

## Chapter 9

# Normal Modes and Waves

©2000 by Harvey Gould and Jan Tobochnik  
6 December 2000

We discuss the physics of wave phenomena and the motivation and use of Fourier transforms.

### 9.1 Coupled Oscillators and Normal Modes

Terms such as period, amplitude, and frequency are used to describe both waves and oscillatory motion. To understand the relation between the latter two phenomena, consider a flexible rope that is under tension with one end fixed. If we flip the free end, a pulse propagates along the rope with a speed that depends on the tension and on the inertial properties of the rope. At the *macroscopic* level, we observe a transverse wave that moves along the length of the rope. In contrast, at the *microscopic* level we see discrete particles undergoing oscillatory motion in a direction perpendicular to the motion of the wave. One goal of this chapter is to use simulations to understand the relation between the microscopic dynamics of a simple mechanical model and the macroscopic wave motion that the model can support. For simplicity, we consider a one-dimensional chain of  $L$  particles each of mass  $M$ . The particles are coupled by massless springs with force constant  $K$ . The equilibrium separation between the particles is  $a$ . We denote the displacement of particle  $j$  from its equilibrium position at time  $t$  by  $u_j(t)$  (see Figure ??). For many purposes the most realistic boundary conditions are to attach particles  $j = 1$  and  $j = L$  to springs which are attached to fixed walls. We denote the walls by  $j = 0$  and  $j = L + 1$ , and require that  $u_0(t) = u_{L+1}(t) = 0$ .

The force on an individual particle is determined by the compression or extension of the adjacent springs. The equation of motion of particle  $j$  is given by

$$\begin{aligned} M \frac{d^2 u_j(t)}{dt^2} &= -K[u_j(t) - u_{j+1}(t)] - K[u_j(t) - u_{j-1}(t)] \\ &= -K[2u_j(t) - u_{j+1}(t) - u_{j-1}(t)]. \end{aligned} \tag{9.1}$$

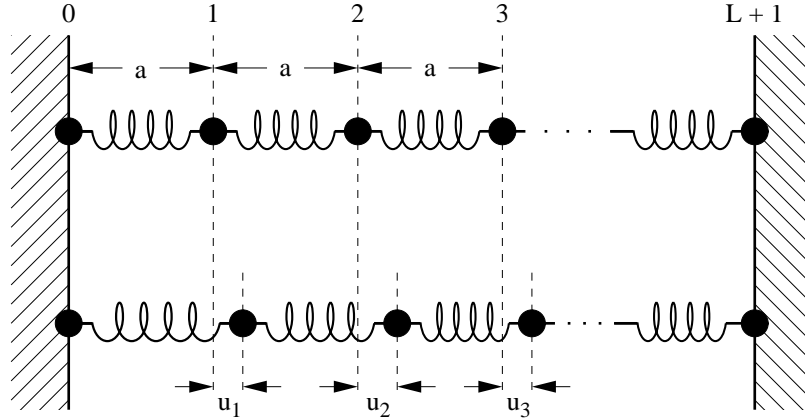


Figure 9.1: A one-dimensional chain of  $L$  particles of mass  $M$  coupled by massless springs with force constant  $K$ . The first and last particles (0 and  $L + 1$ ) are attached to fixed walls. The top chain shows the oscillators in equilibrium. The bottom chain shows the oscillators displaced from equilibrium.

As expected, the motion of particle  $j$  is coupled to its two nearest neighbors. The equations of motion (9.1) describe *longitudinal* oscillations, i.e., motion along the length of the system. It is straightforward to show that identical equations hold for the *transverse* oscillations of  $L$  identical mass points equally spaced on a stretched massless string (cf. French).

The equations of motion (9.1) are linear, that is, only terms proportional to the displacements appear. It is straightforward to obtain analytical solutions of (9.1). Although the analytical solution will help us interpret the numerical solutions in terms of normal modes, it is not necessary to understand the analytical solution in detail to understand the numerical solutions.

To find the normal modes, we look for solutions for which the displacement of each particle is proportional to  $\sin \omega t$  or  $\cos \omega t$ . We write

$$u_j(t) = u_j \cos \omega t, \tag{9.2}$$

where  $u_j$  is the amplitude of vibration of the  $j$ th particle. If we substitute the form (9.2) into (9.1), we obtain

$$-\omega^2 u_j = -\frac{K}{M} [2u_j - u_{j+1} - u_{j-1}]. \tag{9.3}$$

We next assume that  $u_j$  depends sinusoidally on the distance  $ja$ :

$$u_j = C \sin qja. \tag{9.4}$$

The magnitude of the constant  $C$  will be determined later. If we substitute the form (9.4) into (9.3), we find the following condition for  $\omega$ :

$$-\omega^2 \sin qja = -\frac{K}{M} [2 \sin qja - \sin q(j-1)a - \sin q(j+1)a]. \tag{9.5}$$

We write  $\sin q(j \pm 1)a = \sin qja \cos qa \pm \cos qja \sin qa$  and find that (??) is a solution if

$$\omega^2 = 2\frac{K}{M}(1 - \cos qa). \quad (9.6)$$

We need to find the values of the wavenumber  $q$  that satisfy the boundary conditions  $u_0 = 0$  and  $u_{L+1} = 0$ . The former condition is automatically satisfied by assuming a sine instead of a cosine solution in (??). The latter boundary condition implies that

$$q = q_n = \frac{\pi n}{a(L+1)} \quad n = 1, \dots, L \quad (\text{fixed boundary conditions}) \quad (9.7)$$

What are the corresponding possible values of the wavelength  $\lambda$ ? The latter is related to  $q$  by  $q = 2\pi/\lambda$ . The corresponding values of the angular frequencies are given by

$$\omega_n^2 = 2\frac{K}{M}[1 - \cos q_n a] = 4\frac{K}{M}\sin^2 \frac{q_n a}{2} \quad (9.8)$$

or

$$\omega_n = 2\sqrt{\frac{K}{M}}\sin \frac{q_n a}{2}. \quad (9.9)$$

The relation (??) between  $\omega_n$  and  $q_n$  is known as a dispersion relation.

