   $\hat{a}^{+}|n\rangle$ is an eigenket of $\hat{N}$ with the eigenvalue (n + 1).

   Then

   $$\hat{a}^{+}|n\rangle = c|n+1\rangle . \tag{A.36}$$

   Since

   $$\langle n|\hat{a}\hat{a}^{+}|n\rangle = |c|^{2}\langle n+1|n+1\rangle = |c|^{2} , \tag{A.37}$$

   or

   $$\langle n|\hat{a}^{+}\hat{a}+1|n\rangle = n+1 = |c|^{2} , \tag{A.39}$$

   we obtain

   $$|c| = \sqrt{n+1} . \tag{A.40}$$

3. $$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle , \tag{A.41}$$

   $$[\hat{N}, \hat{a}]|n\rangle = -\hat{a}|n\rangle , \tag{A.42}$$

   $$\hat{N}\hat{a}|n\rangle = \hat{a}\hat{N}|n\rangle - \hat{a}|n\rangle = (n-1)\hat{a}|n\rangle , \tag{A.43}$$

   $\hat{a}|n\rangle$ is an eigenket of $\hat{N}$ with the eigenvalue (n - 1)

   Then

   $$\hat{a}|n\rangle = c|n-1\rangle . \tag{A.44}$$

   Since

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle = |c|^2\langle n-1|n-1\rangle = |c|^2 = n, \tag{A.45}$$

$$|c| = \sqrt{n} \tag{A.46}$$

(b) Basis vectors in terms of $|0\rangle$

We use the relation

$$|1\rangle = \hat{a}^{+}|0\rangle,$$

$$|2\rangle = \frac{1}{\sqrt{2}}\hat{a}^{+}|1\rangle = \frac{1}{\sqrt{2!}}\left(\hat{a}^{+}\right)^2|0\rangle,$$

$$|3\rangle = \frac{1}{\sqrt{3}}\hat{a}^{+}|2\rangle = \frac{1}{\sqrt{3!}}\left(\hat{a}^{+}\right)^3|0\rangle,$$

$$|n\rangle = \frac{1}{\sqrt{n}}\hat{a}^{+}|n-1\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^{+}\right)^n|0\rangle, \tag{A.48}$$

The expression for $\hat{x}|n\rangle$ and $\hat{p}|n\rangle$

$$\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\hat{a} + \hat{a}^{+}\right)|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\sqrt{n+1}|n+1\rangle + \sqrt{n}|n-1\rangle\right), \tag{A.49}$$

$$\hat{p}|n\rangle = \sqrt{\frac{m\hbar\omega_0}{2}}i\left(\hat{a}^{+} - \hat{a}\right)|n\rangle = \sqrt{\frac{m\hbar\omega_0}{2}}i\left(\sqrt{n+1}|n+1\rangle - \sqrt{n}|n-1\rangle\right). \tag{A.50}$$

Therefore the matrix elements of $\hat{a}$, $\hat{a}^{+}$, $\hat{x}$, and $\hat{p}$ operators in the $\{|n\rangle\}$ representation are as follows.

$$\langle n'|\hat{a}|n\rangle = \sqrt{n}\delta_{n',n-1}, \tag{A.51}$$

$$\langle n'|\hat{a}^{+}|n\rangle = \sqrt{n+1}\delta_{n',n+1}, \tag{A.52}$$

$$\langle n'|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1}\right), \tag{A.53}$$

$$\langle n'|\hat{p}|n\rangle = i\sqrt{\frac{m\hbar\omega_0}{2}}\left(\sqrt{n+1}\delta_{n',n+1} - \sqrt{n}\delta_{n',n-1}\right). \tag{A.54}$$

Mean values and root-mean-square deviations of $\hat{x}$ and $\hat{p}$ in the state $|n\rangle$.

$$\langle n|\hat{x}|n\rangle = 0, \tag{A.55}$$

$$\langle n|\hat{p}|n\rangle = 0, \tag{A.56}$$

$$(\Delta x)^2 = \langle n|\hat{x}^2|n\rangle = \left(n + \frac{1}{2}\right)\frac{\hbar}{m\omega_0}, \tag{A.57}$$

$$(\Delta p)^2 = \langle n|\hat{p}^2|n\rangle = \left(n + \frac{1}{2}\right)m\hbar\omega_0. \tag{A.58}$$

