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04 Linear Chain of Coupled Oscillators

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Exercise: Just from the form of (3.4), can you explain why the eigenvectors are only determined up to an overall multiplicative factor?

Using these eigenvectors in (3.10) we recover the expression (2.12) – you really should verify this yourself. In particular, it is the eigenvectors of K that determine the column vectors appearing in (2.16) *(exercise)*.

Note that the eigenvectors are linearly independent as advertised (*exercise*). Indeed, using the usual scalar product on the vector space of column vectors $\mathbf{v}$ and $\mathbf{w}$,

$$(\mathbf{v}, \mathbf{w}) = \mathbf{v}^T \mathbf{w},$$

you can check that $\mathbf{e}_1$ and $\mathbf{e}_2$ are orthogonal (see Problems).

To summarize: The resonant frequencies of a system of coupled oscillators, described by the matrix differential equation

$$\frac{d^2}{dt^2}\mathbf{q} = -K\mathbf{q},$$

are determined by the eigenvalues of the matrix K. The normal modes of vibration are determined by the eigenvectors of K.

4. Linear Chain of Coupled Oscillators.

As an important application and extension of the foregoing ideas, and to obtain a first glimpse of wave phenomena, we consider the following system. Suppose we have N identical particles of mass m in a line, with each particle bound to its neighbors by a Hooke's law force, with "spring constant" k. Let us assume the particles can only be displaced in one-dimension; label the displacement from equilibrium for the j^{th} particle by q_j, $j = 1, 2, \ldots, N$. Let us also assume that particle 1 is attached to particle 2 on the right and a rigid wall on the left, and that particle N is attached to particle $N-1$ on the left and another rigid wall on the right. The equations of motion then take the form (*exercise*):

$$\frac{d^2 q_j}{dt^2} + \omega^2(q_j - q_{j-1}) - \omega^2(q_{j+1} - q_j) = 0, \quad j = 1, 2, \ldots, N. \tag{4.1}$$

For convenience, in this equation and in all that follows we have extended the range of the index j on q_j to include $j = 0$ and $j = N+1$. You can pretend that there is a particle fixed to each wall with displacements labeled by q_0 and q_{N+1}. Since the walls are rigid, to obtain the correct equations of motion we must set

$$q_0 = 0 = q_{N+1}. \tag{4.2}$$

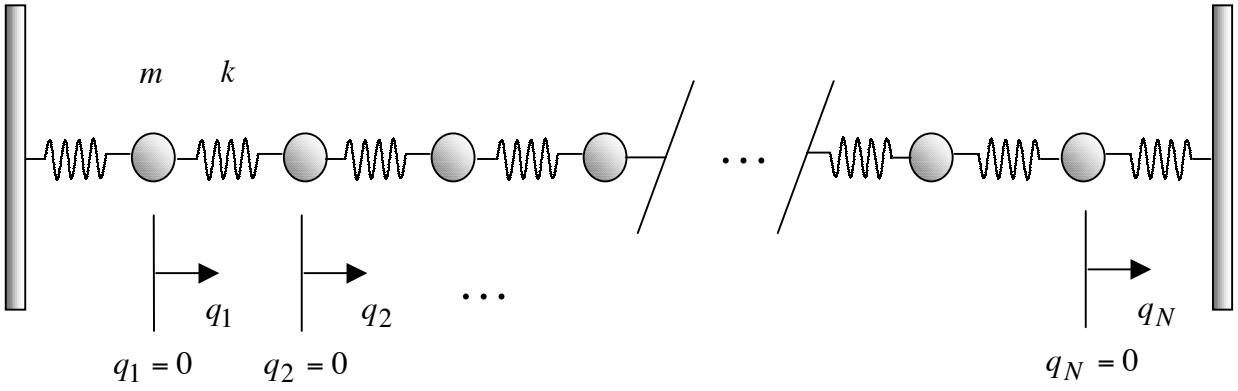

Figure 7. Linear chain of coupled oscillators. Each oscillator of mass m is coupled to its nearest neighbor with a spring with spring constant k. As in the case of the two-coupled oscillator problem, displacement from equilibrium q_i is restricted to be along the chain of oscillators, as illustrated.