A particular value of the integer  $n$  corresponds to the  $n$ th *normal mode*. We write the (time-independent) normal mode solutions as

$$u_{j,n} = C \sin q_n j a. \quad (9.10)$$

The linear nature of the equation of motion (9.1) implies that the time dependence of the displacement of the  $j$ th particle can be written as a superposition of normal modes:

$$u_j(t) = C \sum_{n=1}^L (A_n \cos \omega_n t + B_n \sin \omega_n t) \sin q_n j a \quad (9.11)$$

The coefficients  $A_n$  and  $B_n$  are determined by the initial conditions:

$$u_j(t=0) = C \sum_{n=1}^L A_n \sin q_n j a \quad (9.12a)$$

and

$$v_j(t=0) = C \sum_{n=1}^L \omega_n B_n \sin q_n j a. \quad (9.12b)$$

To solve (??) for  $A_n$  and  $B_n$ , we note that the normal mode solutions,  $u_{j,n}$ , are *orthogonal*, that is, they satisfy the condition

$$\sum_{j=1}^L u_{j,n} u_{j,m} \propto \delta_{n,m}. \quad (9.13)$$

The Kronecker  $\delta$  symbol  $\delta_{n,m} = 1$  if  $n = m$  and is zero otherwise. It is convenient to normalize the  $u_{j,n}$  so that they are *orthonormal*, i.e.,

$$\sum_{j=1}^L u_{j,n} u_{j,m} = \delta_{n,m}. \quad (9.14)$$

It is easy to show that the choice,  $C = 1/\sqrt{(L+1)/2}$ , in (??) and (??) insures that (??) is satisfied.

We now use the orthonormality condition to determine the coefficients  $A_n$  and  $B_n$ . If we multiply both sides of (??) by  $C \sin q_n j a$ , sum over  $j$ , and use the orthogonality condition (??), we obtain

$$A_n = C \sum_{j=1}^L u_j(0) \sin q_n j a \quad (9.15)$$

and

$$B_n = C \sum_{j=1}^L (v_j(0)/\omega_n) \sin q_n j a. \quad (9.16)$$

For example, if the initial displacement of every particle is zero, and the initial velocity of every particle is zero except for  $v_1(0) = 1$ , we find  $A_n = 0$  for all  $n$ , and

$$B_n = \frac{C}{\omega_n} \sin q_n a. \quad (9.17)$$

The corresponding solution for  $u_j(t)$  is

$$u_j(t) = \frac{2}{L+1} \sum_{n=1}^L \frac{1}{\omega_n} \cos \omega_n t \sin q_n a \sin q_n j a. \quad (9.18)$$

What is the solution if the particles start in a normal mode, i.e.,  $u_j(t=0) \propto \sin q_2 j a$ ?

The analytical solution (??) together with the initial conditions represent the complete solution of the displacement of the particles. If we wish, we can use a computer to compute the sum in (??) and plot the time dependence of the displacements  $u_j(t)$ . There are many interesting extensions that are amenable to analytical solutions. What is the effect of changing the boundary conditions? What happens if the spring constants are not all equal, but are chosen from a probability distribution? What happens if we vary the masses of the particles? For these cases we can follow a similar approach and look for the eigenvalues  $\omega_n$  and eigenvectors  $u_{j,n}$  of the matrix equation

$$\mathbf{T} \mathbf{u} = \omega^2 \mathbf{u}. \quad (9.19)$$

The matrix elements  $T_{i,j}$  are zero except for

$$T_{i,i} = \frac{1}{M_i} [K_{i,i+1} + K_{i,i-1}] \quad (9.20a)$$

$$T_{i,i+1} = -\frac{K_{i,i+1}}{M_i} \quad (9.20b)$$

and

$$T_{i,i-1} = -\frac{K_{i,i-1}}{M_i}, \quad (9.20c)$$

where  $K_{i,j}$  is the spring constant between particles  $i$  and  $j$ . The solution of matrix equations is a well studied problem in linear programming, and a commercial subroutine package such as IMSL or a symbolic programming language such as Maple, MatLab, or Mathematica can be used to obtain the solutions.

