Coupled oscillators: lattices
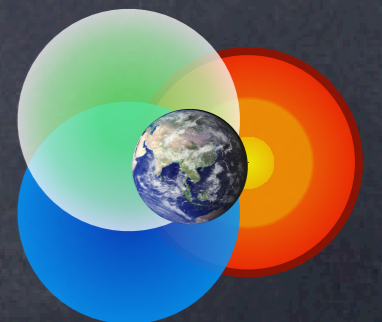
FABIO ROMANELLI
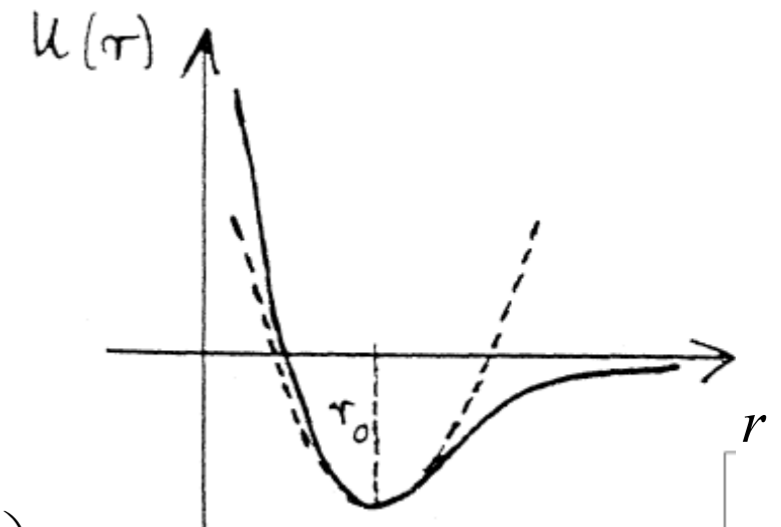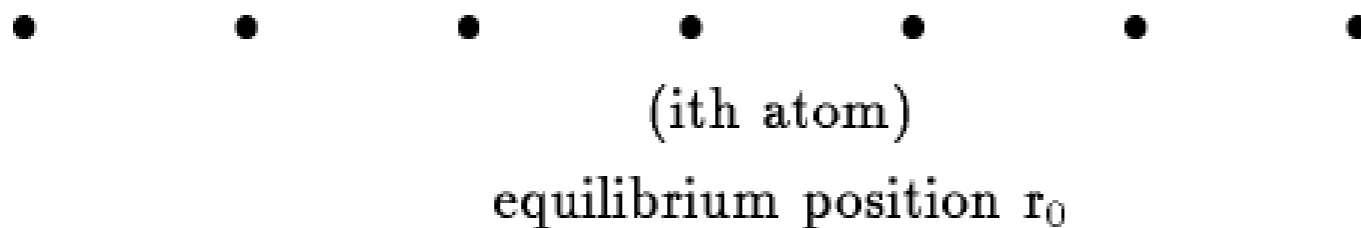
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Interatomic potential

Now we consider a monatomic 1-D lattice in the x-direction. The lattice atoms are very close to eqilibrium. Let us examine a single i-th atom and find the r_i potential as a function of displacement from equilibrium, $U(r_i)$.

(ith atom)

equilibrium position r_0

We expand this potential into a Taylor's series:

$$U(r_i) = U(r_0) + (r_i - r_0)\left(\frac{dU}{dr_i}\right)_{r_0} + \frac{1}{2}(r_i - r_0)^2\left(\frac{d^2U}{dr_i^2}\right)_{r_0} + \frac{1}{6}(r_i - r_0)^3\left(\frac{d^3U}{dr_i^3}\right)_{r_0} + ...$$

The first term of this expansion is just the equilibrium binding energy ($\equiv$ const). The second term is the slope of the potential at its minimum (= 0). The fourth and higher terms become increasingly smaller. We are therefore left with the third term as the only significant change in the potential energy for a small displacement $u = r_i - r_o$. This has the form

$$\Delta U = \tfrac{1}{2}Cu^2 \quad (C = d^2U/dr_i^2 \text{ at } r_i = r_0)$$

representing the *harmonic approximation*, since it is the same as the energy stored in a spring, or the potential energy of a harmonic oscillator. Our simple model of the dynamic crystal structure should therefore be a "ball and spring" model, with the lengths of the springs equivalent to the equilibrium separations of the ion cores.

Monatomic 1D lattice

Let us examine the simplest periodic system within the context of harmonic approximation ($F = dU/du = Cu$) - a one-dimensional crystal lattice, which is a sequence of masses m connected with springs of force constant C and separation a.