The product $\Delta x\Delta p$ is

$$\Delta x \Delta p = \left(n + \frac{1}{2}\right)\hbar \geq \frac{1}{2}\hbar \qquad \text{(Heisenberg's principle of uncertainty),} \qquad (A.59)$$

Note that

$$\hat{x}^2 = \frac{\hbar}{2m\omega_0}\left(\hat{a}^+ + \hat{a}\right)\left(\hat{a}^+ + \hat{a}\right) = \frac{\hbar}{2m\omega_0}\left(\hat{a}^+\hat{a}^+ + \hat{a}\hat{a} + \hat{a}^+\hat{a} + \hat{a}\hat{a}^+\right), \qquad (A.60)$$

$$\hat{p}^2 = \frac{m\hbar\omega_0}{2}\left(\hat{a}^+ - \hat{a}\right)\left(\hat{a}^+ - \hat{a}\right) = \frac{m\hbar\omega_0}{2}\left(\hat{a}^+\hat{a}^+ + \hat{a}\hat{a} - \hat{a}^+\hat{a} - \hat{a}\hat{a}^+\right), \qquad (A.61)$$

and

$$\langle n|\left(\hat{a}^+\right)^2|n\rangle = 0\,, \qquad (A.62)$$

$$\langle n|\hat{a}^2|n\rangle = 0, \qquad (A.63)$$

$$\langle n|\hat{a}^+\hat{a} + \hat{a}\hat{a}^+|n\rangle = \langle n|2\hat{a}^+\hat{a} + 1|n\rangle = 2n + 1\,, \qquad (A.64)$$

Mean potential energy

$$\langle V\rangle = \frac{1}{2}m\omega^2\langle n|\hat{x}^2|n\rangle = \frac{1}{2}m\omega^2(\Delta x)^2 = \frac{1}{2}\varepsilon_n\,. \qquad (A.65)$$

Mean kinetic energy

$$\langle K\rangle = \frac{1}{2m}\langle n|\hat{p}^2|n\rangle = \frac{1}{2m}(\Delta p)^2 = \frac{1}{2}\varepsilon_n\,. \qquad (A.66)$$

Thus we have

$$\langle V\rangle = \langle K\rangle\,. \qquad (A.67)$$

(Virial theorem)

B. Translation operator in quantum mechanics

Here we discuss the translation operator $\hat{T}(a)$ in quantum mechanics,

$$|\psi'\rangle = \hat{T}(a)|\psi\rangle, \qquad (B.1)$$

or

$$\langle\psi'| = \langle\psi'|\hat{T}^+(a)\,. \qquad (B.2)$$

In an analogy from the classical mechanics, it is predicted that the average value of $\hat{x}$ in the new state $|\psi'\rangle$ is equal to that of $\hat{x}$ in the old state $|\psi\rangle$ plus the *x*-displacement *a* under the translation of the system

$$\langle\psi'|\hat{x}|\psi'\rangle = \langle\psi|\hat{x} + a|\psi\rangle,$$

or

$$\langle\psi|\hat{T}^+(a)\hat{x}\hat{T}(a)|\psi\rangle = \langle\psi|\hat{x} + a|\psi\rangle,$$

or

$$\hat{T}^+(a)\hat{x}\hat{T}(a) = \hat{x} + a\hat{1}\,. \qquad (B.3)$$

Normalization condition:

$$\langle\psi'|\psi'\rangle = \langle\psi|\hat{T}^+(a)\hat{T}(a)|\psi\rangle = \langle\psi|\psi\rangle\,,$$

or

$$\hat{T}^+(a)\hat{T}(a) = \widehat{1}\,. \qquad (B.4)$$

[$\hat{T}(a)$ is an unitary operator].