For our purposes it is easier to find the numerical solution of the equations of motion (9.1) directly because we also are interested in the effects of nonlinear forces between the particles, a case for which the matrix approach is inapplicable. In `Program oscillators` we use the Euler-Richardson algorithm to simulate the dynamics of  $L$  linearly coupled oscillators. The particle displacements are displayed as transverse oscillations using techniques similar to `Program animation` in Chapter 5. Note that we have used the `MAT` instruction to assign the array `usave` to `u` (see `SUB initial`). This instruction is equivalent to assigning every element of the array `usave` the corresponding value of the array `u`.

```

PROGRAM oscillators
! simulate coupled linear oscillators in one dimension
DIM u(0 to 21),v(0 to 21),usave(0 to 21)
CALL initial(L,u(),v(),t,dt,usave(),mass$,erase$)
DO
  CALL update(L,u(),v(),ke,t,dt,usave())
  CALL animate(L,u(),ke,t,usave(),mass$,erase$)
LOOP until key input
END

SUB initial(L,u(),v(),t,dt,usave(),mass$,erase$)
  DATA 0,0.5,0,0,0,0,0,0,0,0
  DATA 0,0,0,0,0,0,0,0,0,0
  LET t = 0
  LET dt = 0.025
  LET L = 10                ! number of particles
  SET WINDOW -1,L+1,-4,4
  SET COLOR "red"
  BOX AREA 0.9,1.1,-0.1,0.1
  BOX KEEP 0.9,1.1,-0.1,0.1 in mass$
  SET COLOR "background"
  BOX AREA -0.1,0.1,-0.1,0.1
  BOX KEEP -0.1,0.1,-0.1,0.1 in erase$
  PLOT line -2,0;L+2,0
  FOR j = 1 to L
    READ u(j)                ! initial displacements
    BOX SHOW mass$ at j-0.1,u(j)-0.1
  NEXT j
  FOR j = 1 to L
    READ v(j)                ! initial velocities

```

```

NEXT j
LET u(0) = 0                ! fixed wall boundary conditions
LET u(L+1) = 0
MAT usave = u              ! note use of matrix assignment instruction
END SUB

SUB update(L,u(),v(),ke,t,dt,usave())
! Euler-Richardson algorithm
DIM a(20),amid(20),umid(0 to 21),vmid(20)
LET ke = 0
! K/M equal to unity
FOR j = 1 to L
  LET usave(j) = u(j)
  LET a(j) = -2*u(j) + u(j+1) + u(j-1)
  LET umid(j) = u(j) + 0.5*v(j)*dt
  LET vmid(j) = v(j) + 0.5*a(j)*dt
NEXT j
LET umid(0) = 0
LET umid(L+1) = 0
FOR j = 1 to L
  LET amid(j) = -2*umid(j) + umid(j+1) + umid(j-1)
  LET u(j) = u(j) + vmid(j)*dt
  LET v(j) = v(j) + amid(j)*dt
  LET ke = ke + v(j)*v(j)
NEXT j
LET t = t + dt
END SUB

SUB animate(L,u(),ke,t,usave(),mass$,erase$)
LET pe = (u(1) - u(0))^2    ! interaction with left spring
FOR j = 1 to L
  ! compute potential energy
  LET pe = pe + (u(j+1) - u(j))^2
  ! transverse oscillation
  BOX SHOW erase$ at j-0.1,usave(j)-0.1
  BOX SHOW mass$ at j-0.1,u(j)-0.1
NEXT j
PLOT line -2,0;L+2,0
SET CURSOR 1,1
SET COLOR "black"
PRINT using "t = ###.##": t
LET E = 0.5*(ke + pe)
PRINT using "E = #.####": E
END SUB

```

*Problem 9.1.* Motion of coupled oscillators

1. Run **Program oscillators** for  $L = 2$  and choose the initial values of  $u(1)$  and  $u(2)$  so that the system is in one of its two normal modes, e.g.,  $u(1) = u(2) = 0.5$ . Set the initial velocities equal to zero. Note that the program sets the ratio  $K/M = 1$ . Describe the displacement of the particles. Is the motion of each particle periodic in time? To answer this question, add a subroutine that plots the displacement of each particle versus the time. Then consider the other normal mode, e.g.,  $u(1) = 0.5, u(2) = -0.5$ . What is the period in this case? Does the system remain in a normal mode indefinitely? Finally, choose the initial particle displacements equal to random values between  $-0.5$  and  $+0.5$ . Is the motion of each particle periodic in this case?
2. Consider the same questions as in part (a), but with  $L = 4$  and  $L = 10$ . Consider the  $n = 2$  mode for  $L = 4$  and the  $n = 3$  and  $n = 8$  modes for  $L = 10$ . (See (??) for the form of the normal mode solutions.) Also consider random initial displacements.
3. **Program oscillators** depicts the oscillations as transverse because they are easier to visualize. Modify the program to represent longitudinal oscillations instead. Define the density as the number of particles within a certain range of  $x$ . For example, set  $L = 20$  and describe how the average density varies as a function of the time within the region defined by  $8 < x < 12$ . Use the initial condition  $u_j = \sin(3j\pi/(L + 1))$  corresponding to the third normal mode. Repeat for another normal mode.
4. Write a program to verify that the normal mode solutions (??) are orthonormal. Then compare the analytical results and the numerical results for  $L = 10$  using the initial conditions listed in the **DATA** statements in **Program oscillators**. How much faster is it to calculate the analytical solution? What is the maximum deviation between the analytical and numerical solution of  $u_j(t)$ ? How well is the total energy conserved in **Program oscillators**? How does the maximum deviation and the conservation of the total energy change when the time step  $\Delta t$  is reduced?

*Problem 9.2.* Motion of coupled oscillators with external forces

1. Modify **Program oscillators** so that an external force  $F_e$  is exerted on the first particle,

$$F_e/m = 0.5 \cos \omega_e t, \quad (9.21)$$

where  $\omega_e$  is the angular frequency of the external force. (Note that  $\omega_e$  is an angular frequency, but as is common practice, we frequently refer to  $\omega_e$  as a frequency.) Let the initial displacements and velocities of all  $L$  particles be zero. Choose  $L = 3$  and then  $L = 10$  and consider the response of the system to an external force for  $\omega = 0.5$  to  $4.0$  in steps of  $0.5$ . Record  $A(\omega)$ , the maximum amplitude of any particle, for each value of  $\omega$ . Explain how this system can be used as a high frequency filter.