The collective motion of these springs will correspond to solutions of a wave equation.
Note: by construction we can see that 3 types of wave motion are possible,
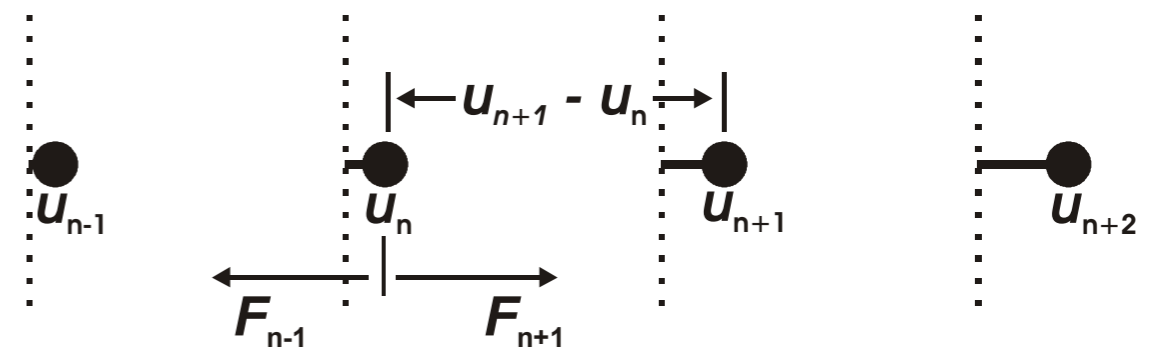2 transverse, 1 longitudinal (or compressional)

Mass M
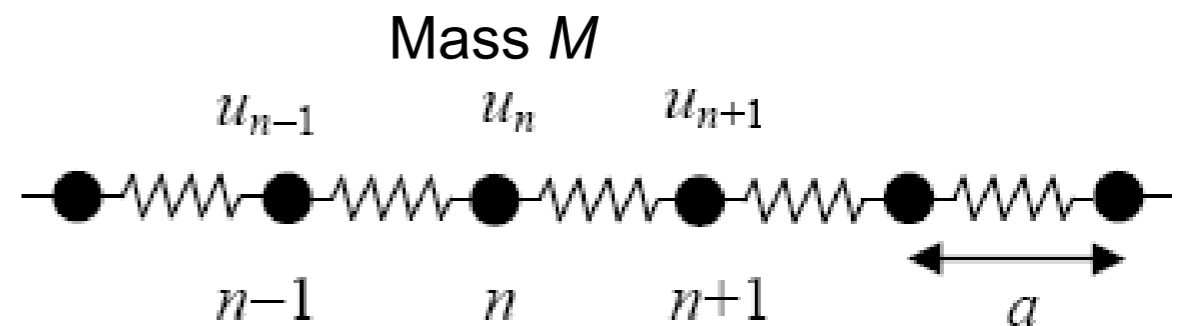
How does the system appear with a longitudinal wave?:

The force exerted on the n-th atom in the lattice is given by

$$F_n = F_{n+1,n} - F_{n-1,n} = C[(u_{n+1} - u_n) - (u_n - u_{n-1})].$$

Applying Newton's second law to the motion of the n-th atom we obtain

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

Note that we neglected hereby the interaction of the n-th atom with all but its nearest neighbors. A similar equation should be written for each atom in the lattice, resulting in N coupled differential equations, which should be solved simultaneously (N - total number of atoms in the lattice). In addition the boundary conditions applied to end atoms in the lattice should be taken into account.

Dispersion

Monatomic 1D lattice - continued

Now let us attempt a solution of the form: $u_n = Ae^{i(kx_n - \omega t)}$,

where x_n is the equilibrium position of the n-th atom so that $x_n = na$. This equation represents a traveling wave, in which all atoms oscillate with the same frequency ω and the same amplitude A and have a wavevector k. Now substituting the guess solution into the equation and canceling the common quantities (the amplitude and the time-dependent factor) we obtain

$$M(-\omega^2)e^{ikna} = -C[2e^{ikna} - e^{ik(n+1)a} - e^{ik(n-1)a}].$$

This equation can be further simplified by canceling the common factor e^{ikna} , which leads to

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

We find thus the dispersion relation for the frequency:

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

which is the relationship between the frequency of vibrations and the wavevector k. The dispersion relation has a number of important properties.