From Eqs.(B3) and (B4), we have

$$\hat{x}\hat{T}(a) = \hat{T}(a)(\hat{x}+a) = \hat{T}(a)\hat{x} + a\hat{T}(a),$$

or the commutation relation:

$$[\hat{x},\hat{T}(a)] = a\hat{T}(a). \qquad \text{(B.5)}$$

From this, we have

$$\hat{x}\hat{T}(a)|x\rangle = \hat{T}(a)\hat{x}|x\rangle + a\hat{T}(a)|x\rangle = (x+a)\hat{T}(a)|x\rangle.$$

Thus, $\hat{T}(a)|x\rangle$ is the eigenket of $\hat{x}$ with the eigenvalue (x+a).

or

$$\hat{T}(a)|x\rangle = |x+a\rangle, \qquad \text{(B.6)}$$

or

$$\hat{T}^{+}(a)\hat{T}(a)|x\rangle = \hat{T}^{+}(a)|x+a\rangle = |x\rangle. \qquad \text{(B.7)}$$

When x is replaced by x-a in Eq.(B7), we get

$$|x-a\rangle = \hat{T}^{+}(a)|x\rangle, \qquad \text{(B.8)}$$

or

$$\langle x-a| = \langle x|\hat{T}(a). \qquad \text{(B.9)}$$

Note that

$$\langle x|\psi'\rangle = \langle x|\hat{T}(a)|\psi\rangle = \langle x-a|\psi\rangle = \psi(x-a). \qquad \text{(B.10)}$$

The average value of $\hat{p}$ in the new state $|\psi'\rangle$ is equal to the average value of $\hat{p}$ in the old state $|\psi\rangle$ under the translation of the system

$$\langle\psi'|\hat{p}|\psi'\rangle = \langle\psi|\hat{p}|\psi\rangle, \qquad \text{(B.11)}$$

or

$$\langle\psi|\hat{T}^{+}(a)\hat{p}\hat{T}(a)|\psi\rangle = \langle\psi|\hat{p}|\psi\rangle,$$

or

$$\hat{T}^{+}(a)\hat{p}\hat{T}(a) = \hat{p}. \qquad \text{(B.12)}$$

So we have the commutation relation

$$[\hat{T}(a),\hat{p}] = \hat{0}.$$

From this commutation relation, we have

$$\hat{p}\hat{T}(a)|p\rangle = \hat{T}(a)\hat{p}|p\rangle = p\hat{T}(a)|p\rangle.$$

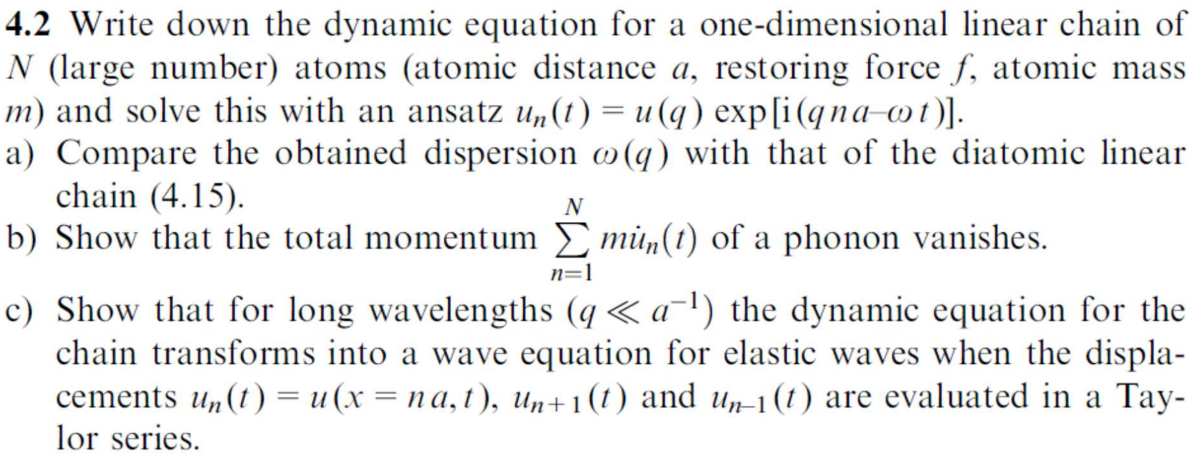
Thus, $\hat{T}(a)|p\rangle$ is the eigenket of $\hat{p}$ associated with the eigenvalue p.