The equations of motion (4.1) are, mathematically speaking, a system of N coupled, linear, homogeneous, ordinary differential equations with constant coefficients. Note that each oscillator is coupled only to its "nearest neighbors" (*exercise*). As it turns out, the system of coupled oscillators described by (4.1) exhibits resonant frequencies and normal modes of vibration. To see this we could set up (4.1) as a matrix equation (see Problems) and use the linear algebraic techniques discussed above. In particular, the generalization of the matrix K from the last section will be symmetric and hence will admit N linearly independent eigenvectors, which define the normal modes and whose eigenvalues define the characteristic frequencies. While this is a perfectly reasonable way to proceed, particularly for relatively low values for N, for arbitrary values of N we can reduce the analysis considerably by employing a shortcut. We shall explain this in a moment.

This picture of a linear chain of coupled oscillators (and its three-dimensional generalization) is used in solid state physics to model the vibrational motion of atoms in a solid. The masses represent the atomic nuclei that make up the solid and the spacing between the masses is the atomic separation. The "springs" coupling the masses represent a harmonic approximation to the forces binding the nuclei into the solid. In the context of applications to solid state physics the normal modes (when treated quantum mechanically) are identified with *phonons*. This phonon picture of vibrational modes of a solid is used to describe thermal conductivity, specific heat, propagation of sound, and other properties of the solid.

Our goal will be to obtain the normal modes and characteristic frequencies of vibration defined by (4.1). Recall that each of the normal modes of vibration for a pair of coupled oscillators has the masses oscillating harmonically, all at the same frequency (*cf.* (2.9) and (2.10)). Let us therefore look for a complex solution to (4.1) of the form

$$q_j(t) = A_j e^{i\Omega t}. \tag{4.3}$$

By convention we assume that the frequency Ω is non-negative. Substituting this into our equations yields a *recursion relation** (*exercise*):

$$-\Omega^2 A_j = \omega^2(A_{j-1} - 2A_j + A_{j+1}), \quad j = 1, 2, \ldots, N, \tag{4.4}$$

still subject to the conditions

$$A_0 = 0 = A_{N+1}.$$

We can solve this relation by further specifying our trial solution. Suppose A_j is of the form:

$$A_j = a\sin(j\phi), \tag{4.5}$$

where ϕ is some real number and a can be complex.† Note that this trial solution satisfies the boundary condition $q_0 = 0$, but we still have to take care of the condition $q_{N+1} = 0$ — we shall do this below by specifying the parameter ϕ. We plug (4.5) into the recursion relation to get (*exercise*)

$$-\Omega^2 a\sin(j\phi) = \omega^2\Big\{a\sin[(j-1)\phi] - 2a\sin[j\phi] + a\sin[(j+1)\phi]\Big\}. \tag{4.6}$$

Note that a will drop out of this condition, that is, a is not determined by (4.4)

Exercise: What property of the equations (4.1) and/or (4.4) guarantees that a will drop out of (4.6)?

To analyze (4.6) we use the trigonometric identity (*exercise*),

$$\sin(\alpha + \beta) = \sin\alpha\cos\beta + \cos\alpha\sin\beta$$

* A recursion relation for a set of variables A_j, $, j = 1, 2, \ldots n$, is a sequence of equations which allows one to determine A_k from the set $A_1, A_2, \ldots, A_{k-1}$.