$\omega_{max} = \sqrt{4\,c\,/\,m}$

1st Brillouin zone
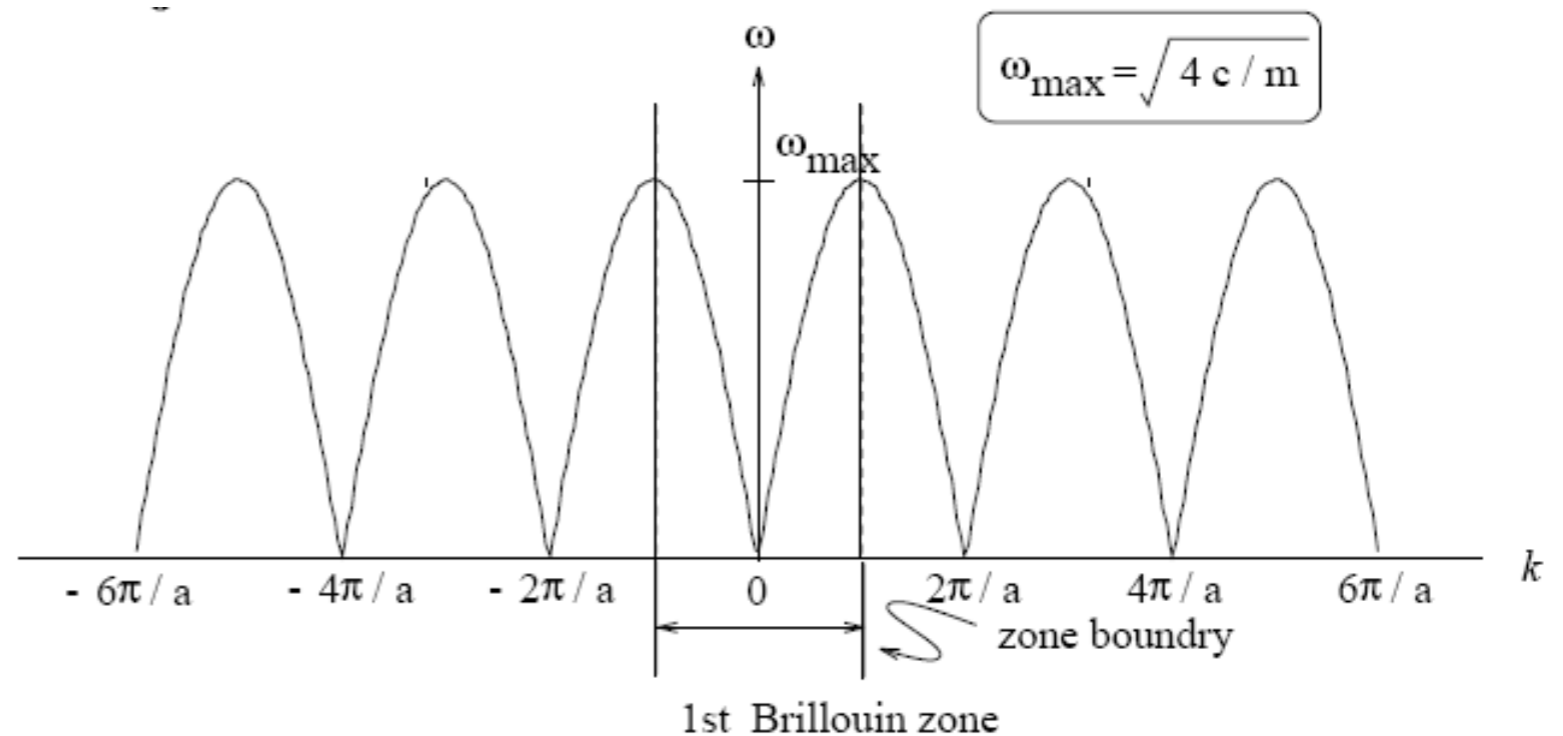
Phase and group velocities

Monatomic 1D lattice – continued


Phase and group velocity. The phase velocity is defined by

$$v_p = \frac{\omega}{k}$$ and the group velocity by $$v_g = \frac{d\omega}{dk}$$

The physical distinction between the two velocities is that v_p is the velocity of propagation of the plane wave, whereas the v_g is the velocity of the propagation of the wave packet. The latter is the velocity for the propagation of energy in the medium. For the particular

dispersion relation $$\omega = \sqrt{\frac{4C}{M}}\left|\sin\frac{ka}{2}\right|$$ the group velocity is given by $$v_g = \sqrt{\frac{Ca^2}{M}}\cos\frac{ka}{2}.$$

Apparently, the group velocity is zero at the edge of the zone where $k = \pm\,\pi/a$. Here the wave is standing and therefore the transmission velocity for the energy is zero.
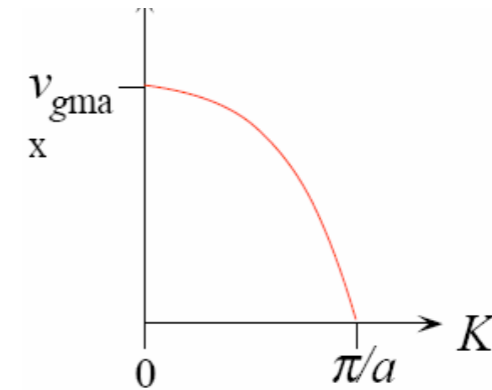
Long wavelength limit. The long wavelength limit implies that $\lambda \gg a$. In this limit $ka \ll 1$.

We can then expand the sine in 'ω' and obtain for the positive frequencies: $$\omega = \sqrt{\frac{C}{M}}ka.$$

We see that the frequency of vibration is proportional to the wavevector. This is equivalent to the statement that velocity is independent of frequency. In this case:

$$v_p = \frac{\omega}{k} = \sqrt{\frac{C}{M}}a.$$ This is the velocity of sound for the one dimensional lattice which is consistent with the expression we obtained earlier for elastic waves.