2. Choose  $\omega_e$  to be one of the normal mode frequencies. Does the maximum amplitude remain constant or does it increase with time? How can you use the response of the system to an external force to determine the normal mode frequencies? Discuss your results in terms of the power input,  $F_e v_1$ ?
3. In addition to the external force exerted on the first particle, add a damping force equal to  $-\gamma v_i$  to all the oscillators. Choose the damping constant  $\gamma = 0.05$ . How do you expect the

system to behave? How does the maximum amplitude depend on  $\omega_e$ ? Are the normal mode frequencies changed when  $\gamma \neq 0$ ?

*Problem 9.3.* Different boundary conditions

1. Modify Program `oscillators` so that periodic boundary conditions are used, i.e.,  $u(L+1) = u(1)$  and  $u(0) = u(L)$ . Choose  $L = 10$ , and the initial condition corresponding to the normal mode (??) with  $n = 2$ . Does this initial condition yield a normal mode solution for periodic boundary conditions? It might be easier to answer this question by plotting  $u(i)$  versus time for two or more particles. For fixed boundary conditions there are  $L + 1$  springs, but for periodic boundary conditions there are  $L$  springs. Why? Choose the initial condition corresponding to the  $n = 2$  normal mode, but replace  $L + 1$  by  $L$  in (??). Does this initial condition correspond to a normal mode? Now try  $n = 3$ , and other values of  $n$ . Which values of  $n$  give normal modes? Only sine functions can be normal modes for fixed boundary conditions (see (??)). Can there be normal modes with cosine functions if we use periodic boundary conditions?
2. Modify Program `oscillators` so that free boundary conditions are used, that is,  $u(L+1) = u(L)$  and  $u(0) = u(1)$ . Choose  $L = 10$ . Use the initial condition corresponding to the  $n = 3$  normal mode found using fixed boundary conditions. Does this condition correspond to a normal mode for free boundary conditions? Is  $n = 2$  a normal mode for free boundary conditions? Are the normal modes purely sinusoidal?
3. Choose free boundary conditions and  $L \geq 10$ . Let the initial condition be a pulse of the form,  $u(1) = 0.2, u(2) = 0.6, u(3) = 1.0, u(4) = 0.6, u(5) = 0.2$ , and all other  $u(j) = 0$ . After the pulse reaches the right end, what is the phase of the reflected pulse, i.e., are the displacements in the reflected pulse in the same direction as the incoming pulse (a phase shift of zero degrees) or in the opposite direction (a phase shift of 180 degrees)? What happens for fixed boundary conditions? Choose  $L$  to be as large as possible so that it is easy to distinguish the incident and reflected waves.
4. Set  $L = 20$  and let the spring constants on the right half of the system be four times greater than the spring constants on the left half. Use fixed boundary conditions. Set up a pulse on the left side. Is there a reflected pulse at the boundary between the two types of springs? If so, what is its relative phase? Compare the amplitude of the reflected and transmitted pulses. Consider the same questions with a pulse that is initially on the right side.

## 9.2 Fourier Transforms

In Section 9.1, we showed that the displacement of a single particle can be written as a linear combination of normal modes, that is, a linear superposition of sinusoidal terms. In general, an arbitrary periodic function  $f(t)$  of period  $T$  can be expressed as a Fourier series of sines and cosines:

$$f(t) = \frac{1}{2}a_0 + \sum_{k=1}^{\infty} (a_k \cos \omega_k t + b_k \sin \omega_k t), \quad (9.22)$$

where

$$\omega_k = k\omega_0 \quad \text{and} \quad \omega_0 = \frac{2\pi}{T}. \quad (9.23)$$

The quantity  $\omega_0$  is the fundamental frequency. The sine and cosine terms in (??) for  $k = 2, 3, \dots$  represent the second, third,  $\dots$ , and higher order harmonics. The *Fourier coefficients*  $a_k$  and  $b_k$  are given by

$$a_k = \frac{2}{T} \int_0^T f(t) \cos \omega_k t \, dt \quad (9.24a)$$

$$b_k = \frac{2}{T} \int_0^T f(t) \sin \omega_k t \, dt. \quad (9.24b)$$

The constant term  $\frac{1}{2}a_0$  in (??) is the average value of  $f(t)$ . The expressions (??) for the coefficients follow from the orthogonality conditions:

$$\frac{2}{T} \int_0^T \sin \omega_k t \sin \omega_{k'} t \, dt = \delta_{k,k'} \quad (9.25a)$$

$$\frac{2}{T} \int_0^T \cos \omega_k t \cos \omega_{k'} t \, dt = \delta_{k,k'}. \quad (9.25b)$$

$$\frac{2}{T} \int_0^T \sin \omega_k t \cos \omega_{k'} t \, dt = 0. \quad (9.25c)$$