APPENDIX II

Ibach and Luth

Chapter 4

Ibach and Luth 4-2



4.2 Write down the dynamic equation for a one-dimensional linear chain of N (large number) atoms (atomic distance a, restoring force f, atomic mass m) and solve this with an ansatz $u_n(t) = u(q)\exp[\mathrm{i}(qna - \omega t)]$.

a) Compare the obtained dispersion $\omega(q)$ with that of the diatomic linear chain (4.15).

b) Show that the total momentum $\sum_{n=1}^{N} m\dot{u}_n(t)$ of a phonon vanishes.

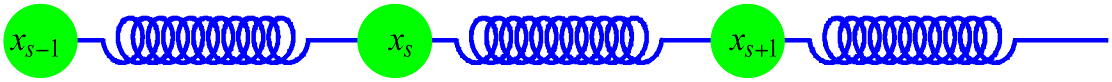
c) Show that for long wavelengths ($q \ll a^{-1}$) the dynamic equation for the chain transforms into a wave equation for elastic waves when the displacements $u_n(t) = u(x = na, t)$, $u_{n+1}(t)$ and $u_{n-1}(t)$ are evaluated in a Taylor series.

((**Solution**))

One dimensional case: longitudinal mode (from my note)

We start our discussion with the Lagrangian for the displacement of the *s*-th plane, given by

$$\begin{aligned} L_s &= T_s - V_s \\ &= \frac{1}{2}M\dot{u}_s{}^2 - \frac{1}{2}C[(x_{s+1} - x_s - a)^2 + (x_s - x_{s-1} - a)^2] \\ &= \frac{1}{2}M\dot{u}_s{}^2 - \frac{1}{2}C[(u_{s+1} - u_s)^2 + (u_s - u_{s-1})^2] \qquad (1) \end{aligned}$$



where x_s is the position of the atom at the *s*-th site and a is assumed to be the length of the un-stretched spring.

$$x_s = u_s + sa$$

where a is the distance between the adjacent atoms in thermal equilibrium. The Lagrange's equation for this system is derived as

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{u}_s}\right) = \frac{\partial L}{\partial u_s}, \qquad (2$$

or

$$\begin{aligned} M\ddot{u}_s &= -\frac{1}{2}C[2(u_{s+1} - u_s)(-1) + 2(u_s - u_{s-1})] \\ &= -C(-u_{s+1} + u_s + u_s - u_{s-1}) \end{aligned}$$

$$= C(u_{s+1} - 2u_s + u_{s-1})$$
$$= F_s$$

(3)

where

$$F_s = C(u_{s+1} - 2u_s + u_{s-1})$$

is the effective force on the *s*-th plane (Hooke's law), *C* is the force constant between nearest-neighbor planes, $C_L \neq C_T$ (C_L: force constant for longitudinal wave, C_T: force constant for transverse wave). 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 the plane *s* is

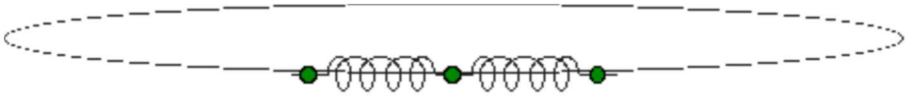
$$M\frac{d^2u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1}), \tag{4}$$

where *M* is the mass of an atom in the *s*-th plane. Suppose that this equation has the traveling wave solutions of the form

$$u_s = ue^{i(ksa-\omega t)}. \tag{2.5}$$

The Born-Karman boundary condition: The object connecting the ion on the extreme left with the spring on the extreme right is a massless rigid rod of length *L* = *Na*.

⇓



The Born-von Karman periodic boundary condition for the linear chain.