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Boundary conditions

Monatomic 1D lattice – continued

Finite chain – Born – von Karman periodic boundary condition.
Unlike a continuum, there is only a finite number of distinguishable vibrational modes. But how many?
Let us impose on the chain ends the Born – von Karman periodic boundary conditions specified as following: we simply join the two remote ends by one more spring in a ring or device in the figure below forcing atom N to interact with ion 1 via a spring with a spring constant C. If the atoms occupy sites a, $2a$, …, Na
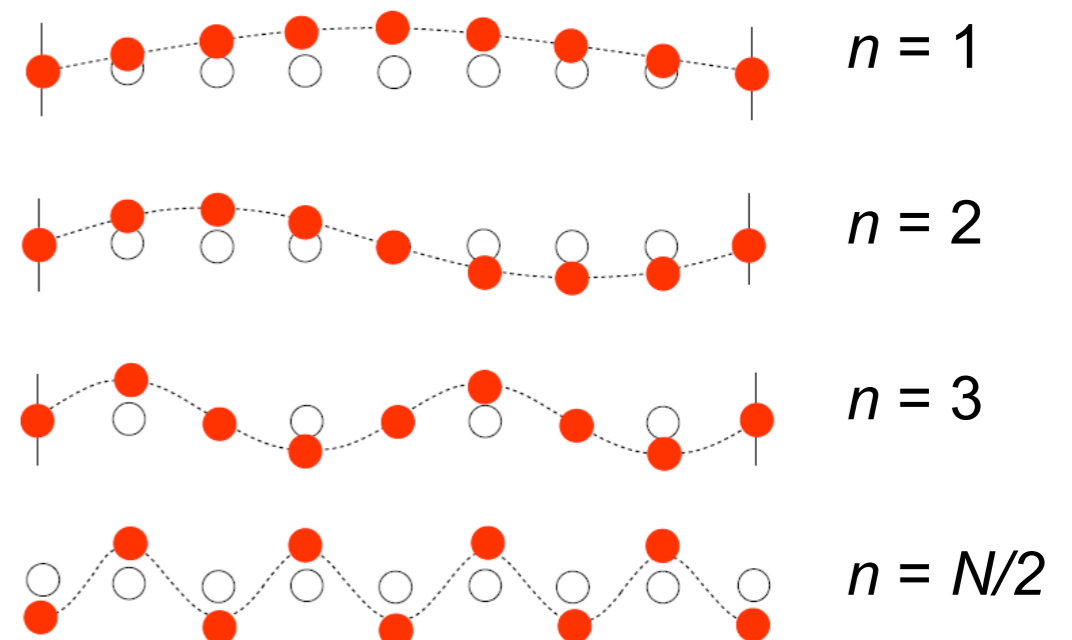The boundary condition is $u_{N+1} = u_1$ or $u_N = u_0$.
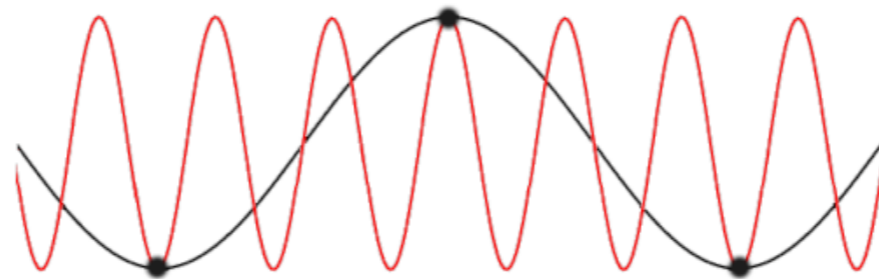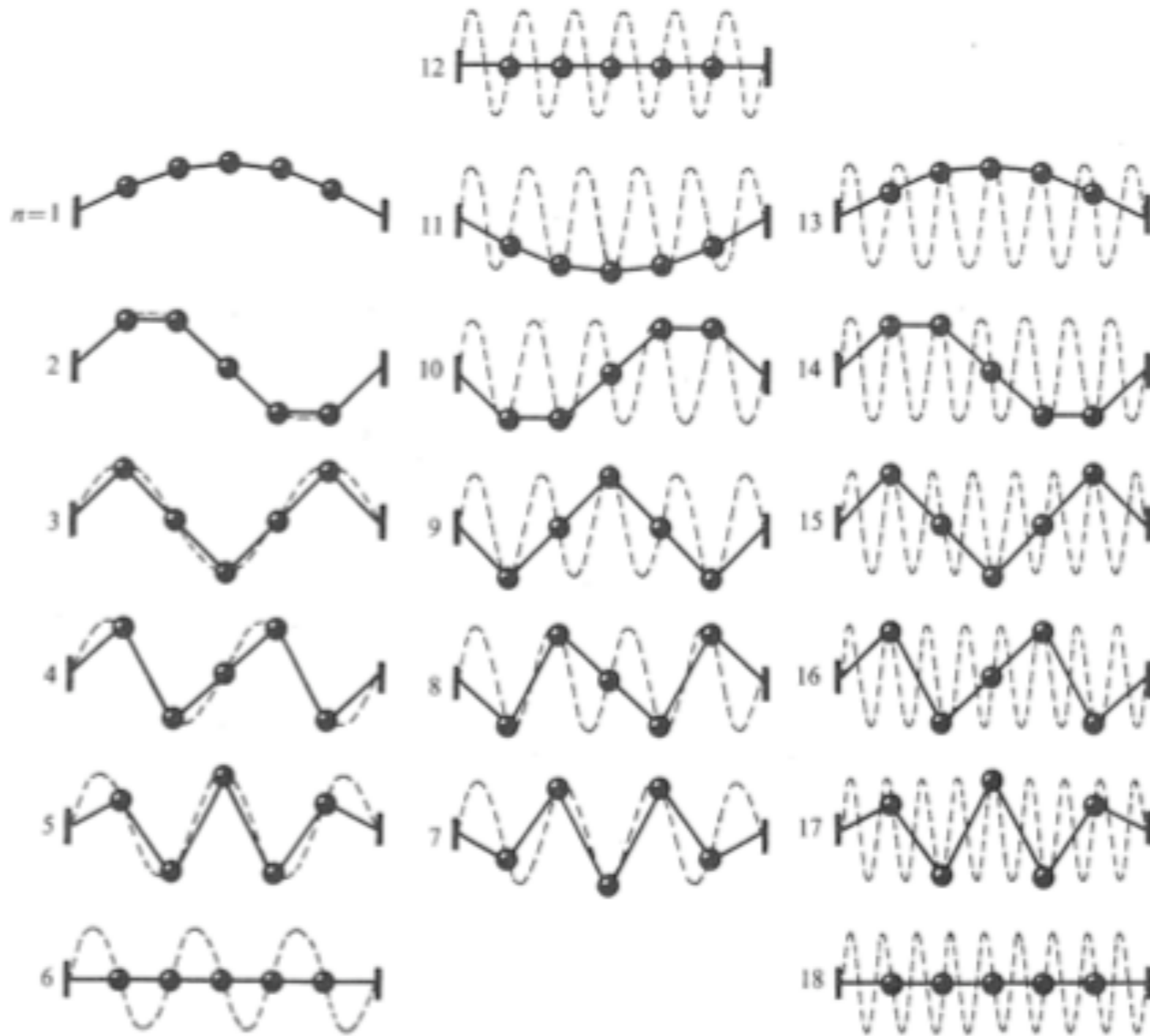
$$\overleftarrow{\quad\quad\quad Na \quad\quad\quad}$$
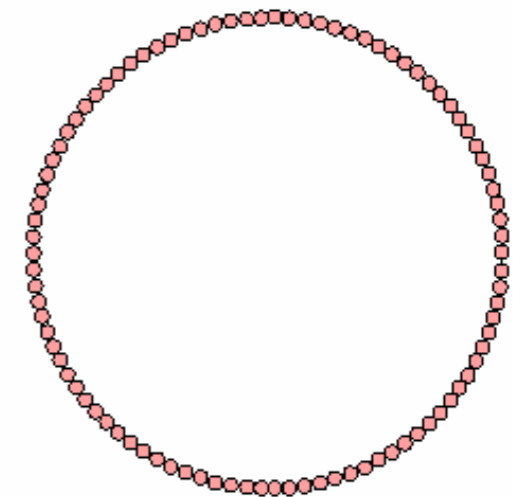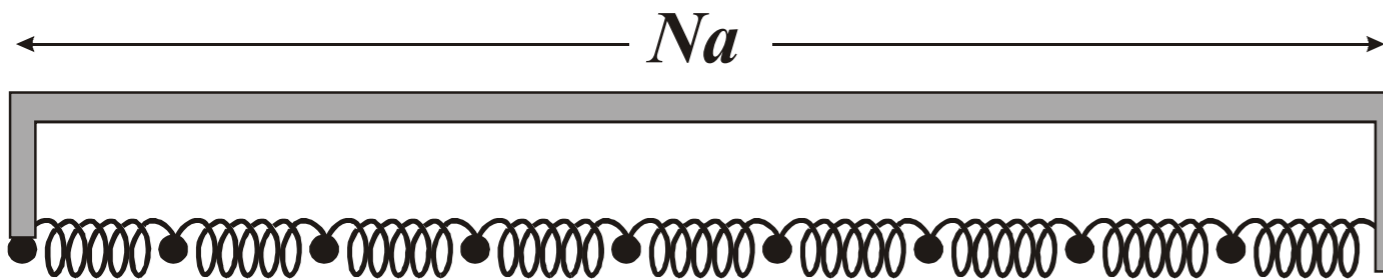
With the displacement solution of the form
$u_n = A\exp[i(kna-wt)]$, the periodic boundary
condition requires that $\exp(\pm ikNa) = 1$,
which in turn requires 'k' to have the form:

