

# Chapter 1

## COUPLED ONE-DIMENSIONAL OSCILLATORS

### 1.1 *Introduction*

Much of the interesting vibrational behavior of periodic systems is revealed by the classical oscillations of chains of masses connected by springs that obey Hooke's Law. Recall that Hooke's Law simply means that when a mass connected to a spring is displaced from its equilibrium position, there is a restoring force,  $F$ , directly proportional to the displacement  $\psi$ , i.e.  $F = -k\psi$ . We will see that the motions of such chains can be analyzed using the physics of simple harmonic oscillators and the concept of normal modes.

### 1.2 *Two coupled simple harmonic oscillators*

We begin by reviewing the simple case of two masses coupled by Hooke's Law springs. We wish to find the possible motions of such a system. Later, we will extend this to linear chains containing finite and infinite numbers of masses. This system is a model for other types of coupled oscillations such as coupled LC circuits, coupled pendulums, etc. The governing equations for all systems consisting of two coupled harmonic oscillators can be put into the same mathematical form. This has the powerful implication that once we have solved for the behavior of one such system, we have effectively solved for all of them.

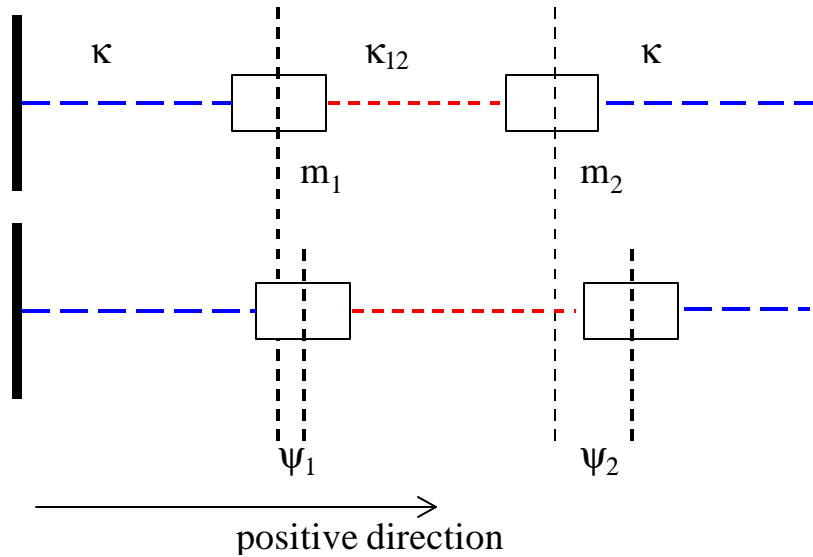
#### 1.2.1 *Equations of motion*

Newton's second law of motion tells us how a point mass moves in response to a force:

$$\vec{F} = \frac{d\vec{p}}{dt} = m \frac{d^2\vec{r}}{dt^2}$$

Thus, if we know what  $F$  is, we can, in principle, solve the differential equation to get the trajectory  $\vec{r}(t)$ !

Now, let  $\psi$  be the displacement from equilibrium in the longitudinal direction (along the line connecting the masses) and apply Hooke's Law,  $F = -k\mathbf{y}$ :



We adopt a systematic approach and define displacements to the right to be positive. Then

$$\text{Force on mass 1} = -(\text{force to left}) + (\text{force to right}) = F_1 = -\kappa\psi_1 + \kappa_{12}(\psi_2 - \psi_1)$$

$$\text{Force on mass 2} = F_2 = -\kappa_{12}\psi_2 + \kappa_{12}\psi_1 - \kappa\psi_2 = -\kappa\psi_2 - \kappa_{12}(\psi_2 - \psi_1)$$

Hint: check each term for the sign of the displacement!

Using our notation, Newton's Law is  $F_{1(2)} = m_{1(2)}\ddot{\mathbf{y}}_{1(2)}$ , so let's plug in the forces and, for simplicity, assume that the masses are equal ( $m_1 = m_2 = m$ ):

$$\ddot{\mathbf{y}}_1 = -\frac{\mathbf{k} + \mathbf{k}_{12}}{m}\mathbf{y}_1 + \frac{\mathbf{k}_{12}}{m}\mathbf{y}_2$$

$$\ddot{\mathbf{y}}_2 = +\frac{\mathbf{k}_{12}}{m}\mathbf{y}_1 - \frac{\mathbf{k} + \mathbf{k}_{12}}{m}\mathbf{y}_2$$

We see that the result is a pair of coupled ordinary differential equations for  $\psi_1$  and  $\psi_2$ . They are coupled because the second derivative of  $\psi_1$  or  $\psi_2$  (acceleration of a given mass) depends on both  $\psi_1$  and  $\psi_2$ . Another way of expressing this result is the matrix equation

$$\begin{pmatrix} \ddot{y}_1 \\ \ddot{y}_2 \end{pmatrix} = \begin{pmatrix} -\frac{k+k_{12}}{m} & \frac{k_{12}}{m} \\ \frac{k_{12}}{m} & -\frac{k+k_{12}}{m} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

### 1.2.2 Normal modes

To proceed further, we make the important assumption that there are particular motions of the system in which both masses oscillate with the same frequency. These special motions are called **normal modes**. We will see as we go along that for one-dimensional chains there are exactly as many normal modes as there are masses in the system. Each normal mode corresponds to motion with a single frequency, but the frequencies of normal modes can be (and usually are) different. Once we have identified the motions associated with the normal modes and have found the normal mode frequencies, we can express the general motion of any mass in terms of a superposition of normal modes.

To find the normal mode frequencies, assume that both masses move with the same frequency

$$\omega: \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} A_1 e^{i\omega t} \\ A_2 e^{i\omega t} \end{pmatrix}. \text{ The coefficients } A_1 \text{ and } A_2 \text{ are complex. Eventually, we will take the real}$$

parts to get the actual motion. The mathematical task is to find the possible values of  $\omega$  and the relationship between the coefficients for each  $\omega$ .

Note that for our assumed time dependence of the displacements, the second derivatives of the displacements (the accelerations) are proportional to the displacements themselves:

$$\begin{aligned} \ddot{y}_1 &= -\omega^2 A_1 e^{i\omega t} = -\omega^2 y_1 \\ \ddot{y}_2 &= -\omega^2 A_2 e^{i\omega t} = -\omega^2 y_2 \end{aligned}$$

If we substitute these expressions for  $\ddot{y}_1$  and  $\ddot{y}_2$  in the equations of motion we get the convenient result that the coupled **differential** equations have been converted to a pair of coupled **linear algebraic** equations. In matrix form,

$$\omega^2 \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} \frac{k+k_{12}}{m} & -\frac{k_{12}}{m} \\ -\frac{k_{12}}{m} & \frac{k+k_{12}}{m} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

This is an eigenvalue equation of the form

$$\mathbf{A} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \omega^2 \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

whose eigenvalues will be the normal mode frequencies ( $\omega$ -values) we seek.

### 1.2.3 Frequencies of normal modes: eigenvalues

To find eigenvalues, we set  $\det(\mathbf{A} - \omega^2 \mathbf{I}) = 0$ . This yields

$$\left(\frac{\mathbf{k} + \mathbf{k}_{12}}{m} - \omega^2\right)^2 - \left(\frac{\mathbf{k}_{12}}{m}\right)^2 = 0$$

Although this appears to be a quartic equation, it is really just a quadratic equation for  $\omega^2$ :

$$\begin{aligned} \left(\frac{\mathbf{k} + \mathbf{k}_{12}}{m}\right)^2 - 2\omega^2 \frac{\mathbf{k} + \mathbf{k}_{12}}{m} + \omega^4 - \left(\frac{\mathbf{k}_{12}}{m}\right)^2 &= 0 \\ \Rightarrow \omega^2 &= \frac{\mathbf{k} + \mathbf{k}_{12}}{m} \pm \sqrt{\left(\frac{\mathbf{k} + \mathbf{k}_{12}}{m}\right)^2 - \left(\frac{\mathbf{k} + \mathbf{k}_{12}}{m}\right)^2 + \left(\frac{\mathbf{k}_{12}}{m}\right)^2} \\ \Rightarrow \omega^2 &= \frac{\mathbf{k} + \mathbf{k}_{12}}{m} \pm \frac{\mathbf{k}_{12}}{m} \end{aligned}$$

Thus there are two eigenvalues (“eigenfrequencies”) and two corresponding normal modes. (We anticipated this with the statement that there would be as many normal modes as there are masses.)

Taking the solution with the minus sign we get a **low frequency mode** with frequency

$$\omega_{low} = \sqrt{\frac{\mathbf{k} + \mathbf{k}_{12}}{m} - \frac{\mathbf{k}_{12}}{m}} = \sqrt{\frac{\mathbf{k}}{m}}$$

This frequency is independent of the spring constant  $\kappa_{12}$  of the coupling spring! What does this suggest about the motion associated with the low frequency normal mode?