(a) Normal modes

We solve the equations of motion

$$M\frac{d^2u_s}{dt^2} = C(u_{s+1} - 2u_s + u_{s-1}), \tag{6}$$

by assuming that

$$u_s = e^{i(ksa-\omega t)}. \tag{7}$$

Then we have

$$\frac{d^2u_s}{dt^2} = -\omega^2 u_s, \tag{8}$$

$$u_{s\pm1} = e^{\pm ika}u_s, \tag{9}$$

$$-\omega^2 M u_s = C\left[e^{ika} + e^{-ika} - 2\right]u_s, \tag{10}$$

leading to the dispersion relation

$$\omega^2 = \frac{C}{M}(2-2\cos ka) = \frac{2C}{M}(1-\cos ka) = \frac{4C}{M}\sin^2(\frac{ka}{2}), \tag{11}$$

or

$$\omega = \sqrt{\frac{4C}{M}}\,|\sin(\frac{ka}{2})|. \tag{12}$$

It is usual for one to assume that ω is positive. Then the wave propagates along the positive x direction for $k>0$ and along the negative x direction for $k<0$.

The boundary of the first Brillouin zone lies at $k = \pm\frac{\pi}{a}$.

(b) The total momentum

The total momentum:

$$P = \sum_{s=1}^{N} m\dot{u}_s$$

$$= -im\omega u(q)\sum_{s=1}^{N} e^{iqsa}$$

$$\sum_{s=1}^{N} e^{iqsa} = e^{iqa}\left[1 + e^{iqa} + e^{i2qa} + \cdots + e^{i(N-1)qa}\right]$$

$$= \frac{e^{iqa}}{1-e^{iqa}}(1-e^{iNqa})$$

$$=0$$

since

$$Nqa = N\frac{2\pi l}{Na}a = 2\pi l, \qquad e^{iNqa} = 1$$

(c) Wave equation

We start with

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

In the continuous elastic wave, we assume that

$$u_s = u(x), \quad u_{s+1} = u(x + \Delta x), \quad u_{s-1} = u(x - \Delta x)$$

Using the Taylor expansion for the continuous wave

$$M\frac{d^2}{dt^2}u(x) = C[u(x + \Delta x) - 2u(x) + u(x - \Delta x)$$

$$= C(\Delta x)^2\frac{\partial^2}{\partial x^2}u(x)$$

or

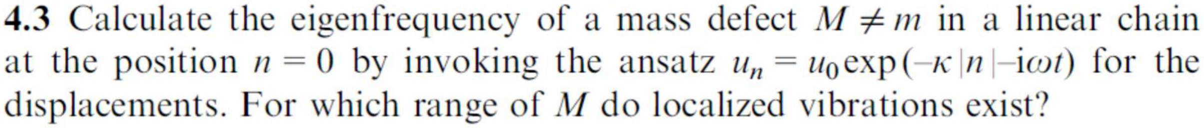
$$\frac{1}{v^2}\frac{d^2}{dt^2}u(x) = \frac{\partial^2}{\partial x^2}u(x)$$

where the velocity is defined by

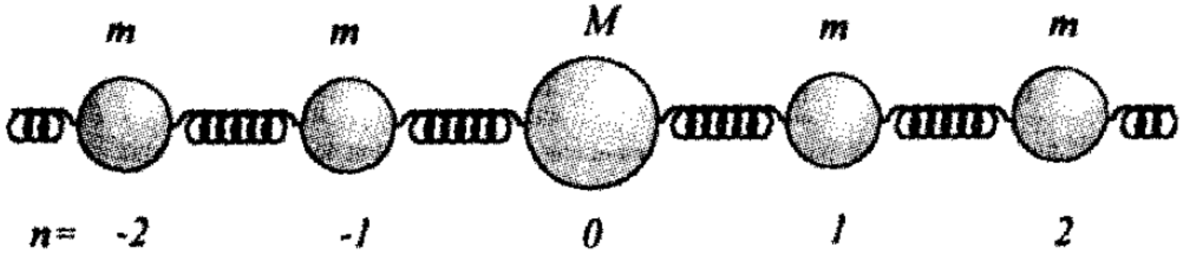
$$v = \sqrt{\frac{C}{M}}\Delta x.$$

APPENDIX-III

Ibach and Luth Problem 4-3



4.3 Calculate the eigenfrequency of a mass defect $M \neq m$ in a linear chain at the position $n = 0$ by invoking the ansatz $u_n = u_0 \exp(-\kappa|n| - \mathrm{i}\omega t)$ for the displacements. For which range of M do localized vibrations exist?