$$k = \frac{2\pi}{a}\frac{n}{N} \quad (n - \text{an integer}), \quad \text{and} \quad -\frac{N}{2} \leq n \leq \frac{N}{2}, \quad \text{or}$$

$$k = \pm\frac{2\pi}{Na}, \pm\frac{4\pi}{Na}, \pm\frac{6\pi}{Na}, ..., \pm\frac{\pi}{a} \quad (N \text{ values of } k).$$

$n = 1$

$n = 2$

$n = 3$

$n = N/2$

Modes of vibration

Diatomic 1D lattice

We can treat the motion of this lattice in a similar fashion as for the monatomic lattice. However, in this case, because we have two different kinds of atoms, we should write two equations of motion:

$$M_1 \frac{d^2 u_n}{dt^2} = -C(2u_n - u_{n+1} - u_{n-1})$$

$$M_2 \frac{d^2 u_{n+1}}{dt^2} = -C(2u_{n+1} - u_{n+2} - u_n)$$

In analogy with the monatomic lattice we are looking for the solution in the form of traveling mode for the two atoms:

$$\begin{bmatrix} u_n \\ u_{n+1} \end{bmatrix} = \begin{bmatrix} A_1 e^{ikna} \\ A_2 e^{ik(n+1)a} \end{bmatrix} e^{-i\omega t} \qquad \text{in matrix form.}$$