If we take the plus sign, we get the frequency of the high frequency mode:

$$\omega_{high} = \sqrt{\frac{\mathbf{k} + \mathbf{k}_{12}}{m} + \frac{\mathbf{k}_{12}}{m}} = \sqrt{\frac{\mathbf{k} + 2\mathbf{k}_{12}}{m}}$$

The high frequency **does** depend on the coupling  $\kappa_{12}$ . What is the implication for this mode?

### 1.2.4 Symmetries of normal modes: eigenvectors

We don’t really have to guess about the nature of the motions of the two normal modes. If we find the eigenvectors of the normal modes we will know the relation between the coefficients  $A_1$  and  $A_2$  for a given mode. This will define the symmetry of the motion.

The procedure is to substitute a particular eigenfrequency into the matrix equation and find the relationship between  $A_1$  and  $A_2$  (amplitudes of the displacements) for that mode.

For the low frequency mode:

$$\begin{pmatrix} \frac{k+k_{12}}{m} - \frac{k}{m} & -\frac{k_{12}}{m} \\ -\frac{k_{12}}{m} & \frac{k+k_{12}}{m} - \frac{k}{m} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = 0$$

$$\begin{aligned} \left(\frac{k+k_{12}}{m} - \frac{k}{m}\right)y_1 - \frac{k_{12}}{m}y_2 &= 0 & \frac{k_{12}}{m}y_1 - \frac{k_{12}}{m}y_2 &= 0 \\ -\frac{k_{12}}{m}y_1 + \left(\frac{k+k_{12}}{m} - \frac{k}{m}\right)y_2 &= 0 & \frac{k_{12}}{m}y_1 - \frac{k_{12}}{m}y_2 &= 0 \end{aligned} \Rightarrow$$

so that  $y_1 = y_2$  and therefore  $A_1 = A_2$ . The mode is **symmetric** with the masses moving **in phase**. Since the masses maintain their separation in this mode, the frequency is independent of the spring constant of the coupling spring.

If we let  $A_1 = A_2 = A_0 e^{i\varphi}$  with  $A_0$  real, we can express the displacements for the low frequency mode in the form  $\begin{pmatrix} x \\ \xi \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \begin{pmatrix} \bar{0} \\ \bar{0} \end{pmatrix} = \begin{pmatrix} x \\ \xi \end{pmatrix} \begin{pmatrix} A_0 e^{i\varphi} \\ A_0 e^{i\varphi} \end{pmatrix} e^{i\sqrt{\frac{k}{m}}t}$ . The real constants  $A_0$  and  $\varphi$  are determined by the initial conditions. To get the actual displacements, take the real parts:

$$\text{Re}(\psi_1) = \text{Re}(\psi_2) = A_0 (\cos \varphi \cos \omega t - \sin \varphi \sin \omega t) \quad \omega = \sqrt{\frac{k}{m}}$$

For the high frequency mode, the same procedure yields  $\begin{pmatrix} x \\ \xi \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \begin{pmatrix} \bar{0} \\ \bar{0} \end{pmatrix} = \begin{pmatrix} x \\ \xi \end{pmatrix} \begin{pmatrix} A_0 e^{i\varphi} \\ -A_0 e^{i\varphi} \end{pmatrix} e^{i\sqrt{\frac{k+2k_{12}}{m}}t}$ .

This mode is **anti-symmetric** with the masses moving out of phase (equal and opposite displacements). In this mode, the coupling spring is alternately stretched and compressed so the frequency must depend on the coupling constant  $k_{12}$ .

### 1.2.5 General motions: Principle of Superposition

We know that the system has 2 eigenfrequencies,  $\omega_{low}$  for the symmetric mode in which  $\psi_1 = \psi_2$ , and  $\omega_{high}$  for the antisymmetric mode in which  $\psi_1 = -\psi_2$ . If we start the system with initial conditions corresponding to one of these modes, say by displacing both masses symmetrically (antisymmetrically), then the system will oscillate with a single frequency  $\omega_{low}$  ( $\omega_{high}$ ). For more general initial conditions, both modes will be excited and the system

will execute complex motion corresponding to a superposition of the two eigenfrequencies. Applying the Principle of Superposition, we should be able to express the motions of masses 1 and 2 as

$$\psi_1 = Ae^{i\omega_a t} + Be^{i\omega_b t} \quad \text{and} \quad \psi_2 = Ae^{i\omega_a t} + Be^{i\omega_b t}$$

where, for simplicity we let  $\omega_{low} = \omega_a$  and  $\omega_{high} = \omega_b$ .

The amplitudes  $A, B, A\zeta$  and  $B\zeta$  are complex constants to be determined by the initial conditions. (We will take the real part when we need to.) However, these constants are not completely independent of each other.

We know, for example, that if  $B = B\zeta = 0$  so that the system is oscillating only with frequency  $\omega_{low} = \omega_a$ , then the motion must be symmetric, i.e.  $\psi_1 = \psi_2$   $\Rightarrow A\zeta = A$ . Similarly, to get the antisymmetric mode, we need  $\psi_1 = -\psi_2$   $\Rightarrow B\zeta = -B$ . We can assure this by writing

$$\psi_1 = Ae^{i\omega_a t} + Be^{i\omega_b t} \quad \text{and} \quad \psi_2 = Ae^{i\omega_a t} - Be^{i\omega_b t}$$

Putting in the complex nature of the coefficients explicitly, we see that we have 4 undetermined constants, the (real) amplitudes  $A_0, B_0$  and the phase factors,  $\phi, \delta$ .

$$\psi_1(t) = A_0 e^{i\phi} e^{i\omega_a t} + B_0 e^{i\delta} e^{i\omega_b t} \quad \text{and} \quad \psi_2(t) = A_0 e^{i\phi} e^{i\omega_a t} - B_0 e^{i\delta} e^{i\omega_b t}$$

Now, let's choose a particular set of initial conditions: mass 1 at the equilibrium position with zero velocity and mass 2 displaced a distance  $2C$ , also with zero velocity. Expressing this algebraically we have

$$\begin{aligned} \psi_1(0) = \text{Re}(A_0 e^{i\phi} + B_0 e^{i\delta}) &= 0 \quad \text{and} \quad \psi_2(0) = \text{Re}(A_0 e^{i\phi} - B_0 e^{i\delta}) = 2C \\ \left. \frac{d\psi_1}{dt} \right|_0 = \text{Re}(i\omega_a A_0 e^{i\phi} + i\omega_b B_0 e^{i\delta}) &= 0 \quad \text{and} \quad \left. \frac{d\psi_2}{dt} \right|_0 = \text{Re}(i\omega_a A_0 e^{i\phi} - i\omega_b B_0 e^{i\delta}) = 0 \end{aligned}$$

Rewriting the two equations for the velocity initial conditions by taking the real parts of the exponentials, we find

$$-\omega_a A_0 \sin \phi - \omega_b B_0 \sin \delta = 0 \quad \text{and} \quad -\omega_a A_0 \sin \phi + \omega_b B_0 \sin \delta = 0$$

Adding and subtracting these two equations gives

$$-2\omega_a A_0 \sin \phi = 0 \quad \text{and} \quad -2\omega_b B_0 \sin \delta = 0$$

from which we conclude  $\phi = \delta = 0$ . If we had forgotten about the velocity initial condition, it would have been the same as assuming  $A$  and  $B$  real, which would have been OK for this case. But this can't be done in general!

Now, go back to the displacement initial conditions, which now read,

$$A_0 + B_0 = 0 \quad \text{and} \quad A_0 - B_0 = 2C$$

whence,  $A_0 = -B_0 = C$ .

So now our equations for the displacements read

$$\psi_1(t) = \text{Re} \left[ C(e^{i\omega_a t} - e^{i\omega_b t}) \right] = C[\cos(\omega_a t) - \cos(\omega_b t)]$$

$$\psi_2(t) = \text{Re} \left[ C(e^{i\omega_a t} + e^{i\omega_b t}) \right] = C[\cos(\omega_a t) + \cos(\omega_b t)]$$

These are equivalent to

$$\psi_1(t) = 2C \sin \frac{\omega_b + \omega_a}{2} t \sin \frac{\omega_b - \omega_a}{2} t$$

$$\psi_2(t) = 2C \cos \frac{\omega_b + \omega_a}{2} t \cos \frac{\omega_b - \omega_a}{2} t$$

To show this takes a bit of algebra: use the trig identities  $\sin(x \pm y) = \sin x \cos y \pm \cos y \sin x$  in the preceding equations, carry out the multiplication, and introduce the identities

$$\sin^2 \frac{x}{2} = \frac{1}{2} - \frac{1}{2} \cos x \quad \text{and} \quad \cos^2 \frac{x}{2} = \frac{1}{2} + \frac{1}{2} \cos x.$$

### Beats

This result shows that the general motion of the system consists of a high frequency oscillation with frequency  $\frac{(\omega_b + \omega_a)}{2}$  modulated by a lower frequency  $\frac{(\omega_b - \omega_a)}{2}$ . The effect of the lower frequency (frequency difference) term is known as “beats” in analogy to the throbbing sound that is heard when two acoustical tones with slightly different frequencies are heard simultaneously. The mathematical description is identical – superposition of two sines or cosines.