((**Solution**))

If the displacement of the n-th mass is s_n, the equations of motion for the masses are

$$m\ddot{s}_{-1} = C(s_{-2} - 2s_{-1} + s_0)$$

$$M\ddot{s}_0 = C(s_{-1} - 2s_0 + s_1)$$

$$m\ddot{s}_1 = C(s_0 - 2s_1 + s_2)$$

We use the assumption that

$$s_n = s_0 \exp(-\kappa|n| - i\omega t)$$

Note that K is the spring constant and κ is the wave number.

Inserting this into the equations of motion, we obtain

$$-m\omega^2 = C(e^{\kappa} - 2 + e^{-\kappa}) \qquad \text{for } n>0$$

$$-M\omega^2 = 2C(-1 + e^{-\kappa}) \qquad \text{for } n = 0$$

$$-m\omega^2 = C(e^{\kappa} - 2 + e^{-\kappa}) \qquad \text{for } n<0$$

This reduces to two equations,

$$M\omega^2 = 2C(1 - e^{-\kappa})$$

$$m\omega^2 = C(2 - e^{\kappa} - e^{-\kappa})$$

The solutions are given as

$$\frac{M}{m} = \frac{2(1 - e^{-\kappa})}{2 - e^{\kappa} - e^{-\kappa}}$$

or

$$\kappa = \ln(1 - \frac{2m}{M})$$

$$\omega = \sqrt{\frac{4C}{M}}\sqrt{\frac{m}{2m - M}} = \sqrt{\frac{4C}{M}}\sqrt{\frac{1}{2 - \frac{M}{m}}}$$

(i) $\boldsymbol{M > 2m}$

ω: pure imaginary; $\omega = i\omega_0$

with

$$\omega_0 = \sqrt{\frac{4C}{M}}\sqrt{\frac{1}{\frac{M}{m}-2}}$$

$(\omega_0>0)$

κ: real and negative; $\kappa = -\kappa_0$ $(\kappa_0 > 0)$

leading to

$s_n = s_0\exp(\kappa_0|n| + \omega_0 t)$ (which explodes in space and time)

(ii) $M < 2m$

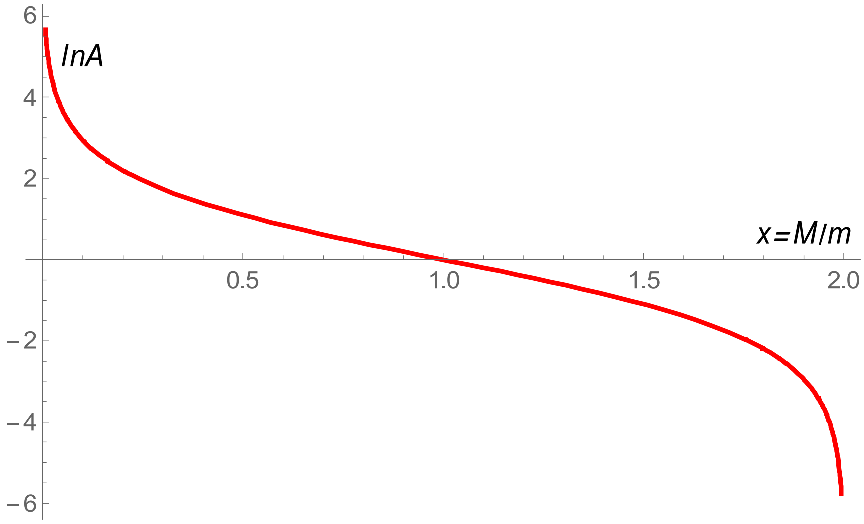
ω: positive and real

$|1-2m/M| = A$ (A>0; amplitude)