In general, an infinite number of terms is needed to represent an arbitrary periodic function exactly. In practice, a good approximation usually can be obtained by including a relatively small number of terms. Unlike a power series, which can approximate a function only near a particular point, a Fourier series can approximate a function at all points. **Program synthesize**, listed in the following, plots the sum (??) for various values of  $N$ , the number of terms in the series. One purpose of the program is to help us visualize how well a finite sum of harmonic terms can represent an arbitrary periodic function.

```
PROGRAM synthesize
CALL plotf(0,0.5,0.5,1)
CALL plotf(0,0.5,0,0.5)
CALL plotf(0.5,1,0.5,1)
CALL plotf(0.5,1,0,0.5)
END

SUB plotf(xmin,xmax,ymin,ymax)
  OPEN #1: screen xmin,xmax,ymin,ymax
  SET WINDOW -4,4,-2,2
  PLOT LINES: -pi,0;pi,0
  PLOT LINES: 0,-1.5;0,1.5
  INPUT prompt "number of modes = ": N
  SET COLOR "red"
```

```

CALL fourier(N)
CLOSE #1
END SUB

SUB fourier(N)
! compute Fourier series and plot function
DIM a(0 to 1000),b(1000)
CALL coefficients(N,a(),b())
LET nplot = 100
LET t = -pi
LET dt = pi/100
DO while t <= pi
  LET f = a(0)/2
  FOR k = 1 to N
    IF a(k) <> 0 then LET f = f + a(k)*cos(k*t)
    IF b(k) <> 0 then LET f = f + b(k)*sin(k*t)
  NEXT k
  PLOT LINES: t,f;
  LET t = t + dt
LOOP
END SUB

SUB coefficients(N,a(),b())
! generate Fourier coefficients for special case
LET a(0) = 0
FOR k = 1 to N
  LET a(k) = 0
  IF mod(k,2) <> 0 then
    LET b(k) = 2/(k*pi)
  ELSE
    LET b(k) = 0
  END IF
NEXT k
END SUB

```

*Problem 9.4.* Fourier synthesis

1. The process of constructing a function by adding together a fundamental frequency and harmonics of various amplitudes is called *Fourier synthesis*. Use **Program synthesize** to visualize how a sum of harmonic functions can represent an arbitrary periodic function. Consider the series

$$f(t) = \frac{2}{\pi} \left( \sin t + \frac{1}{3} \sin 3t + \frac{1}{5} \sin 5t + \cdots \right). \quad (9.26)$$

Describe the nature of the plot when only the first three terms in (??) are retained. Increase the number of terms until you are satisfied that (??) represents the function sufficiently accurately. What function is represented by the infinite series?

2. Modify Program `synthesize` so that you can “zoom in” on the visual representation of  $f(t)$  for different intervals of  $t$ . Consider the series (??) with at least 32 terms. For what values of  $t$  does the finite sum most faithfully represent the exact function? For what values of  $t$  does it not? Why is it necessary to include a large number of terms to represent  $f(t)$  where it has sharp edges? The small oscillations that increase in amplitude as a sharp edge is approached are known as the Gibbs phenomenon.
3. Use Program `synthesize` to determine the function that is represented by the Fourier series with coefficients  $a_k = 0$  and  $b_k = (2/k\pi)(-1)^{k-1}$  for  $k = 1, 2, 3, \dots$ . Approximately how many terms in the series are required?

So far we have considered how a sum of sines and cosines can approximate a known periodic function. More typically, we measure a time series consisting of  $N$  data points,  $f(t_i)$ , where  $t_i = 0, \Delta, 2\Delta, \dots, (N-1)\Delta$ . We assume that the data repeats itself with a period  $T$  given by  $T = N\Delta$ . (The time interval  $\Delta$  between the measurements should not be confused with the finite time step  $\Delta t$  used in the numerical solution of a differential equation.) Our goal is to determine the Fourier coefficients  $a_k$  and  $b_k$  because, as we will see, these coefficients contain important physical information.

If we know only a finite number of terms in a time series, it is possible to find only a finite set of Fourier coefficients. For a given value of  $\Delta$ , what is the largest frequency component we can extract? In the following, we give a plausibility argument that suggests that the maximum frequency we can analyze is

$$\omega_c = \frac{\pi}{\Delta}. \quad (\text{Nyquist critical frequency}) \quad (9.27)$$

One way to understand this result is to imagine that  $f(t)$  is a sine wave. If  $f(t_i)$  has the same value for all  $t_i$ , the period is equal to either  $\Delta$  or  $\Delta/n$ , where  $n$  is an integer. The largest frequency component we can determine in this case is  $\omega = 2\pi n/\Delta$ , an arbitrarily large quantity. Hence, a constant data set does not impose any limitations on the maximum frequency. Now suppose that  $f(t_i)$  has one value for even  $i$  and another value for odd  $i$ . In this case we know that the period is  $2\Delta$ , and hence the maximum possible frequency of this function is  $\omega = 2\pi/(2\Delta) = \pi/\Delta$ . More variations in  $f(t_i)$  would correspond to lower frequencies, and hence we conclude that the highest frequency is  $\pi/\Delta$ .

One consequence of (??) is that there are  $\omega_c/\omega_0 + 1$  independent coefficients for  $a_k$  (including  $a_0$ ), and  $\omega_c/\omega_0$  independent coefficients for  $b_k$ , a total of  $N + 1$  independent coefficients. (Recall that  $\omega_c/\omega_0 = N/2$ , where  $\omega_0 = 2\pi/T$  and  $T = N\Delta$ .) However, because  $\sin \omega_c t = 0$  for all values of  $t$  that are multiples of  $\Delta$ , we have that  $b_{N/2} = 0$  from (??). Consequently, there are  $N/2 - 1$  values for  $b_k$ , and hence a total of  $N$  Fourier coefficients that can be computed. This conclusion is reasonable because the number of meaningful Fourier coefficients should be the same as the number of data points.