The functional forms of  $\psi_1(t)$  and  $\psi_2(t)$  are shown below for a case where  $\frac{\omega_b - \omega_a}{\omega_b + \omega_a} = 0.1$ .

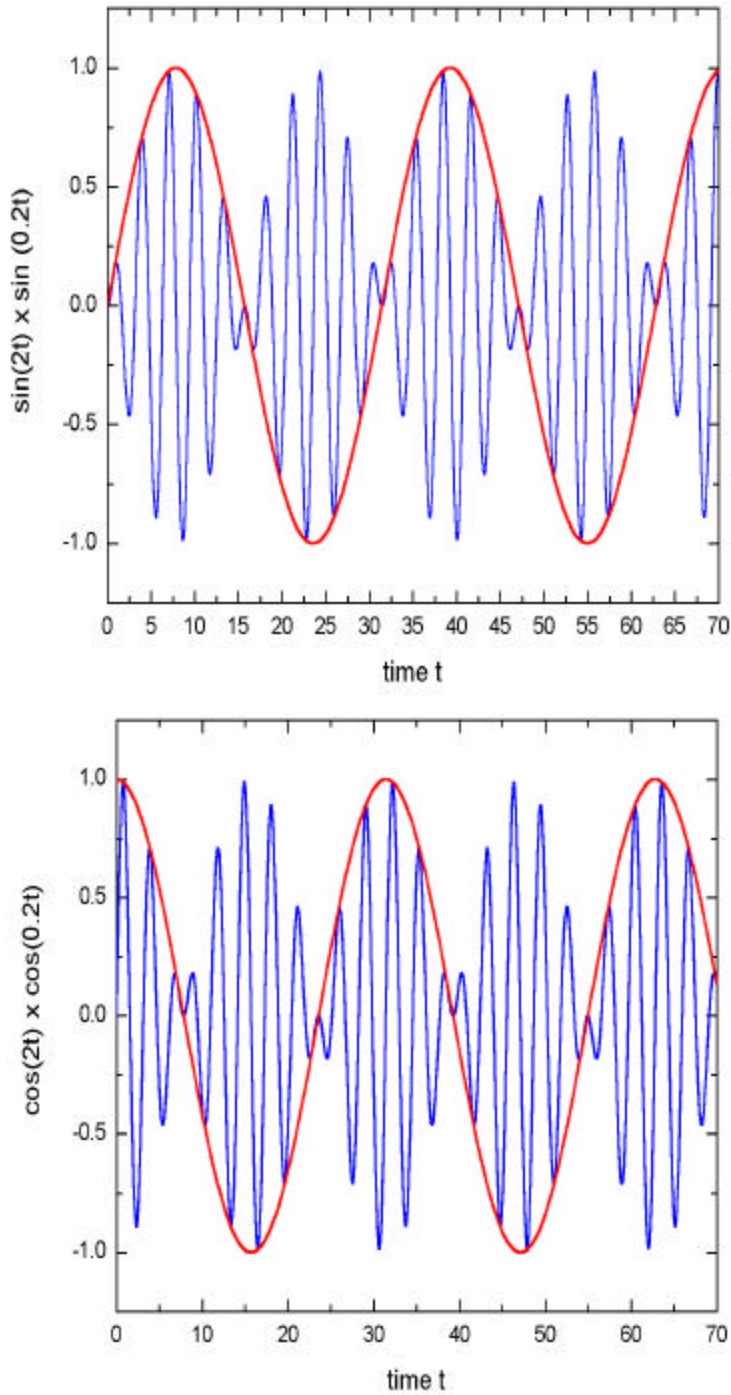


Fig. X. Displacements  $\psi_1(t)$  (upper plot) and  $\psi_2(t)$  (lower plot) for the case  $\frac{\omega_b - \omega_a}{\omega_b + \omega_a} = 0.1$ .

Notice that the “envelopes” of the displacements for the two masses are  $90^\circ$  out of phase. When mass 1 is oscillating with maximum amplitude, mass 2 has minimum amplitude and *vice versa*.



Energy is periodically exchanged (with frequency  $\omega_b - \omega_a$ ) between the two individual harmonic oscillators.

### Weak coupling limit

Recall the expressions for the two eigenfrequencies:

$$\omega_{low} = \omega_a = \sqrt{\frac{\kappa}{m}} \quad \text{and} \quad \omega_{high} = \omega_b = \sqrt{\frac{\kappa + 2\kappa_{12}}{m}}$$

and recall that it is the coupling ( $\kappa_{12}$ ) that distinguishes the two frequencies. (If  $\kappa_{12} = 0$ , we simply have two, completely independent simple harmonic oscillators.) Now, suppose that the coupling is weak, i.e.  $\kappa_{12} \ll \kappa$ . Then, using the approximation  $\sqrt{1 + \epsilon} \approx 1 + \frac{1}{2}\epsilon$  for  $\epsilon \ll 1$  we can write

$$\omega_{high} = \omega_b = \sqrt{\frac{\kappa + 2\kappa_{12}}{m}} = \sqrt{\frac{\kappa}{m}} \times \sqrt{1 + \frac{2\kappa_{12}}{\kappa}} \approx \sqrt{\frac{\kappa}{m}} \times \left(1 + \frac{\kappa_{12}}{\kappa}\right) = \omega_a + \omega_a \frac{\kappa_{12}}{\kappa}$$

The modulation frequency in this limit is  $\frac{(\omega_b - \omega_a)}{2} = \omega_a \frac{\kappa_{12}}{2\kappa}$  which is directly proportional to the strength of the coupling.

#### Discussion question:

Given a pair of identical coupled mechanical oscillators with known masses  $m$ , how could you determine the strength of the coupling by an experiment?

### 1.3 Many coupled masses: the “monatomic” $N$ -membered chain

**Lab #1 is the study of chains of  $N$  masses using the CUPS simulations programs.**

The simulations studied in Lab #1 yielded the following results:

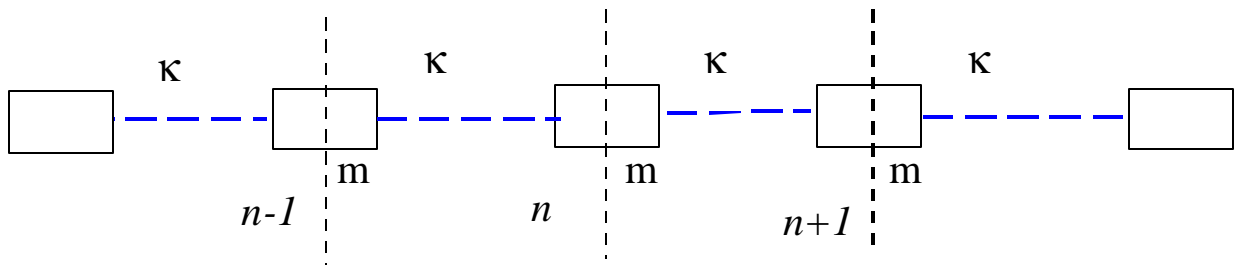
1. An experimentally determined dispersion relation (frequency  $\omega$  versus wave vector  $k = 2\pi/\lambda$ ) for a 5-mass chain.
2. The dispersion relation  $\omega(k)$  is linear at low frequency.
3. There is a maximum frequency for the normal modes of the chain.

4. The normal mode frequencies are repeated for higher wave vectors – no new physics for  $k$ -values beyond the maximum in  $\omega(k)$ .

Now let's see how these results follow from an analysis of the mechanics of the chain using Newton's equation of motion.

### 1.3.1 Equations of motion

We continue with many masses coupled to their nearest neighbors by Hooke's Law springs and find the possible longitudinal motion of such a system. (Coupling with other springs to next neighbors is a homework example). This system is a model for other types of coupled oscillations (transverse motion of these masses, coupled LC circuits, pendulums ...)