† This form of the trial solution is certainly not obvious. It can be motivated by studying several special cases with N small. Alternatively, one can consider (4.4) for very large values of j, in which case one can pretend that A_j is a function of the continuous variable j. One can then interpret the recursion relation as (approximately) saying that the second derivative of this function is proportional to the function itself. Using $A_0 = 0$ one arrives at (4.5) (*exercise*).

to write

$$\sin[(j \pm 1)\phi] = \sin(j\phi)\cos(\phi) \pm \cos(j\phi)\sin(\phi).$$

Using this in (4.6) gives (*exercise*)

$$\Omega^2 \sin(j\phi) = 2\omega^2[1 - \cos(\phi)]\sin(j\phi).$$

Given (4.3) and (4.5), we naturally assume that $\sin(j\phi)$ does not vanish identically for all j. Thus the recursion relation (and hence the equations of motion (4.1)) are satisfied by (4.3) and (4.5) if and only if

$$\Omega^2 = 2\omega^2[1 - \cos(\phi)] = 4\omega^2 \sin^2(\phi/2), \tag{4.7}$$

that is,

$$\Omega = 2\omega|\sin(\phi/2)|. \tag{4.8}$$

Note that we are adhering to our convention that Ω be non-negative.

We still must enforce the condition $q_{N+1} = 0$, which is now $A_{N+1} = 0$. This condition means

$$\sin[(N+1)\phi] = 0, \tag{4.9}$$

so that

$$(N+1)\phi = n\pi, \quad n = 1, 2, \ldots, N. \tag{4.10}$$

In (4.10) we take the maximum value for n to be N to avoid redundant solutions; if $n > N$ then we obtain solutions for A_j that were already found when $n \leq N$ (see below and also the homework problems). We exclude the solution corresponding to $n = 0$ because this solution has $\phi = 0$, which forces $A_j = 0$, *i.e.,* this is the trivial solution $q_j(t) = 0$ (for all values of j) of the coupled oscillator equations.

Exercise: What property of (4.1) guarantees that $q_j = 0$ is a solution?

To summarize thus far, there are N distinct resonant frequencies, which we label by an integer n, where $n = 1, 2, \ldots, N$. They take the form

$$\Omega_n = 2\omega|\sin\left(\frac{n\pi}{2N+2}\right)|, \quad n = 1, 2, \ldots, N. \tag{4.11}$$

Compare this with the case of two coupled oscillators, treated earlier, where there were 2 resonant frequencies.

We can now return to our trial solution for the complex amplitudes A_j. For each resonant frequency there will be a corresponding set of complex amplitudes. (In the case of two coupled oscillators there were two resonant frequencies and two sets of amplitudes,

representing the normal modes.) For the resonant frequency Ω_n (for some choice of n) we denote the corresponding complex amplitudes by $A_{(n)j}$, $j = 1, 2, \ldots, N$. We have (*exercise*)

$$A_{(n)j} = a_n \sin\left(\frac{n\pi j}{N+1}\right), \tag{4.12}$$

where a_n is any complex number. Let us pause to keep track of our notation: j labels the masses, N is the total number of masses, and n labels the normal modes of vibration and their resonant frequencies. If you view the N amplitudes for each n, $A_{(n)j}$, $j = 1, 2, \ldots, N$, n fixed, as forming the entries of a column vector, *i.e.,*

$$\begin{pmatrix} A_{(n)1} \\ A_{(n)2} \\ \cdot \\ \cdot \\ \cdot \\ A_{(n)N-1} \\ A_{(n)N} \end{pmatrix}$$

then the totality of the column vectors (obtained by letting $n = 1, 2, \ldots, N$) would form a basis for the N-dimensional space of column vectors with N entries. This basis is in fact the basis of eigenvectors defined by the matrix K which we mentioned (but didn't explicitly write down) at the beginning of this section. As guaranteed by general results in linear algebra, all the vectors in this basis are orthogonal. You will investigate this in the Problems.

The solution of the equations of motion for the n^{th} normal mode has oscillator displacements given by (*exercise*)

$$\begin{aligned} q_{(n)j} &= Re\left[a_n \sin\left(\frac{n\pi j}{N+1}\right) e^{i\Omega_n t}\right], \\ &= |a_n| \sin\left(\frac{n\pi j}{N+1}\right) \cos(\Omega_n t + \alpha_n), \quad j = 1, 2, \ldots, N, \end{aligned} \tag{4.13}$$

where we have written $a_n = |a_n| e^{i\alpha_n}$.