Program `analyze` computes the Fourier coefficients  $a_k$  and  $b_k$  of a function  $f(t)$  defined between  $t = 0$  and  $t = T$  at intervals of  $\Delta$ , and plots  $a_k$  and  $b_k$  versus  $k$ . To compute the coefficients we do the integrals in (??) numerically using the simple rectangular approximation (see Section ??):

$$a_k \approx \frac{2\Delta}{T} \sum_{i=0}^{N-1} f(t_i) \cos \omega_k t_i \quad (9.28a)$$

$$b_k \approx \frac{2\Delta}{T} \sum_{i=0}^{N-1} f(t_i) \sin \omega_k t_i, \quad (9.28b)$$

where the ratio  $2\Delta/T = 2/N$ .

```

PROGRAM analyze
! determine the Fourier coefficients a_k and b_k
CALL parameters(N,nmax,delta,period)
CALL screen(nmax,period,#1,#2)
CALL coefficients(N,nmax,delta,period,#1,#2)
END

SUB parameters(N,nmax,delta,period)
  INPUT prompt "number of data points N (even) = ": N
  INPUT prompt "sampling time dt = ": delta
  LET period = N*delta          ! assumed period
  ! maximum value of mode corresponding to Nyquist frequency
  LET nmax = N/2
END SUB

SUB screen(nmax,period,#1,#2)
  LET ymax = 2
  LET ticksize = ymax/50
  OPEN #1: screen 0,1,0.5,1
  PRINT "    a_k";
  PRINT "    ";
  PRINT using "frequency interval = #.#####": 2*pi/period
  SET WINDOW -1,nmax+1,-ymax,ymax
  CALL plotaxis(nmax,ticksize)
  SET COLOR "red"
  OPEN #2: screen 0,1,0,0.5
  PRINT "    b_k"
  SET WINDOW -1,nmax+1,-ymax,ymax
  CALL plotaxis(nmax,ticksize)
  SET COLOR "red"
END SUB

SUB plotaxis(nmax,ticksize)
  PLOT LINES: 0,0;nmax,0
  FOR k = 1 to nmax
    PLOT LINES: k,-ticksize;k,ticksize
  
```

```

    NEXT k
END SUB

SUB coefficients(N,nmax,delta,period,#1,#2)
  DECLARE DEF f
  FOR k = 0 to nmax
    LET ak = 0
    LET bk = 0
    LET wk = 2*pi*k/period
    ! rectangular approximation
    FOR i = 0 to N - 1
      LET t = i*delta
      LET ak = ak + f(t)*cos(wk*t)
      LET bk = bk + f(t)*sin(wk*t)
    NEXT i
    LET ak = 2*ak/N
    LET bk = 2*bk/N
    WINDOW #1
    PLOT LINES: k,0;k,ak
    WINDOW #2
    PLOT LINES: k,0;k,bk
  NEXT k
END SUB

FUNCTION f(t)
  LET w0 = 0.1*pi
  LET f = sin(w0*t)           ! simple example
END DEF

```

In Problem ?? we compute the Fourier coefficients for several known functions. We will see that if  $f(t)$  is a sum of sinusoidal functions with different periods, it is essential that the period  $T$  in Program `analyze` be an integer multiple of the periods of all the functions in the sum. If  $T$  does not satisfy this condition, then the results for some of the Fourier coefficients will be spurious. In practice, the solution to this problem is to vary the sampling rate and the total time over which the signal  $f(t)$  is sampled. Fortunately, the results for the power spectrum (see below) are less ambiguous than the values for the Fourier coefficients themselves.

*Problem 9.5.* Fourier analysis

1. Use Program `analyze` with  $f(t) = \sin \pi t/10$ . Determine the Fourier coefficients by doing the integrals in (??) analytically before running the program. Choose the number of data points to be  $N = 200$  and the sampling time  $\Delta = 0.1$ . Which Fourier components are nonzero? Repeat your analysis for  $N = 400, \Delta = 0.1$ ;  $N = 200, \Delta = 0.05$ ;  $N = 205, \Delta = 0.1$ ; and  $N = 500, \Delta = 0.1$ , and other combinations of  $N$  and  $\Delta$ . Explain your results by comparing the period of  $f(t)$  with  $N\Delta$ , the assumed period. If the combination of  $N$  and  $\Delta$  are not chosen properly, do you find any spurious results for the coefficients?

2. Consider the functions  $f_1(t) = \sin \pi t/10 + \sin \pi t/5$ ,  $f_2(t) = \sin \pi t/10 + \cos \pi t/5$ , and  $f_3(t) = \sin \pi t/10 + \frac{1}{2} \cos \pi t/5$ , and answer the same questions as in part (a). What combinations of  $N$  and  $\Delta$  give reasonable results for each function?
3. Consider a function that is not periodic, but falls to zero for large  $\pm t$ . For example, try  $f(t) = t^4 e^{-t^2}$  and  $f(t) = t^3 e^{-t^2}$ . Interpret the difference between the Fourier coefficients of these two functions.