Hooke's Law gives us the force on the  $n^{\text{th}}$  mass when it is displaced a distance  $\psi_n$  from its equilibrium position,  $F_n = -\kappa\psi_n$ . We are considering only longitudinal motion (along the chain) in one dimension. For the present, we assume that all masses ( $m$ ) and spring constants ( $\kappa$ ) are equal. Later we will relax this restriction. Then the force on mass  $n$  is

$$F_n = -\mathbf{k}(\mathbf{y}_n - \mathbf{y}_{n-1}) - \mathbf{k}(\mathbf{y}_n - \mathbf{y}_{n+1})$$

Hint: again, check each term for the sign of the force relative to that of the displacement

Now, apply Newton's equation of motion,  $F_n = m_n\ddot{\mathbf{y}}$  and plug in the forces for mass  $n$  and its nearest neighbors:

$$\begin{aligned} m\ddot{\mathbf{y}}_{n-1} &= -\mathbf{k}(\mathbf{y}_{n-1} - \mathbf{y}_{n-2}) - \mathbf{k}(\mathbf{y}_{n-1} - \mathbf{y}_n) \\ m\ddot{\mathbf{y}}_n &= -\mathbf{k}(\mathbf{y}_n - \mathbf{y}_{n-1}) - \mathbf{k}(\mathbf{y}_n - \mathbf{y}_{n+1}) \\ m\ddot{\mathbf{y}}_{n+1} &= -\mathbf{k}(\mathbf{y}_{n+1} - \mathbf{y}_n) - \mathbf{k}(\mathbf{y}_{n+1} - \mathbf{y}_{n+2}) \end{aligned}$$

### 1.3.2 Dispersion Relation

Once again, we have a set of coupled differential equations. The acceleration of a particular mass depends not only on its own displacement, but also those of its neighbors. The route to a solution is to assume, as we did for two coupled oscillators, that the system has a set of normal modes in which all masses oscillate with the same frequency.

For a particular normal mode with frequency  $\omega$ , the displacement of mass  $n$  can be expressed as  $\mathbf{y}_n = A_n e^{i\omega t}$ . The coefficients  $A_n$  give the amplitudes of the oscillations for the various masses  $n$  and are, in general, complex.

Note that the frequency has no subscript (particle label) – all particles oscillate with the same frequency in a given normal mode.

Furthermore, as we saw in in Lab 1, the amplitudes of the particles' oscillations form the envelope of a sinusoid in the normal modes, so we'll further assume:  $\mathbf{y}_n = A e^{i(nka - \omega t)}$  where  $na$  is the particle's position along the chain, and  $k = \frac{2\pi}{\lambda}$  is the "wave vector." (In one-dimension, the "vector" property is expressed only by the sign ( $\pm$ ) of  $k$ ; in a two- or three-dimensional system, this is a true vector,  $\vec{k}$ ). The wavelength  $\lambda$  is that of the envelope that describes the instantaneous positions of the masses in that particular mode.

Substitute the normal mode solution into Newton's equation of motion:

$$-m\omega^2 A e^{inka - i\omega t} = -k(A e^{inka - i\omega t} - A e^{i(n-1)ka - i\omega t}) - k(A e^{inka - i\omega t} - A e^{i(n+1)ka - i\omega t})$$

$$\frac{m\omega^2}{k} e^{inka} = -e^{i(n-1)ka} + 2e^{inka} - e^{i(n+1)ka}$$

$$\omega^2 = \frac{2k}{m} \left( 1 - \frac{e^{ika} + e^{-ika}}{2} \right) = \frac{2k}{m} (1 - \cos ka)$$

$$\omega^2 = \frac{4k}{m} \sin^2 \frac{ka}{2}$$

$$\omega(k) = 2\sqrt{\frac{k}{m}} \sin \frac{ka}{2}$$

Our assumption of wave-like, oscillatory normal modes has led us to a dispersion relation  $\omega(k)$ .

This function is plotted below for  $\omega_{\max} = 2\sqrt{\frac{k}{m}} = 1$  and  $a = 1$ .

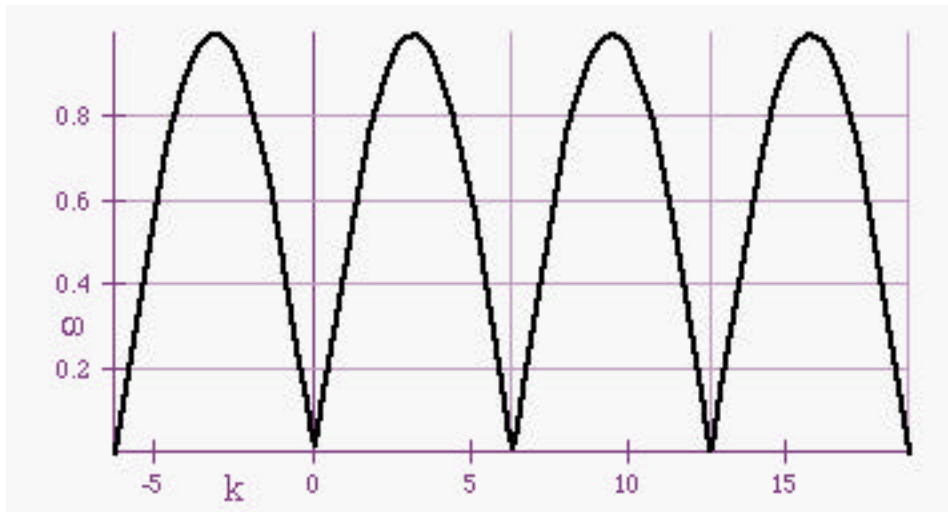


Fig. X. Dispersion relation  $\omega(k)$  for a monatomic chain (equal masses and spring constants).

#### Important features of the dispersion relation:

1. Information is repeated after  $k = \frac{\pi}{a}$ . This is called the Brillouin zone boundary and corresponds to a wavelength of  $\lambda = 2a$ . Smaller wavelengths are physically meaningless as we found in lab.
2. There is a maximum frequency  $\omega_{\max} = 2\sqrt{\frac{\kappa}{m}}$  above which there are no wave-like normal modes.
3. For small values of  $k$ , the dispersion relation is linear:  $\omega \approx 2\sqrt{\frac{\kappa}{m}} \frac{a}{2} k = v_s k$ .

The proportionality constant  $v_s = a\sqrt{\frac{\kappa}{m}}$  is just the speed of longitudinal “sound” (long wavelength waves) along the chain. Here “long wavelength” means  $ka \ll 2\pi$ , or  $\lambda \gg a$ .

The dispersion relation gives us the relation between  $\omega$  and  $k$  for the normal modes, but we have not yet found the specific frequencies (and  $k$ -values) of the modes. These will depend on the number of masses in the chain and the boundary conditions at the ends of the chain.

### 1.3.3 Boundary conditions: normal mode frequencies and wave vectors

To find particular values of  $\omega$  and  $k$  for the normal modes, we need to specify boundary conditions, and the total number of masses  $N$ . Let us introduce a new index  $q$  to label the frequency  $\omega_q$  and wave vector  $k_q$  of the  $q^{\text{th}}$  normal mode. Then, the dispersion relation for the monatomic chain becomes  $\mathbf{w}_q = \mathbf{w}_{\max} \sin\left(\frac{k_q a}{2}\right)$ .

#### Fixed boundary conditions

One approach to finding the normal modes is to apply **fixed boundary conditions**. This means that we fix the ends of the chain at all times, *i.e.* we require the fictitious  $0^{\text{th}}$  and  $(N+1)^{\text{th}}$  masses to be fixed. In this case, the normal modes will be **standing waves**.

Recall  $\mathbf{y}_n = A e^{i(nka - \mathbf{d})} e^{i\omega t}$ . The boundary condition  $\psi_0 = \text{Re}\left(A e^{i(k \cdot 0 - \mathbf{d})} e^{i\omega t}\right) = 0$  at all times requires that  $A_0 = \text{Re}\left(A e^{i(k \cdot 0 - \mathbf{d})}\right) = A \cos(-\mathbf{d}) = 0$  which implies  $\mathbf{d} = \frac{\pi}{2}$ . Thus, for any mass  $n$  on the chain,  $A_n = \text{Re}\left(A e^{i(kna - \pi/2)}\right) = A \cos(kna - \pi/2) = A \sin kna$ . These are the wave-like amplitudes of the eigenmodes.

Now, at the other end of the chain, the boundary condition  $\psi_{N+1} = 0$  implies

$$A_{N+1} = A \sin k_q(N+1)a = 0 \Rightarrow k_q(N+1)a = q\pi \Rightarrow k_q = \frac{q\pi}{(N+1)a}$$

The mode index  $q$  has values  $1, 2 \dots N$  ( $N$  distinct modes) which will give  $N$  distinct values of  $k_q$  and  $\omega_q$ . Now that we have  $k_q$ , we can find the related frequencies,  $\omega_q$ , using the dispersion relation and our problem is solved. The dispersion relation, normal mode frequencies and wave vectors for  $N = 5$  are illustrated in the following plot.