For the n^{th} mode we have the following behavior. By considering (4.13) for a fixed value of j, you can see that each mass is undergoing a harmonic oscillation at frequency Ω_n. The amplitude of oscillation for the j^{th} oscillator is $|a_n| \sin\left(\frac{n\pi j}{N+1}\right)$ – it depends sinusoidally on the location of the mass and has an overall scale set by a_n. In particular, for the nth mode at a fixed time, as you move from one mass to the next the displacement of each mass advances in phase by $\frac{n\pi}{N+1}$, leading to the patterns shown in figure 8. Figure 8 depicts snapshots at a fixed time of the displacement profile of the masses. A number of different normal modes are shown.

Another point of view on these displacement profiles is as follows. Let us suppose that the equilibrium positions of the masses are separated by a distance d, and that the first ($j = 1$) and last ($j = N$) masses are separated from their walls also by d when in equilibrium. Then the j^{th} mass, in its equilibrium position, will be a distance $x = jd$ from the wall attached to q_1 (*exercise*). According to (4.13), if you examine the system at a fixed time t, *i.e.,* take a photograph of the system at time t, then the displacement from equilibrium as a function of location on the chain of oscillators will be a function of the form $P\sin(Qx)$ (*exercise*), where P and Q are some real constants. Thus the displacement is a discrete form of a *standing wave*, which should be familiar to you from introductory physics. Recall that a standing wave in a continuous medium (*e.g.,* a guitar string) is a motion of the medium in which each point of the medium oscillates harmonically (*i.e.,* sinusoidally) in time from its equilibrium position, while the amplitude of the oscillation at any fixed time varies sinusoidally from point to point in the medium.

Also recall that standing waves have *nodes*, which are points which have zero oscillation amplitude, that is, they do not move at all. For our linear chain of coupled oscillators nodes will occur where the sine vanishes, that is, where

$$j = \frac{(N+1)}{n}l, \quad l = 0, 1, 2, \ldots, n. \tag{4.14}$$

Note that we include the cases $j = 0$ and $j = N+1$, which are always nodes corresponding to the (pretend) masses fixed on the walls. Of course, (4.14) only applies when j works out to be an integer, or else there is no mass at the putative node. Indeed, for the discrete chain of oscillators the continuum standing wave picture must be augmented by the knowledge that the wave is only "sampled" at the points $x = jd$, $j = 0, 1, 2, \ldots, N+1$, which is why the displacement profiles in figure 8 are somewhat more intricate than one would expect when thinking of a sine function.

Still using the standing wave point of view, equation (4.11) is a relation between the frequency of vibration of the (discrete) standing wave and the mode number n. Using the interpretation for (4.12) given above, the wavelength of the discrete standing wave is inversely proportional to n. Thus one can also view (4.11) as a relationship between frequency and wavelength of the standing wave and hence as a relationship between wavelength and wave speed. We will find such a relationship in each instance of wave phenomena.* For reasons we shall discuss later, such a relation is called a *dispersion relation.*

Exercises: Show that when $n << N$ the frequency is approximately proportional to n, and when $n \approx N >> 1$ the frequency is approximately 2ω.

* The existence of the dispersion relation follows from the linearity of the equation describing the wave and from Fourier analysis – both topics we shall discuss soon.