Fourier analysis can be simplified by using exponential notation and combining the sine and cosine functions in one expression. We express  $f(t)$  as

$$f(t) = \sum_{k=-\infty}^{\infty} c_k e^{i\omega_k t}, \quad (9.29)$$

and use (??) to express the complex coefficients  $c_k$  in terms of  $a_k$  and  $b_k$ :

$$c_k = \frac{1}{2}(a_k - ib_k) \quad (9.30a)$$

$$c_0 = \frac{1}{2}a_0 \quad (9.30b)$$

$$c_{-k} = \frac{1}{2}(a_k + ib_k). \quad (9.30c)$$

The coefficients  $c_k$  can be expressed in terms of  $f(t)$  by using (??) and (??) and the fact that  $e^{\pm i\omega_k t} = \cos \omega_k t \pm i \sin \omega_k t$ . The result is

$$c_k = \frac{1}{T} \int_0^T f(t) e^{-i\omega_k t} dt. \quad (9.31)$$

As in (??), we can approximate the integral in (??) using the rectangular approximation. We write

$$g(\omega_k) \equiv c_k \frac{T}{\Delta} \approx \sum_{j=0}^{N-1} f(j\Delta) e^{-i\omega_k j\Delta} = \sum_{j=0}^{N-1} f(j\Delta) e^{-i2\pi k j/N}. \quad (9.32)$$

If we multiply (??) by  $e^{i2\pi k j'/N}$ , sum over  $k$ , and use the orthogonality condition

$$\sum_{k=0}^{N-1} e^{i2\pi k j/N} e^{-i2\pi k j'/N} = N \delta_{j,j'}, \quad (9.33)$$

we obtain the inverse Fourier transform

$$f(j\Delta) = \frac{1}{N} \sum_{k=0}^{N-1} g(\omega_k) e^{i2\pi k j/N} = \frac{1}{N} \sum_{k=0}^{N-1} g(\omega_k) e^{i\omega_k t_j}. \quad (9.34)$$

The frequencies  $\omega_k$  for  $k > N/2$  in the summations in (??) are greater than the Nyquist frequency  $\omega_c$ . However, from (??), we see that  $g(\omega_k) = g(\omega_k - \omega_N)$ . Hence, we can interpret all frequencies

for  $k > N/2$  as negative frequencies equal to  $(k - N)\omega_0$ . If  $f(t)$  is real, then  $g(-\omega_k) = g(\omega_k)$ . The occurrence of negative frequency components is a consequence of the use of the exponential functions rather than a sum of sines and cosines.

The importance of a particular frequency component within a signal is measured by the power  $P(\omega)$  associated with that frequency. To obtain this power, we use the discrete form of Parseval's theorem which can be written as

$$\sum_{j=0}^{N-1} |f(t_j)|^2 = \frac{1}{N} \sum_{k=0}^{N-1} |g(\omega_k)|^2. \quad (9.35)$$

In most measurements the function  $f(t)$  corresponds to an amplitude, and the power or intensity is proportional to the square of this amplitude or for complex functions, the modulus squared. Note that the left-hand sum in (9.35) (and hence the right-hand side) is proportional to  $N$ , and hence we need to divide both sides by  $N$  to obtain a quantity independent of  $N$ . The power in the frequency component  $\omega_k$  is proportional to

$$P(\omega_k) = \frac{1}{N^2} [|g(\omega_k)|^2 + |g(-\omega_k)|^2] = \frac{2}{N^2} |g(\omega_k)|^2. \quad (0 < \omega_k < \omega_c) \quad (9.36a)$$

The last equality follows if  $f(t)$  is real. Because the Fourier coefficients for  $\omega = \omega_c$  and  $\omega = -\omega_c$  are identical, we write for this case:

$$P(\omega_c) = \frac{1}{N^2} |g(\omega_c)|^2. \quad (9.36b)$$

Similarly, there is only one term with zero frequency, and hence  $P(0)$  is given by

$$P(0) = \frac{1}{N^2} |g(0)|^2. \quad (9.36c)$$

The *power spectrum*  $P(\omega)$  defined in (9.36) is proportional to the power associated with a particular frequency component embedded in the quantity of interest.

What happens to the power associated with frequencies greater than the Nyquist frequency? To answer this question, consider two choices of the Nyquist frequency,  $\omega_c^a$  and  $\omega_c^b > \omega_c^a$ , and the corresponding sampling times,  $\Delta^b < \Delta^a$ . The calculation with  $\Delta = \Delta^b$  represents the more accurate calculation because the sampling time is smaller. Suppose that this calculation of the spectrum yields the result that  $P(\omega > \omega_c^a) > 0$ . What happens if we compute the power spectrum using  $\Delta = \Delta^a$ ? The power associated with  $\omega > \omega_c^a$  must be “folded” back into the  $\omega < \omega_c^a$  frequency components. For example, the frequency component at  $\omega + \omega_c^a$  is added to the true value at  $\omega - \omega_c^a$  to produce an incorrect value at  $\omega - \omega_c^a$  in the computed power spectrum. This phenomenon is called *aliasing* and leads to spurious results. Aliasing occurs in calculations of  $P(\omega)$  if the latter does not vanish above the Nyquist frequency. To avoid aliasing, it is necessary to sample more frequently, or to remove the high frequency components from the signal before computing the Fourier transform.

The power spectrum can be computed by a simple modification of **Program analyze**. The procedure is order  $N^2$ , because there are  $N$  integrals for the  $N$  Fourier components, each of which is divided into  $N$  intervals. However, many of the calculations are redundant, and it is possible to organize the calculation so that the computational time is order  $N \log N$ . Such an algorithm is called a *fast Fourier transform* (FFT) and is discussed in **Appendix 9A**. It is a good idea to use the FFT for many of the following problems.