Substituting this solution into the equations of the previous slide we obtain:

$$\begin{bmatrix} 2C - M_1\omega^2 & -2C\cos ka \\ -2C\cos ka & 2C - M_2\omega^2 \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = 0.$$

This is a system of linear homogeneous equations for the unknowns A_1 and A_2. A nontrivial solution exists only if the determinant of the matrix is zero. This leads to the secular equation

$$\left(2C - M_1\omega^2\right)\left(2C - M_2\omega^2\right) - 4C\cos^2 ka = 0.$$

$$-\qquad)(\qquad)$$

This is a quadratic equation, which can be readily solved:

$$\omega^2 = C\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2 ka}{M_1 M_2}}$$

Depending on sign in this formula there are two different solutions corresponding to two different dispersion curves, as is shown in the figure:

The lower curve is called the **acoustic** branch, while the upper curve is called the **optical** branch.

The acoustic branch begins at $k = 0$ and $\omega = 0$, and as k $\Rightarrow$ 0:

With increasing k the frequency increases in a linear fashion. This is why this branch is called *acoustic*: it corresponds to elastic waves, or sound. Eventually, this curve saturates at the edge of the Brillouin zone.
On the other hand, the optical branch Has a nonzero frequency at zero k,
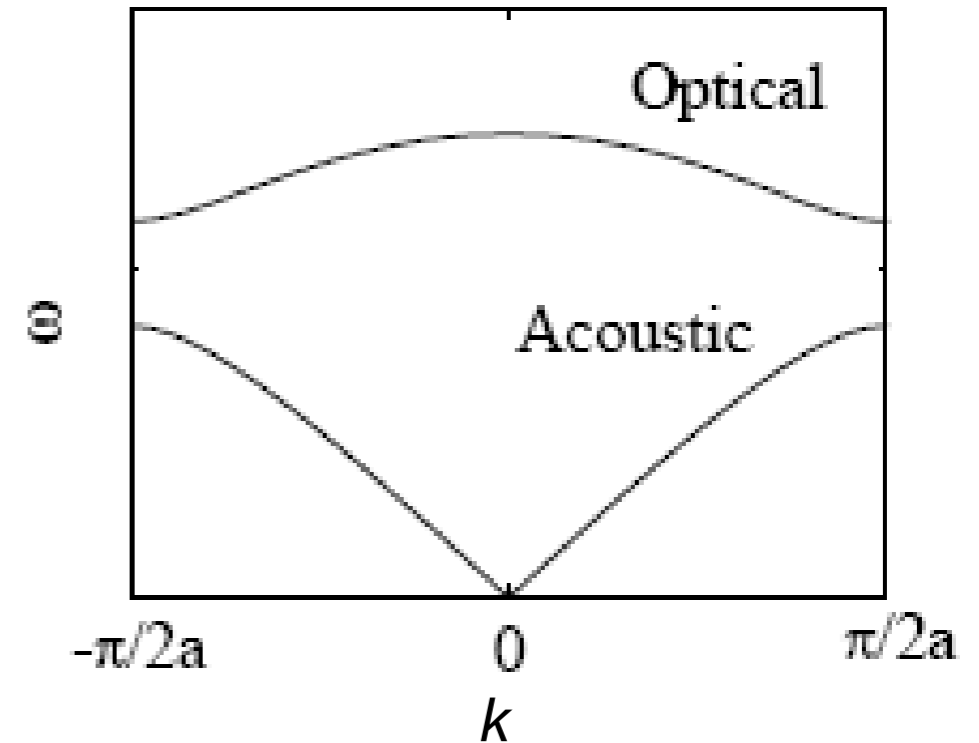
$$\omega_a(0) = \sqrt{\frac{C}{2(M_1 + M_2)}} \cdot ka$$

$$\omega_o = \sqrt{2C\left(\frac{1}{M_1} + \frac{1}{M_2}\right)}$$

and it does not change much with k.

Phonons

- From quantum mechanics, we learn that all energy is quantized (it comes only in discrete values).
- So, on this dispersion curve, there will only be discrete values of ω (since energy is released in packets of $E = \hbar\omega$)
- These quanta of lattice vibrations (waves) are called **phonons** in analogy with the photons of electromagnetic waves.

$$\left[2C\left(\frac{1}{M_1} + \frac{1}{M_2}\right)\right]^{1/2}$$

Optical phonon branch

$(2C/M_2)^{1/2}$

$M_1 > M_2$

$(2C/M_1)^{1/2}$

Discrete values

Acoustical phonon branch

K

$\pi/2a$

- These waves are quantized just like harmonic oscillator waves. For a wave of frequency ω:

$$E = (n + \tfrac{1}{2})\,\hbar\omega$$

- In this case, the mode is occupied by n phonons, each has an energy of $\hbar\omega$. The zero point energy of the mode is $\tfrac{1}{2}\hbar\omega$, where $n = 0$. According to quantum mechanics, there is a zero-point energy associated with every system.