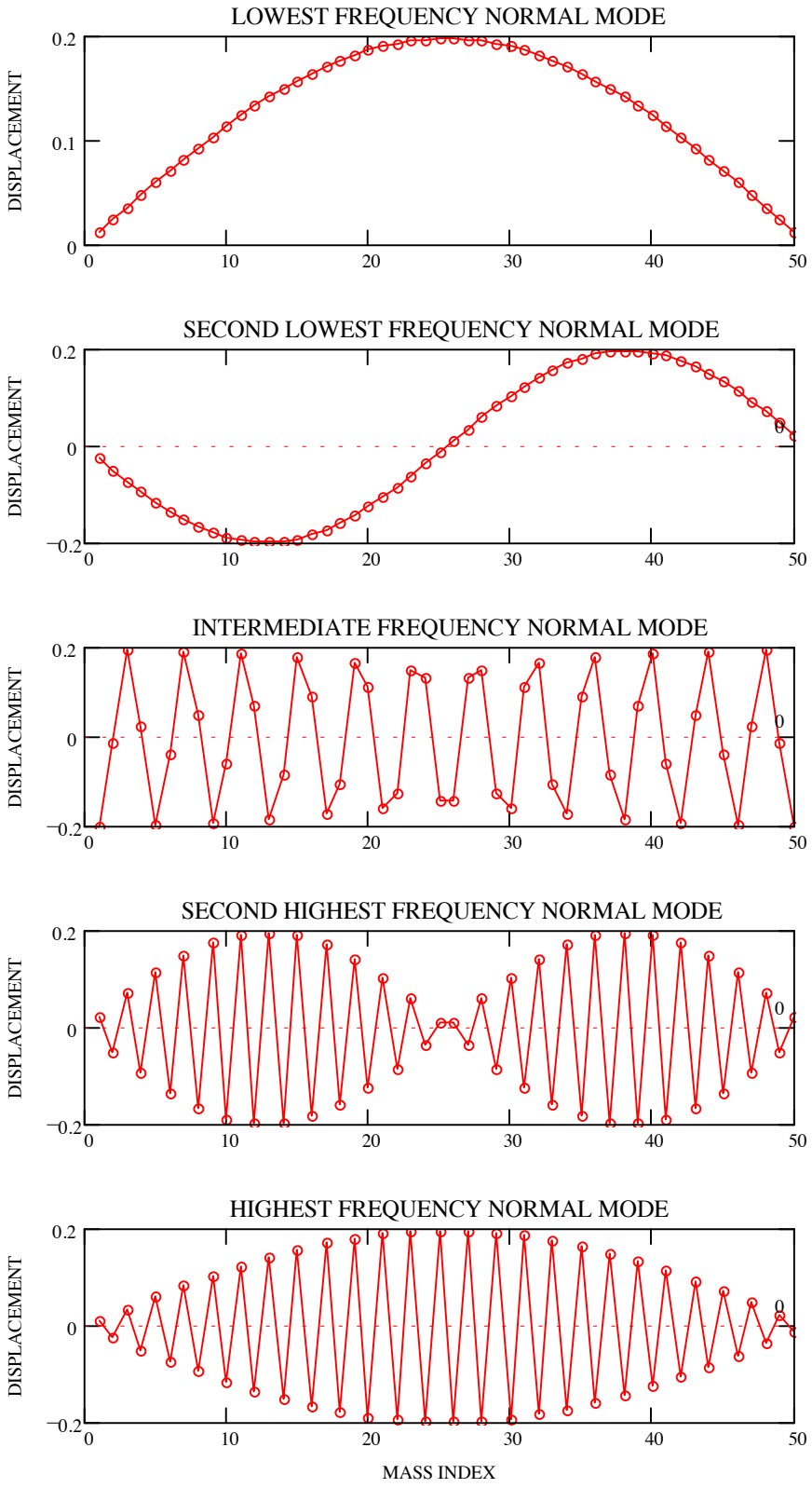

Figure 8. Selected normal modes for an $N = 50$ linear chain of coupled oscillators.