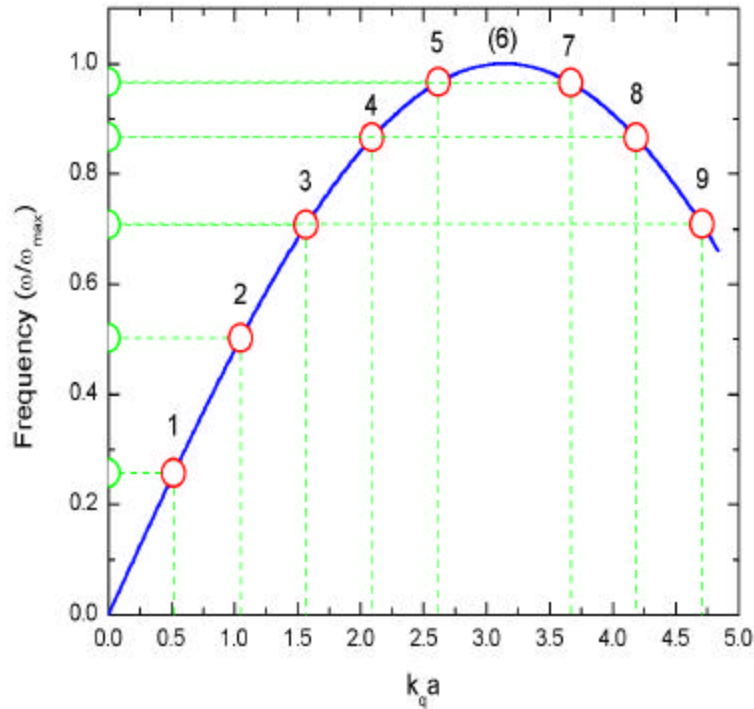


Figure X. Dispersion relation for the monatomic chain with normal mode frequencies and wave vectors for the case  $N = 5$  with fixed boundary conditions.

**Important features of the normal modes for fixed boundary conditions:**

1. For  $q < 0$ , we get no new information, since  $\sin(x) = -\sin(-x)$  and the entire displacement is the same except for a phase which can be absorbed into the time dependence.
2. For  $q = N + 1$ ,  $k_{N+1} = \pi/a$  and  $A_n = A \sin(n\pi) = 0$  for **all**  $n$ . This is a “null mode” – the displacements of all masses are zero at all times. This  $k$ -value ( $\pi/a$ ) defines the **Brillouin zone boundary**.
3. For  $q > N + 1$ , the frequencies repeat those for  $1 \leq q \leq N$  due to the periodicity of the dispersion relation.

## Periodic boundary conditions

**Periodic boundary conditions** are an alternative to fixed boundary conditions. Here we have no requirement on the amplitude, but rather on the displacement as a whole. We require only that the motion of the 0<sup>th</sup> mass be the same as the motion of the (N+1)<sup>th</sup>, or generally that the motion of the  $n^{\text{th}}$  mass be the same as the motion of the (N+n)<sup>th</sup>:

$$\begin{aligned} \mathbf{y}_n &= \mathbf{y}_{n+N+1} \\ \Rightarrow \operatorname{Re} \left( A e^{i(kna - \mathbf{d})} \right) &= \operatorname{Re} \left( A e^{i(k(n+N+1)a - \mathbf{d})} \right) \\ \Rightarrow kna - \mathbf{d} &= k(n+N+1)a - \mathbf{d} \pm 2\pi q \end{aligned}$$

which simplifies to  $k_q = \pm \frac{2\pi q}{(N+1)a}$  (with no requirement on  $\delta$ ).

The normal modes and corresponding  $q$ -values for periodic boundary conditions are compared with those for fixed boundary conditions for  $N = 5$  in Figure X.

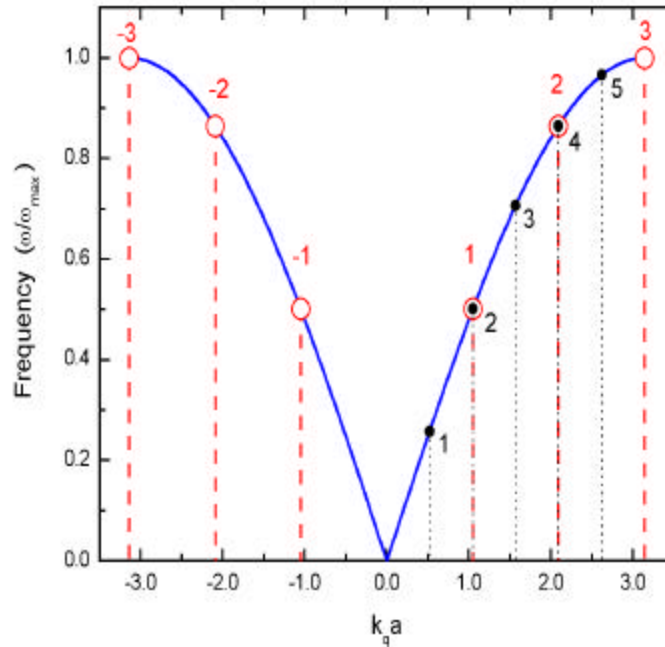


Figure X. Dispersion relation for the monatomic chain for  $N = 5$  showing normal modes and associated  $q$ -values for periodic boundary conditions (open points) and fixed boundary conditions (closed points). Note that for periodic boundary conditions there are actually  $N + 1 = 6$  moving masses in the chain and 6 normal modes (explained below).

**Important features of the normal modes for periodic boundary conditions:**

1. We see that the  $k$  spacing has doubled ( $q = (N+1)/2$  gives the Brillouin zone boundary). Have we lost half the modes? No! In this case the different signs of  $q$  ARE distinct. Positive and negative  $q$  values correspond to oppositely propagating traveling waves. Thus  $q = \pm 1, \pm 2, \dots, \pm(N+1)/2$  give physically distinct modes (now it's clear why the minus sign above was dropped). This running wave set of states is simply a different basis set from the standing wave set
2. Note that one generally sees periodic boundary conditions written as  $\mathbf{y}_n = \mathbf{y}_{n+N}$  and not  $\mathbf{y}_n = \mathbf{y}_{n+N+1}$  as written above. Why? In our problem of  $N$  masses with fixed boundary conditions, we really introduced a fictitious  $0^{\text{th}}$  and  $(N+1)^{\text{th}}$  mass and made them stationary. So we really had  $N + 1$  unit cells in our problem. With the periodic boundary conditions, we let the  $0^{\text{th}}$  and  $N^{\text{th}}$  atom (which are really the same atom) participate in the motion, so again we really had  $N + 1$  unit cells.



## 1.4 Diatomic chain

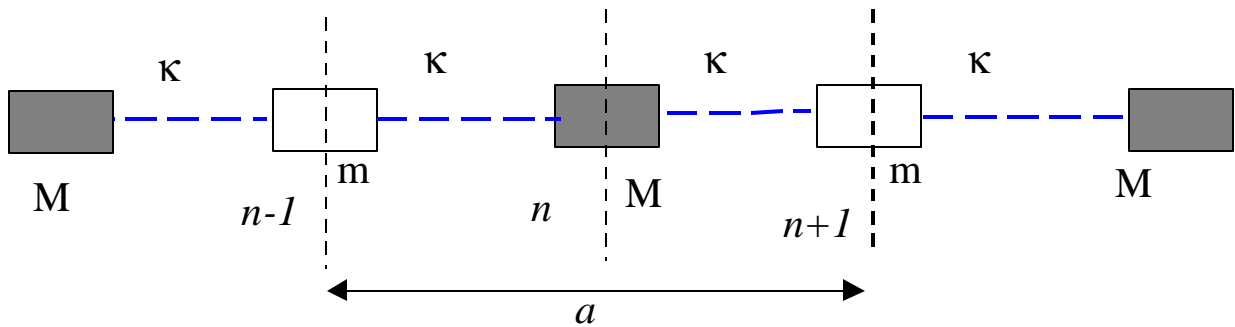
**Lab #2 is the study of an  $N$ -membered chain containing alternating masses (“diatomic chain”)**

### 1.4.1 Equations of motion

Following the procedure we used to analyze the monatomic chain, we will set up Newton’s equations of motion using Hooke’s Law for the forces. Again we constrain the motion to one-dimension along the direction of the chain (longitudinal oscillations).

Each “cell” or repeating unit contains two masses,  $M$  and  $m$ , and two identical springs with spring constant  $\kappa$ . In the diagram below, the dark masses ( $M$ ) are the larger, the light ones ( $m$ ) are the smaller. The distance from cell to cell (“lattice constant”) is  $a$ , therefore equilibrium spacing between the masses (“interatomic distance”) is  $a/2$ . The equilibrium position of mass  $n$  is

$x_n^0 = \frac{na}{2}$  so the actual position of the mass along the chain is  $x_n = \frac{na}{2} + y_n$ .



The force on the heavy mass  $n$  is  $F_n = -\kappa(y_n - y_{n-1}) - \kappa(y_n - y_{n+1})$ . Newton’s law gives  $F_n = M\ddot{y}_n$ , so we have

$$M\ddot{y}_n = \kappa(y_{n+1} - 2y_n + y_{n-1})$$

For the neighboring light mass  $n-1$ , the equation of motion is

$$F_{n-1} = m\ddot{\psi}_{n-1} = \kappa(\psi_{n-2} - 2\psi_{n-1} + \psi_n).$$

For the monatomic chain, we were able to obtain the dispersion relation from the equation of motion for a single mass in the chain. For the diatomic chain, we have two distinct equations because  $M \neq m$ .