$$\kappa = \ln\left(1-\frac{2m}{M}\right) = \ln(Ae^{i\pi}) = i\pi + lnA$$

leading to

$s_n = s_0\exp(-lnA|n| - i(\omega + \pi|n|t)$



We consider the two cases

(a) $m < M < 2m$

Since $lnA < 0$

$s_n = s_0\exp(-lnA|n| - i(\omega + \pi|n|t)$

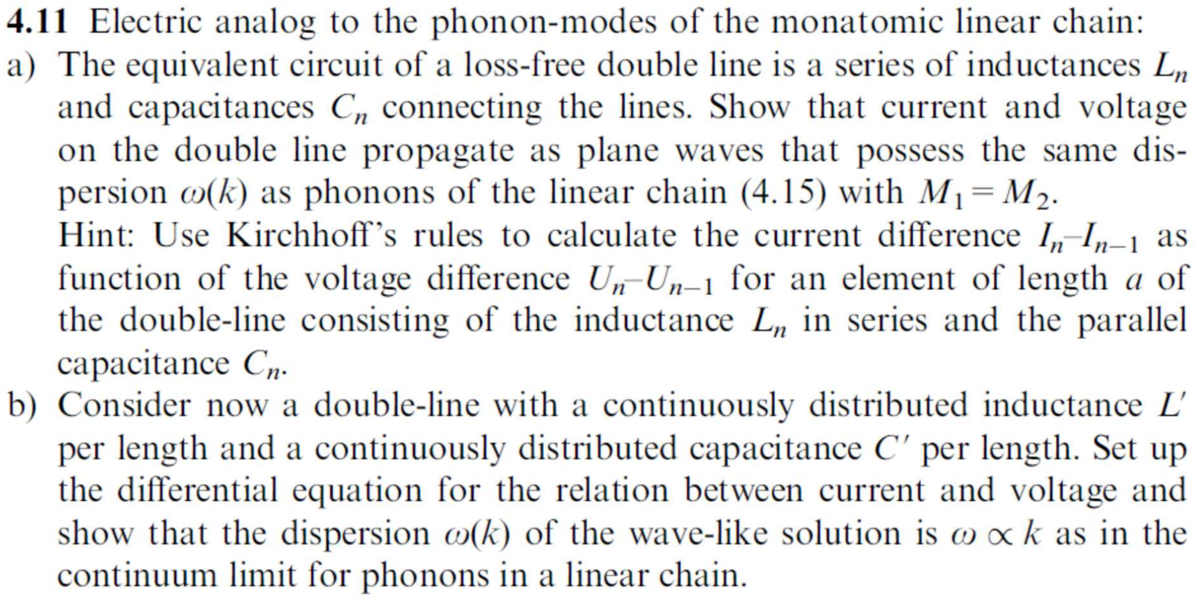
(which explodes in space, but oscillates in time)

(b) $0 < M < m$

Since $lnA > 0$

$s_n = s_0 \exp(-lnA|n| - i(\omega + \pi|n|t)$ (localized in space, but oscillates in time)