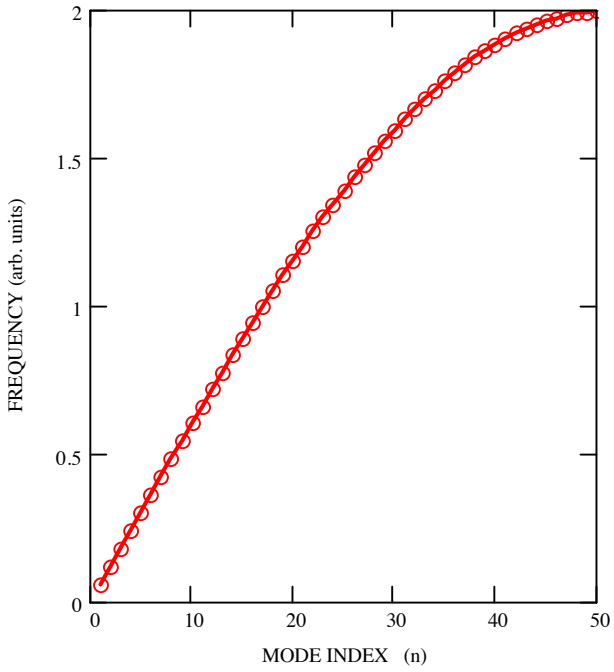

Figure 9. Dispersion relation Ω_n for the $N = 50$ linear chain of coupled oscillators.

The general solution to the equations of motion (4.1) is a superposition of all the normal modes:

$$q_j(t) = Re\left\{\sum_{n=1}^{N} a_n \sin\left(\frac{n\pi j}{N+1}\right) e^{i\Omega_n t}\right\}, \tag{4.15}$$

where a_n is a freely specifiable complex constant for each n. Note we can take the real part before or after the summation (*exercise*). An equivalent form of the general solution is therefore (*exercise*)

$$q_j(t) = \left\{\sum_{n=1}^{N} |a_n| \sin\left(\frac{n\pi j}{N+1}\right) \cos(\Omega_n t + \alpha_n)\right\}, \tag{4.16}$$

where $|a_n|$ and α_n are real numbers. In any case, the solution depends on $2N$ real constants via the complex numbers a_n in (4.15) or the real numbers $(|a_n|, \alpha_n)$ in (4.16). You should not be surprised by this. There are N particles, each obeying Newton's second law. Each particle will require specification of an initial position (displacement) and initial velocity to uniquely determine its motion. This is the same as giving an initial *displacement profile* and *velocity profile* along the chain. Specifying the initial conditions is equivalent to specifying the amplitudes $|a_n|$ and phases α_n. Thus one can accommodate every possible set of initial conditions using (4.15) or (4.16) and so one is indeed justified in claiming these formulas provide the general solution to the coupled oscillator problem.

Let me emphasize two key results that we can glean from the preceding analysis. First, note how the *boundary conditions* — *i.e.,* the rigid wall conditions $q_0 = 0 = q_{N+1}$ — serve to fix the form of the characteristic frequencies and the normal modes and hence the form of the general solution. Second, it is the *initial conditions* (requirements for all space at a fixed time, *e.g.,* initial displacement and velocity profiles) that pick out specific solutions of the equations of motion from the general solution, *i.e.,* determine the constants a_n. In other words, the boundary conditions determine the normal modes and the initial conditions determine the specific linear combination of normal modes that should describe a given situation.

4.1 Other Boundary Conditions

As it turns out, the normal modes have the form of (discrete) standing waves because we have fixed the ends of our chain of oscillators to rigid walls, *i.e.,* $q_0 = 0 = q_{N+1}$. If we change our boundary conditions we can obtain discrete versions of traveling wave solutions. Let us briefly have a look at this.

To begin, let us consider what happens if there are no boundary conditions at all. To do this with a minimum of fuss, we assume that the chain of oscillator extends "to infinity". Of course, no such thing exists. Rather, this is a just a convenient mathematical *model* for a situation where we have a long chain of many oscillators and we are only interested in the behavior of oscillators far from the ends of the chain. The idea is that near the center of a very long chain the effect of the boundary conditions should be negligible.* In this model we still have the equations of motion (4.1) for the displacements q_l, but we let l run over all integer values. We can still use the *ansatz* (4.3) and we obtain (4.4). Since we don't have to satisfy the rigid wall boundary conditions (4.2), we try a solution of the form