### 1.4.2 Normal modes and dispersion relation

We assume, as usual, that there exist normal modes of motion in which all masses oscillate with the same frequency. However, the small and large masses can oscillate with different amplitudes. Thus we need to write

$$\begin{aligned} \mathbf{y}_n &= A e^{i(kna/2 - \omega t)} \text{ for } M \text{ masses.} \\ \mathbf{y}_n &= \alpha A e^{i(kna/2 - \omega t)} \text{ for } m \text{ masses} \end{aligned}$$

where  $\alpha$  determines the amplitude and phase of  $m$  oscillations relative to  $M$  oscillations. Once again note that the frequency  $\omega$  has no subscript  $n$  relating it to a particular mass – all masses move with same frequency in given mode. The wave vector,  $k$ , is determined by the wavelength of the pattern of displacement along the chain,  $k = \frac{2\pi}{\lambda}$ .

Now, substitute the assumed displacements for a normal mode into the two equations of motion and cancel the time-dependent factor  $e^{-i\omega t}$  that is common to all terms.

$$\begin{aligned} -M\omega^2 e^{inka/2} &= -\kappa \left( e^{inka/2} - \alpha e^{i(n-1)ka/2} \right) - \kappa \left( e^{inka/2} - \alpha e^{i(n+1)ka/2} \right) \\ -\alpha m\omega^2 e^{i(n-1)ka/2} &= -\kappa \left( \alpha e^{i(n-1)ka/2} - e^{i(n-2)ka/2} \right) - \kappa \left( \alpha e^{i(n-1)ka/2} - e^{inka/2} \right) \end{aligned}$$

We can also cancel the common factors  $e^{inka/2}$  and  $e^{i(n-1)ka/2}$  in the first and second equations, respectively to get

$$\begin{aligned} -M\omega^2 &= \mathbf{k}(\alpha e^{ika/2} + \alpha e^{-ika/2} - 2) \\ -\alpha m\omega^2 &= \mathbf{k}(e^{ika/2} + e^{-ika/2} - 2\alpha) \end{aligned}$$

which can be further simplified to get two equations in the two unknowns  $\alpha$  and  $\omega^2$ :

$$\begin{aligned} -M\omega^2 &= 2\mathbf{k}\alpha \cos(ka/2) - 2\mathbf{k} \\ -\alpha m\omega^2 &= 2\mathbf{k}\cos(ka/2) - 2\alpha\mathbf{k} \end{aligned}$$

Now eliminate  $\alpha$  by solving each equation for  $\alpha$ ,

$$\begin{aligned} \alpha &= \frac{2\mathbf{k} - M\omega^2}{2\mathbf{k}\cos(ka/2)} \\ \alpha &= \frac{2\mathbf{k}\cos(ka/2)}{2\mathbf{k} - m\omega^2} \end{aligned}$$

and equating them to get the DISPERSION RELATION  $\omega(k)$ :

$$\frac{2\mathbf{k} \cos(ka/2)}{2\mathbf{k} - m\mathbf{w}^2} = \frac{2\mathbf{k} - M\mathbf{w}^2}{2\mathbf{k} \cos(ka/2)}$$

$$\Rightarrow 4\mathbf{k}^2 \cos^2(ka/2) = (2\mathbf{k} - m\mathbf{w}^2)(2\mathbf{k} - M\mathbf{w}^2)$$

$$\mathbf{w}^2 = \mathbf{k} \left( \frac{1}{M} + \frac{1}{m} \right) \pm \mathbf{k} \left[ \left( \frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4}{Mm} \sin^2(ka/2) \right]^{1/2}$$

We can anticipate that we will want to label frequencies and wave vectors with an index  $q$  to identify the normal mode they are associated with. Thus, the final form of the dispersion relation is

$$\boxed{\mathbf{w}_q^2 = \mathbf{k} \left( \frac{1}{M} + \frac{1}{m} \right) \pm \mathbf{k} \left[ \left( \frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4}{Mm} \sin^2(k_q a / 2) \right]^{1/2}}$$

Remember, frequencies  $\omega_q$  and wave vectors  $k_q$  as associated with the  $q^{\text{th}}$  **mode** and not any particular mass. The masses are identified by their “address” along the chain,  $n$ .

A new feature has emerged in the dispersion relation of the diatomic chain. Because of the  $\pm$  signs, there are **two branches to the dispersion curve**. Each value of the index  $q$  has two frequencies. We will need to distinguish these frequencies. We could do this by introducing an additional index, say, by writing  $\omega_q^+$  and  $\omega_q^-$ . However, it is conventional to label the two branches of the dispersion curve with the following names:

the lower frequency branch is called the **ACOUSTIC** branch;  
the higher frequency branch is called the **OPTIC** branch.

There are sound physical reasons for these names, which we shall discuss shortly.

Note the repetition of frequency information after  $k = \frac{\pi}{a}$ , i.e. beyond the boundary of the Brillouin zone. Wavelengths less than  $2a$  are physically meaningless, as we found in Lab #2.

The two branches of the dispersion curve are shown in the following figure. They were calculated for the parameters:  $m = 1$ ,  $M = 2$ ,  $\kappa = 0.5$ ,  $a = \pi$ .

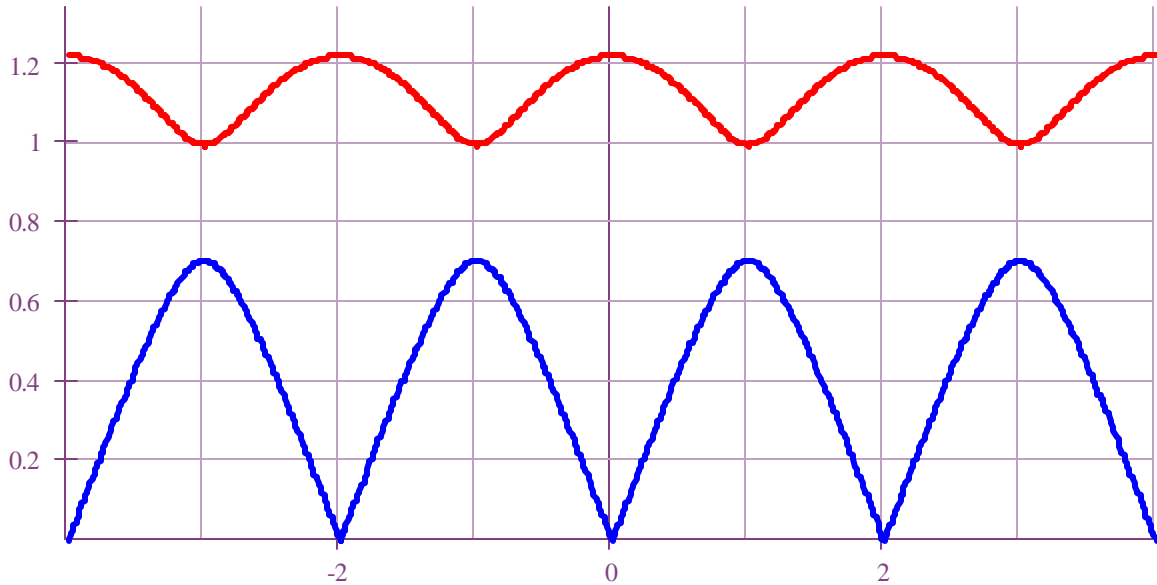


Figure X. Acoustic branch (lower curve) and optic branch (upper curve) of the dispersion relation for a diatomic chain with parameters  $m = 1$ ,  $M = 2$ ,  $\kappa = 0.5$ ,  $a = \pi$ .

#### Important features of the dispersion relation for a diatomic chain:

1. There is a **maximum** frequency for the acoustic branch, and **both maximum and minimum** frequencies for the optic branch.
2. Both branches are **periodic in  $k$**  and all possible frequencies can be obtained with wave vectors in the range  $0 \leq k \leq \pi/a$  (**Brillouin zone**).
3. Because the “lattice constant”  $a$  equals twice the spacing between masses, the Brillouin zone for the diatomic chain is **half the size** of the Brillouin zone for a monatomic chain with the same spacing between masses.
4. The acoustic branch is qualitatively similar to the dispersion relation of a monatomic chain and, in particular, is **linear for small values of  $k$**  (or  $k$ -values that are integer multiples of  $2\pi$ ).
5. At the Brillouin zone boundary, there is a **gap** (a range of forbidden frequencies) between the acoustic and optic branches. The magnitude of the gap depends on the ratio  $m/M$  and the gap closes when  $m = M$ .

Now that we know the frequencies, we can go back and calculate two values for  $\alpha$  at a given  $k$ -value (one for the acoustic modes and one for the optical modes). The results are:

$$\alpha_a = \frac{2\kappa \cos\left(\frac{ka}{2}\right)}{2\kappa - \omega_a^2} \quad \text{and} \quad \alpha_o = \frac{2\kappa \cos\left(\frac{ka}{2}\right)}{2\kappa - \omega_o^2}$$

These expressions for alpha are shown below plotted versus  $k$  for the same parameters used in Fig. X.