APPENDIX-IV
Ibach and Lűth Problem 4-11
Loss-free transmission line

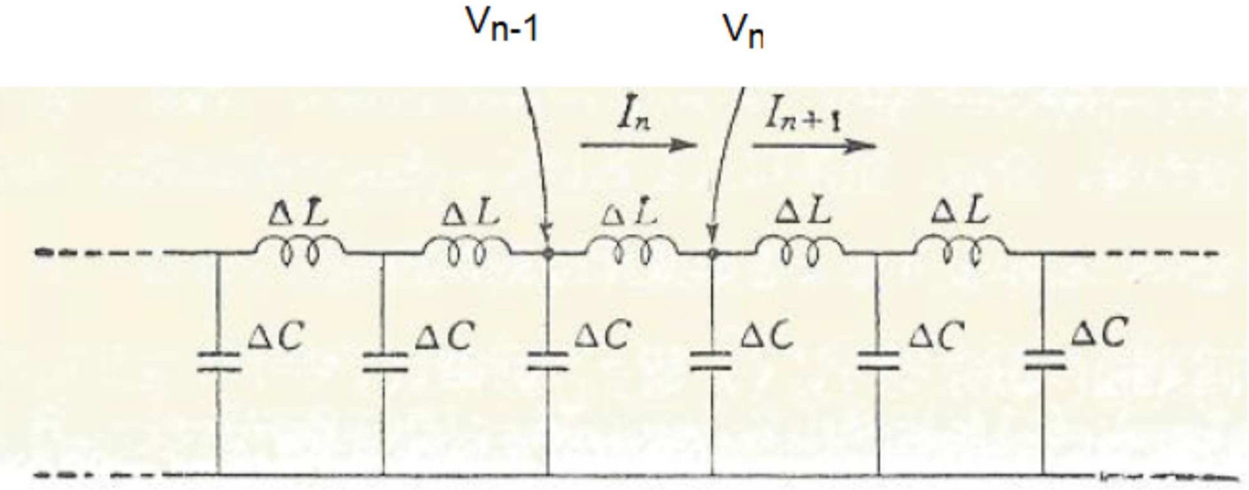


4.11 Electric analog to the phonon-modes of the monatomic linear chain:

a) The equivalent circuit of a loss-free double line is a series of inductances L_n and capacitances C_n connecting the lines. Show that current and voltage on the double line propagate as plane waves that possess the same dispersion $\omega(k)$ as phonons of the linear chain (4.15) with $M_1 = M_2$.
Hint: Use Kirchhoff's rules to calculate the current difference $I_n - I_{n-1}$ as function of the voltage difference $U_n - U_{n-1}$ for an element of length a of the double-line consisting of the inductance L_n in series and the parallel capacitance C_n.

b) Consider now a double-line with a continuously distributed inductance L' per length and a continuously distributed capacitance C' per length. Set up the differential equation for the relation between current and voltage and show that the dispersion $\omega(k)$ of the wave-like solution is $\omega \propto k$ as in the continuum limit for phonons in a linear chain.

((Solution))



Using the Kirchhoff law for the ladder circuit, we get

$$\Delta C\,\dot{V}_n = I_n - I_{n-1}$$

$$\Delta L\,\dot{I}_n = V_{n-1} - V_n$$

Thus we have

$$\Delta C\,\ddot{V}_n = \dot{I}_n - \dot{I}_{n-1}$$

or

$$\begin{aligned}\Delta L\Delta C\,\ddot{V}_n &= \Delta L(\dot{I}_n - \dot{I}_{n-1})\\ &= (V_{n-1} - V_n) - (V_n - V_{n+1})\\ &= V_{n-1} - 2V_n + V_{n+1}\end{aligned}$$

This equation is similar to that for the phonon for the monoatomic atom.

(b)
Suppose that

$$V_n = V(x)$$

$$V_{n+1} = V(x + \Delta x)$$

$$V_{n-1} = V(x - \Delta x)$$

Using the Taylor expansion, we get

$$\begin{aligned}\Delta L\Delta C\,\ddot{V}(x) &= V(x - \Delta x) - 2V(x) + V(x + \Delta x)\\ &= \frac{\partial^2 V}{\partial x^2}(\Delta x)^2\end{aligned}$$

We define the capacitance and the inductance per unit length as

$$\frac{\Delta L}{\Delta x} = L$$

$$\frac{\Delta C}{\Delta x} = C$$

Thus we have

$$LC\,\frac{\partial^2 V}{\partial t^2} = \frac{\partial^2 V}{\partial x^2}$$

or

$$\frac{1}{v^2}\frac{\partial^2 V}{\partial t^2} = \frac{\partial^2 V}{\partial x^2}$$

(wave equation)

(1)

where the velocity is defined as

$$v = \frac{1}{\sqrt{LC}}$$

The solution of Eq.(1) is of the form

$$V(x,t) = f(x - vt)$$

Suppose that

$$V(x,t) = A\exp[i(kx - \omega t)]$$

Then we have the dispersion relation of the propagating wave,

$$\omega = vk$$