$$A_l = ae^{il\phi}. \tag{4.17}$$

This gives (*exercise*)

$$-\Omega^2 e^{il\phi} = \omega^2\Big\{e^{i(l-1)\phi} - 2e^{il\phi} + e^{i(l+1)\phi}\Big\}, \tag{4.18}$$

from which it follows (again!) that

$$\Omega(\phi) = 2\omega|\sin(\phi/2)|.$$

This time, however, there are no boundary conditions and hence no conditions upon ϕ. The normal mode solutions are determined/labeled by ϕ; they take the form

$$q_{\phi,l} = Re\left\{a(\phi)e^{i(l\phi+\Omega(\phi)t)}\right\}. \tag{4.19}$$

* This sort of model (suitably generalized to 3-dimensions) is used to describe the bulk properties of crystalline solids.

Notice that the exponential in (4.19) is unchanged if $\phi \to \phi + 2\pi$. This means that a non-redundant description of the normal modes of vibration is achieved by restricting ϕ to a region of size 2π, *e.g.,* $0 \leq \phi < 2\pi$. Notice also that when $\phi = 0$ the normal mode has zero frequency. What can this mean? Evidently, in this case all of the displacements $(q_1, q_2, \ldots)$ are equal and constant in time. It might help to picture a chain of masses connected by springs and free to move only in one dimension (parallel to the chain). Now visualize the chain of oscillators displaced rigidly as a whole (in one dimension, along its length) with no compression or stretching of the springs. This is the zero frequency mode. In our previous example, the fixed-wall boundary conditions prevented this mode from appearing. For $\phi > 0$, the form of the normal modes given in (4.19) is a discrete version of a *traveling sinusoidal wave*. In particular, at each time t the displacement profile is a (discretely sampled) sinusoidal pattern which moves with velocity $v = -\frac{\Omega d}{\phi}$ (*exercise*). (Here d is the equilibrium separation of the oscillators.)

Aside from rigid displacements of the chain, the general motion of the chain is obtained by a superposition of the normal modes with non-zero frequency. This is an integral of the form:

$$q_l(t) = Re \int_0^{2\pi} d\phi \, a(\phi) e^{i(l\phi + \Omega(\phi)t)}. \tag{4.20}$$

Let us now consider a different type of boundary condition — periodic boundary conditions. Imagine we have $N+1$ oscillators, as before, but now we identify the first and the last oscillators, that is, we assume that they always have the same displacement, which need not vanish:

$$q_1(t) = q_{N+1}(t). \tag{4.21}$$

This could be done by physically identifying the two oscillators — you might try imagining the chain of oscillators connected into a circle — or by some other means. Our analysis goes through as above in the case of no boundary conditions. In particular, we have the normal modes

$$q_{\phi,l}(t) = Re \left\{ a(\phi) e^{i(l\phi + \Omega(\phi)t)} \right\}, \tag{4.22}$$

with

$$\Omega(\phi) = 2\omega |\sin(\phi/2)|. \tag{4.23}$$

but the periodic boundary conditions (4.21) mean that (*exercise*)

$$e^{i\phi} = e^{i(N+1)\phi}, \tag{4.24}$$

so that (*exercise*)

$$\phi = \frac{2\pi}{N} n, \quad n = 0, 1, 2, \ldots N-1. \tag{4.25}$$

As in the case of fixed wall boundary conditions, the periodic boundary conditions force the normal modes to come in a discrete set. We have limited the range of n so that we

have a non-redundant set of modes (*exercise*). As in the case of no boundary conditions, there is a zero frequency normal mode corresponding to a rigid displacement of all the oscillators. The normal modes are again in the form of (discretely sampled) traveling waves. The general motion of the oscillators is a superposition of the normal modes. This superposition takes the form (*exercise*) :

$$q_l(t) = Re \sum_{n=0}^{N-1} a_n e^{i(2\pi nl/N + 2\omega t|\sin(\pi n/N)|)}$$