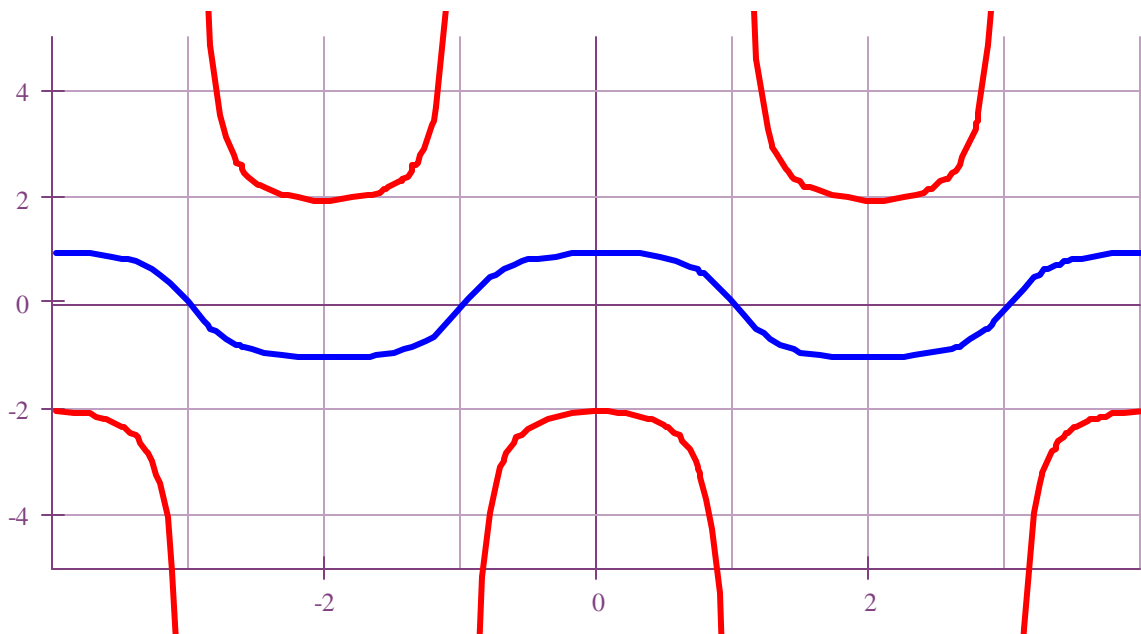


Figure XX. Amplitude ratio  $\alpha$  versus  $k$  for the acoustic modes (central curve) and optic modes (upper and lower curves) for a diatomic chain with parameters  $m = 1$ ,  $M = 2$ ,  $\kappa = 0.5$ ,  $a = \pi$ .

#### Important features of the amplitude ratio $\alpha$ for a diatomic chain:

1. For the acoustic branch near at small  $k$  values,  $\alpha_a \rightarrow 1$ . This means that masses  $m$  and  $M$  are **moving in phase with equal amplitudes**. Since the wavelengths are long in this limit ( $\lambda \gg a$ ), this corresponds to ordinary longitudinal sound waves, hence the name “**acoustic**” for this branch.
2. For the optic branch near  $k = 0$ ,  $\alpha_o \neq 1$  and is negative. This means that masses  $m$  and  $M$  are **moving out of phase with unequal amplitudes**. For the parameters used for Figs. X and XX,  $\alpha_o = -2$  so that the small masses  $m$  are oscillating out of phase and with twice the amplitude as the large masses  $M$ . In real solids where the different masses may also carry differing ionic electric charges, such out-of-phase motions couple strongly to electromagnetic waves (discussed in section x.x), hence the name “**optic**” for this branch.
3. For the acoustic branch at the Brillouin zone boundary,  $\alpha_a = 0$  so that in this mode, the **light masses  $m$  are not moving at all** and only the heavy masses  $M$  are oscillating.
4. For the optic branch and the Brillouin zone boundary,  $\alpha_o \rightarrow \infty$  so that in this mode, the **heavy masses  $M$  are not moving** and only the light masses  $m$  are oscillating.

We asserted previously that the “gap” between the optic and acoustic frequencies at the Brillouin zone boundary depends on the ratio  $m/M$  and that the gap vanishes when  $m = M$ . This is illustrated in Fig. Y where the dispersion relation is plotted for the case  $m = 1, M = 1.1$ . It can be seen that the gap is now very small compared with that in Fig. X. The two branches almost join together to form sets of repeating monatomic dispersion relations.

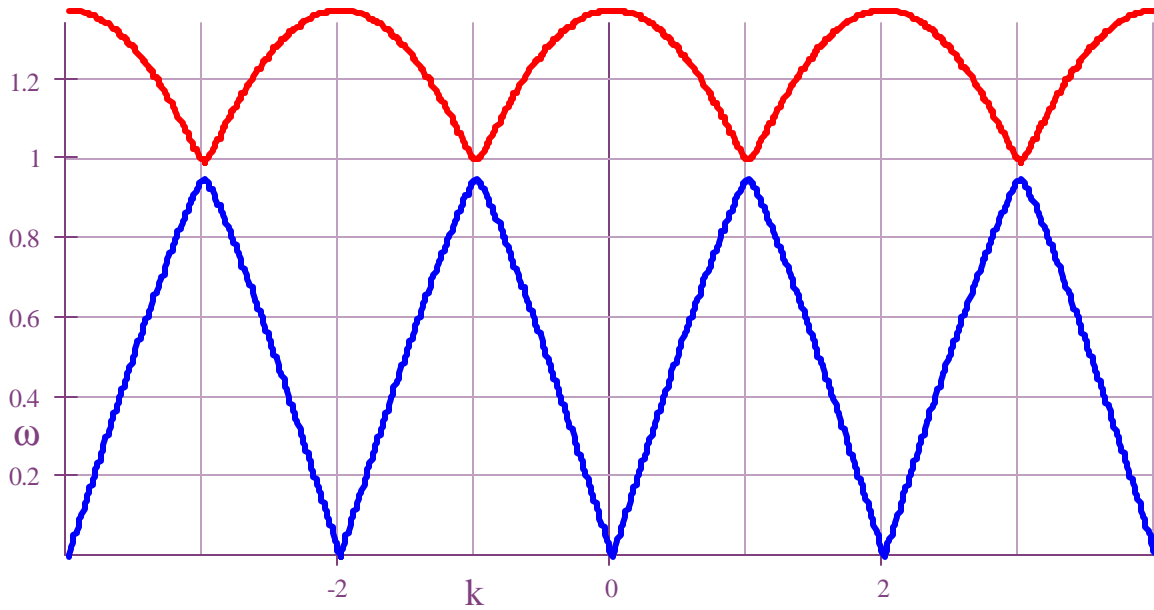


Figure Y. Acoustic branch (lower curve) and optic branch (upper curve) of the dispersion relation for a diatomic chain with parameters  $m = 1, M = 1.1, \kappa = 0.5, a = \pi$ .

The amplitude ratios  $\alpha_a$  and  $\alpha_o$  are shown below in Fig. YY for  $m = 1$  and  $M = 1.1$ . The main effect of nearly equal masses is that  $\alpha_a$  and  $\alpha_o$  are almost constant across the Brillouin zone except very close to the zone boundary.

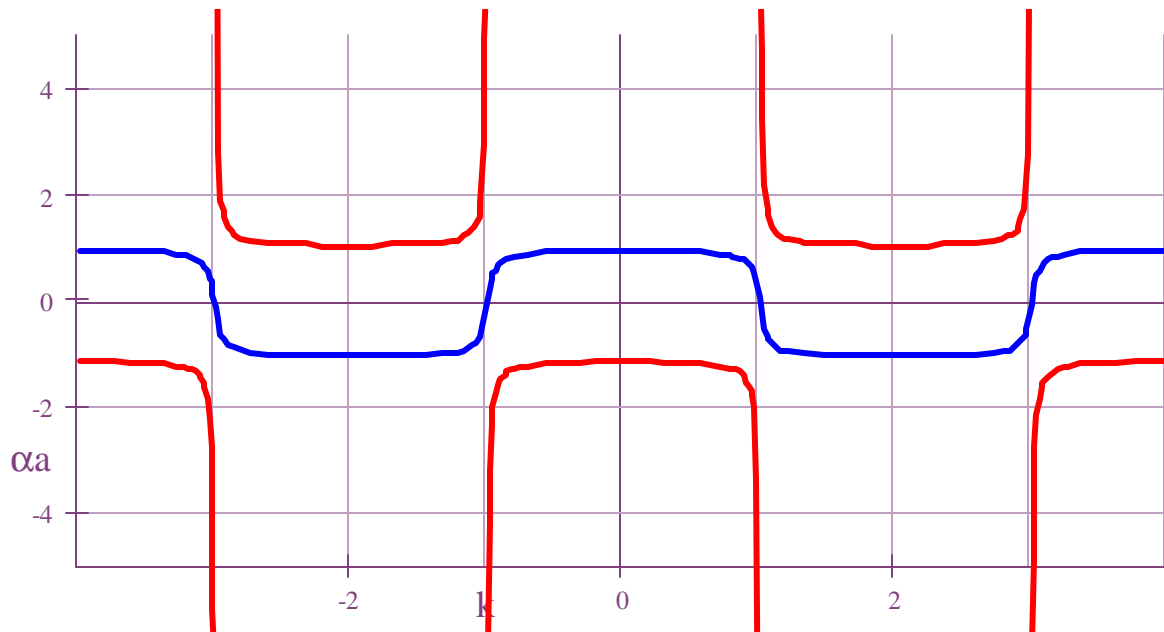


Figure YY. Amplitude ratio  $\alpha$  versus  $k$  for the acoustic modes (central curve) and optic modes (upper and lower curves) for a diatomic chain with parameters  $m = 1$ ,  $M = 1.1$ ,  $\kappa = 0.5$ ,  $a = \pi$ .