Energy

Distance

$\hbar\omega$
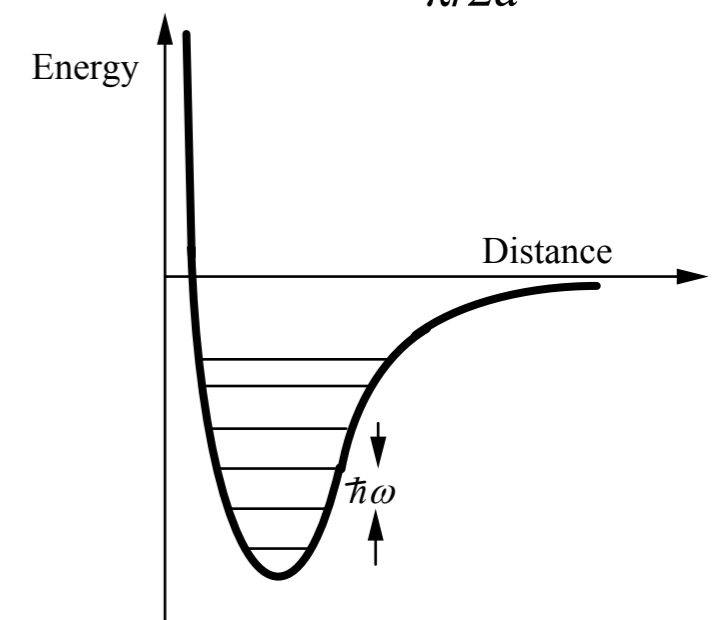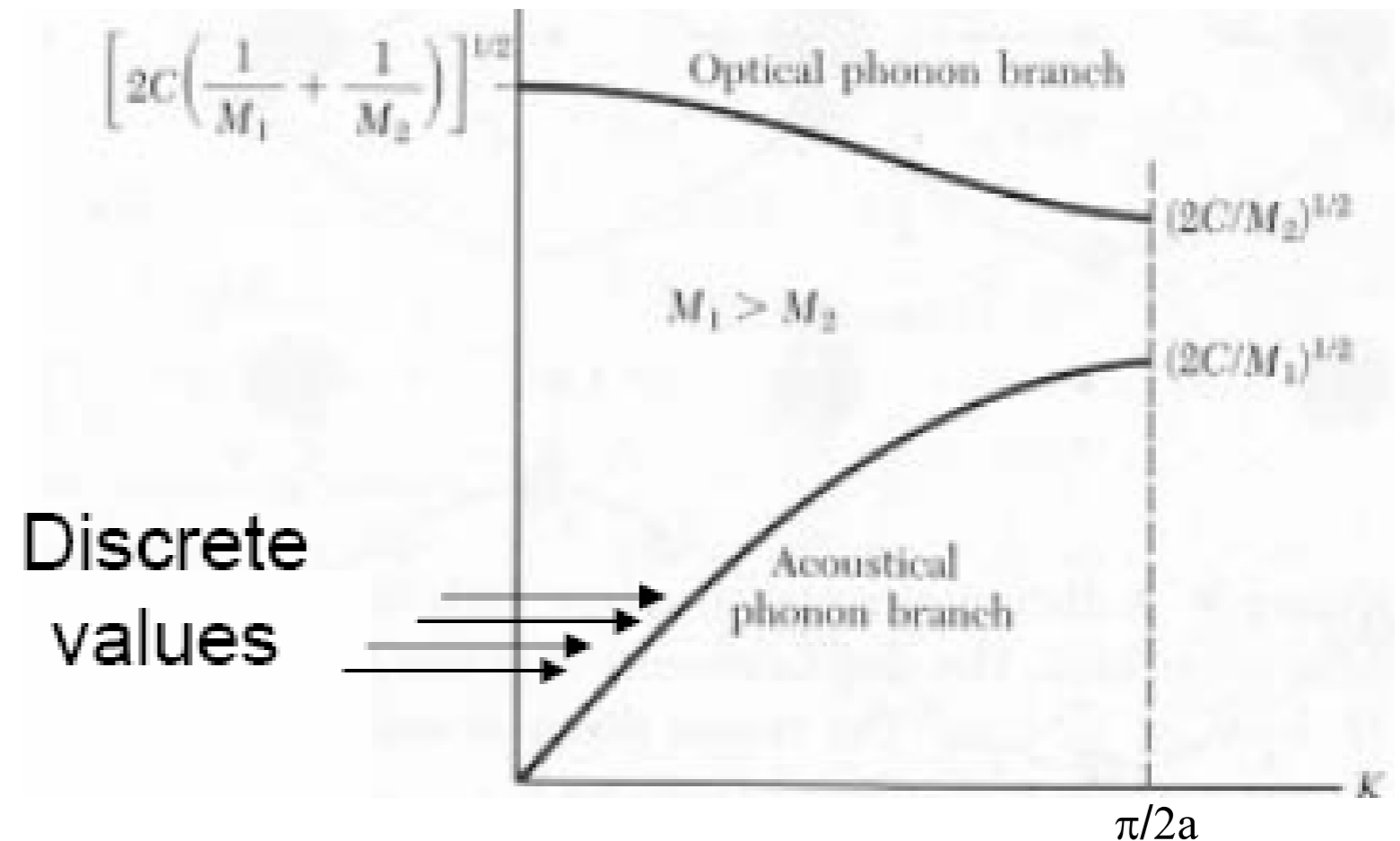
Acoustic and optical modes