**Group activity: For the diatomic chain, find the wave vectors, vibration frequencies, and values of the constant  $\alpha$  at the following special points:**

**Group 1: Long wavelength optical vibration**

**Group 2: Brillouin zone optical vibration**

**Group 3: Brillouin zone acoustic vibration**

**Interpret your results in a way that illustrates the physical behavior of the system. Articulate what distinguishes an acoustic from an optical vibration.**

**If you finish early, move on to another task, swapping roles of taskmaster, cynic, & recorder. Interpret your results in a way that illustrates the physical behavior of the system. Articulate what distinguishes an acoustic from an optical vibration.**

## 1.5 Evanescent waves: forbidden frequencies

From our study of various systems of coupled oscillators we have learned that the normal mode frequencies are confined to certain ranges, depending on the specific type of system. For example, there is a maximum frequency for the allowed modes of linear chains of coupled masses (monatomic or diatomic). The same is true for a “beaded string,” a set of masses connected by a continuous string instead of Hooke’s Law springs. In some cases, there is a minimum frequency. Examples are the coupled pendula (hwk 1) or optic branch of diatomic chain (Lab 2).

The existence of these maximum and minimum allowed frequencies means that there are certain frequency ranges for which no modes exist in coupled systems. Of course, even within the ranges of allowed frequencies, boundary conditions require that only certain discrete frequencies (eigenfrequencies) are allowed. But these discrete frequencies can be made arbitrarily close together in a system with a large number of masses.

The laws of mechanics and the properties of a particular system determine the frequencies of allowed vibrational modes for that system. If the system is excited, say by displacing the masses from equilibrium and then leaving it undisturbed, the system will move in some superposition of the allowed normal modes that depends on the initial conditions. However, there is nothing to prevent us from *driving* a system at *any frequency* of our choice. In particular, we might choose to drive the system at a frequency that is not allowed. We could, for example, oscillate one end of a linear chain of masses and try to excite waves along the chain at a forbidden frequency. What happens?

Let’s consider the example of a monatomic chain. We know that the dispersion relation is

$$\omega(k) = 2\sqrt{\frac{k}{m}} \sin \frac{ka}{2} = \omega_{\max} \sin \frac{ka}{2}$$

We also know that depending on the number of masses and the type of boundary conditions, there are normal modes with discrete frequencies in the range  $0 < \omega \leq \omega_{\max}$  and discrete wave vectors in the Brillouin zone  $0 < k \leq \pi/a$ . But now suppose that we pick a driving frequency  $\omega > \omega_{\max}$ . Then  $\sin\left(\frac{ka}{2}\right) = \frac{\omega}{\omega_{\max}} > 1$  and  $k$  must necessarily be complex since the  $\sin(x)$  cannot exceed 1 for real  $x$ .

To see how this goes, first recall that the sine and cosine of purely imaginary arguments leads to the hyperbolic functions,  $\sinh$  and  $\cosh$ , respectively:

$$\begin{aligned} \sin i\theta &= \frac{e^{i(i\theta)} - e^{-i(i\theta)}}{2i} = \frac{e^{-\theta} - e^{+\theta}}{2i} = i \frac{e^{+\theta} - e^{-\theta}}{2} = i \sinh \theta \\ \cos i\theta &= \frac{e^{i(i\theta)} + e^{-i(i\theta)}}{2} = \frac{e^{-\theta} + e^{+\theta}}{2} = \cosh \theta \end{aligned}$$



Now, letting  $k = \text{Re}(k) + i \text{Im}(k)$ ,

$$\frac{w(k)}{w_{\max}} = \sin \frac{(\text{Re}(k) + i \text{Im}(k))a}{2}$$

$$\frac{w(k)}{w_{\max}} = \sin \frac{\text{Re}(k)a}{2} \cos \frac{i \text{Im}(k)a}{2} + \cos \frac{\text{Re}(k)a}{2} \sin \frac{i \text{Im}(k)a}{2}$$

$$\frac{w(k)}{w_{\max}} = \sin \frac{\text{Re}(k)a}{2} \cosh \frac{\text{Im}(k)a}{2} + i \cos \frac{\text{Re}(k)a}{2} \sinh \frac{\text{Im}(k)a}{2}$$

The frequency  $\omega$  must be real for **any** value of  $k$ , so

$$\cos \frac{\text{Re}(k)a}{2} = 0 \Rightarrow \text{Re}(k) = \frac{\pi}{a}, \frac{3\pi}{a} \dots$$

It is sufficient to take  $\text{Re}(k) = \delta/a$ . This means  $\lambda = 2a$  and the masses **always** vibrate in antiphase. Further,

$$\frac{w(k)}{w_{\max}} = \sin \frac{\pi}{2} \cosh \frac{\text{Im}(k)a}{2} = \cosh \frac{\text{Im}(k)a}{2}$$

$$\frac{\text{Im}(k)a}{2} = \cosh^{-1} \frac{w(k)}{w_{\max}}$$

Now look at displacements again:

$$\psi_n = A e^{i(kna - \delta)} e^{i\omega t}$$

$$\psi_n = A e^{i\left(\frac{\pi n}{a} + i 2n \cosh^{-1} \frac{\omega}{\omega_{\max}} - \delta\right)} e^{i\omega t}$$

$$\psi_n = A e^{-\frac{2n}{a} \cosh^{-1} \frac{\omega}{\omega_{\max}}} e^{i(\pi n - \delta)} e^{i\omega t} = A e^{-\beta n} e^{i(\pi n - \delta)} e^{i\omega t}$$

where  $\beta = 2 \cosh^{-1} \frac{\omega}{\omega_{\max}}$ . The real part is  $\psi_n = A e^{-\beta n} \cos(\pi n - \delta + \omega t)$ .

This describes a wave that is exponentially damped along the chain with a damping length  $(1/\beta)$  that depends on how far above  $\omega_{\max}$  we attempt to drive the chain.

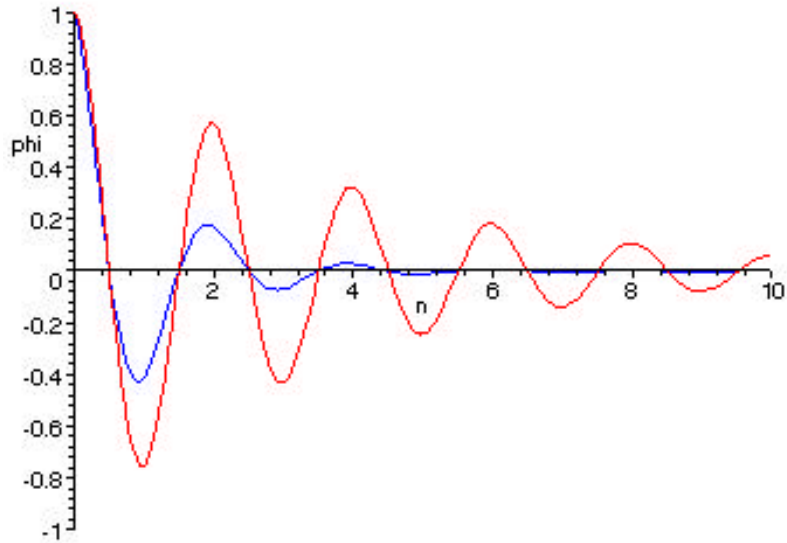


Figure Z. Instantaneous amplitudes of oscillations for a monatomic chain driven at a frequency  $\omega > \omega_{\max}$ . The more strongly damped wave results from a driving frequency that is further into the forbidden frequency range. The horizontal axis represents the distance along from the chain from the point at which it is driven.

**Discussion questions :**

Consider a set of coupled masses in which the middle masses are replaced by heavier ones. What will happen? (Demonstrate with CUPS session?)

Suppose a wave propagating with an allowed frequency along a chain encounters a region in which the frequency of the wave is forbidden. What will happen? What happens to the energy carried by the propagating wave?