Another feature of the dispersion curves is the existence of a forbidden gap between $\omega_a = (2C/M_1)^{1/2}$ and $\omega_o = (2C/M_2)^{1/2}$ at the zone boundaries ($k = \pm \pi/2a$).
The forbidden region corresponds to frequencies in which lattice waves cannot propagate through the linear chain without attenuation. It is interesting to note that a similar situation also exists in the energy band scheme of a solid to be discussed later.

The distinction between the acoustic and optical branches of lattice vibrations can be seen most clearly by comparing them at $k = 0$ (infinite wavelength). As follows from the equations of motion, for the acoustic branch $\omega = 0$ and $A_1 = A_2$. So, in this limit the two atoms in the cell have the same amplitude and phase. Therefore, the molecule oscillates as a rigid body, as shown in the left figure for the acoustic mode.

Acoustic

Optical

optical made

acustical made
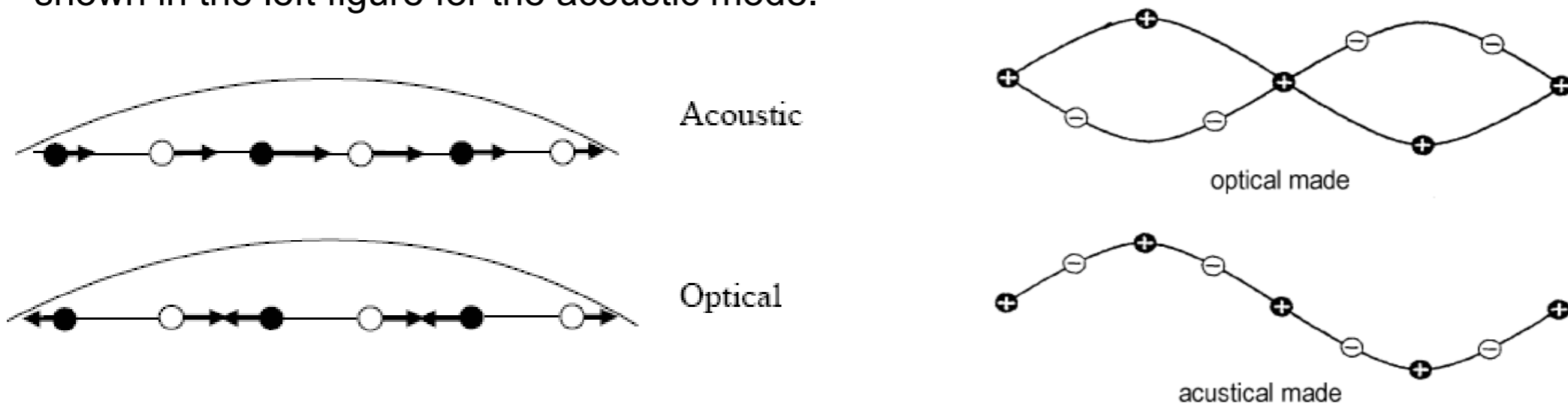
On the other hand, for the optical vibrations, by substituting ω_o we obtain for $k = 0$:

$$M_1A_1 + M_2A_2 = 0 \quad (M_1/M_2 = -A_2/A_1).$$

This implies that the optical oscillation takes place in such a way that the center of mass of a molecule remains fixed. The two atoms move in out of phase as shown. The frequency of these vibrations lies in the infrared region (10^{12} to 10^{14} Hz) which is the reason for referring to this branch as *optical*. If the two atoms carry opposite charges, we may excite a standing wave motion with the electric field of a light wave.
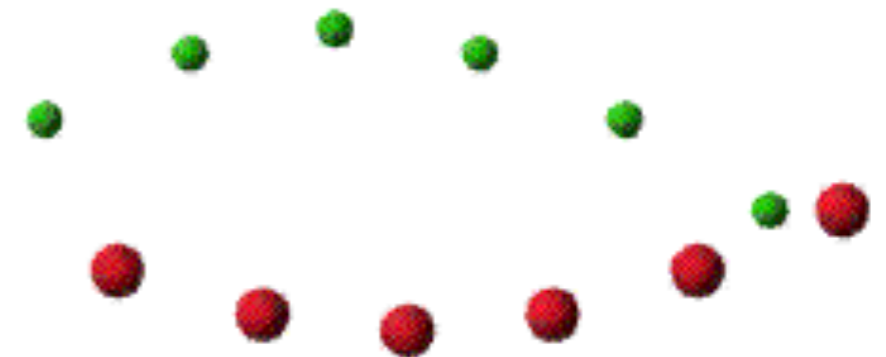
Acoustic and optical modes

Monoatomic chain
acoustic longitudinal mode

Monoatomic chain
acoustic transverse mode

Diatomic chain
acoustic transverse mode

Diatomic chain
optical transverse mode