*Problem 9.6.* Examples of power spectra

1. Create a data set corresponding to  $f(t) = 0.3 \cos(2\pi t/T) + r$ , where  $r$  is a random number between 0 and 1. Plot  $f(t)$  versus  $t$  in intervals of  $\Delta = 4T/N$  for  $N = 128$  values. Can you visually detect any periodicity? Then compute the power spectrum using the same sampling interval  $\Delta = 4T/N$ . Does the behavior of the power spectrum indicate that there are any special frequencies?
2. Simulate a one-dimensional random walk, and compute  $x^2(t)$ , where  $x(t)$  is the distance from the origin of the walk after  $t$  steps. Compute the power spectrum for a walk of  $t = 256$ . In this case  $\Delta = 1$ , the time between steps. Do you observe any special frequencies? Remember to average over several samples.
3. Let  $f_n$  be the  $n$ th number of a random number sequence so that the time  $t = n$  with  $\Delta = 1$ . Compute the power spectrum of the random number generator. Do you detect any periodicities? If so, is the random number generator acceptable?

*Problem 9.7.* Power spectrum of coupled oscillators

1. Modify `Program oscillators` so that the power spectrum of one of the  $L$  particles is computed at the end of the simulation. Set  $\Delta = 0.1$  so that the Nyquist frequency is  $\omega_c = \pi/\Delta \approx 31.4$ . Choose the time of the simulation equal to  $T = 25.6$  and let  $K/M = 1$ . Plot the power spectrum  $P(\omega)$  at frequency intervals equal to  $\Delta\omega = \omega_0 = 2\pi/T$ . First choose  $L = 2$  and choose the initial conditions so that the system is in a normal mode. What do you expect the power spectrum to look like? What do you find? Then choose  $L = 10$  and choose initial conditions corresponding to various normal modes.
2. Repeat part (a) for  $L = 2$  and  $L = 10$  with the initial particle displacements equal to random values between  $-0.5$  and  $0.5$ . Can you detect all the normal modes in the power spectrum? Repeat for a different set of random initial displacements.
3. Repeat part (a) for initial displacements corresponding to the sum of two normal modes.
4. Recompute the power spectrum for  $L = 10$  with  $T = 6.4$ . Is this time long enough? How can you tell?

*\*Problem 9.8.* Quasiperiodic power spectra

1. Write a program to compute the power spectrum of the circle map (6.56). Begin by exploring the power spectrum for  $K = 0$ . Plot  $\ln P(\omega)$  versus  $\omega$ , where  $P(\omega)$  is proportional to the modulus squared of the Fourier transform of  $x_n$ . Begin with  $N = 256$  iterations. How does the power spectra differ for rational and irrational values of the parameter  $\Omega$ ? How are the locations of the peaks in the power spectra related to the value of  $\Omega$ ?
2. Set  $K = 1/2$  and compute the power spectra for  $0 < \Omega < 1$ . Does the power spectra differ from the spectra found in part (a)?
3. Set  $K = 1$  and compute the power spectra for  $0 < \Omega < 1$ . How does the power spectra compare to those found in parts (a) and (b)?

In Problem ?? we found that the peaks in the power spectrum yield information about the normal mode frequencies. In Problem ?? and ?? we compute the power spectra for a system of coupled oscillators where disorder is present. Disorder can be generated by having random masses and/or random spring constants. We will see that one effect of disorder is that the normal modes are no longer simple sinusoidal functions. Instead, some of the modes are localized, meaning that only some of the particles move significantly while the others remain essentially at rest. This effect is known as *Anderson localization*. Typically, we find that modes above a certain frequency are *localized*, and those below this threshold frequency are *extended*. This threshold frequency is well defined for large systems. In one dimension with a finite disorder (e.g., a finite density of defects) all states are localized in the limit of an infinite chain.

*Problem 9.9.* Localization with a single defect

1. Modify Program `oscillators` so that the mass of one oscillator is equal to one fourth that of the others. Set  $L = 20$  and use fixed boundary conditions. Compute the power spectrum over a time  $T = 51.2$  using random initial displacements between  $-0.5$  and  $0.5$  and zero initial velocities. Sample the data at intervals of  $\Delta = 0.1$ . The normal mode frequencies correspond to the well defined peaks in  $P(\omega)$ . Consider at least three different sets of random initial displacements to insure that you find all the normal mode frequencies.
2. Apply an external force  $F_e = 0.3 \sin \omega_e t$  to each particle. (The steady state behavior occurs sooner if we apply an external force to each particle instead of just one particle.) Because the external force pumps energy into the system, it is necessary to add a damping force to prevent the oscillator displacements from becoming too large. Add a damping force equal to  $-\gamma v_i$  to all the oscillators with  $\gamma = 0.1$ . Choose random initial displacements and zero initial velocities and use the frequencies found in part (a) as the driving frequencies  $\omega_e$ . Describe the motion of the particles. Is the system driven to a normal mode? Take a “snapshot” of the particle displacements after the system has run for a sufficiently long time so that the patterns repeat themselves. Are the particle displacements simple sinusoidal functions of position? Sketch the approximate normal mode patterns for each normal mode frequency. Which of the modes appear localized and which modes appear to be extended? What is the approximate cutoff frequency that separates the localized from the extended modes?

*Problem 9.10.* Localization in a disordered chain of oscillators

1. Modify Program `oscillators` so that the spring constants can be varied by the user. Set  $L = 10$  and use fixed wall boundary conditions. Consider the following set of 11 spring constants:

DATA 0.704,0.388,0.707,0.525,0.754,0.721

DATA 0.006,0.479,0.470,0.574,0.904

To help you determine all the normal modes, we provide two of the normal mode frequencies:  $\omega \approx 0.28$  and  $1.15$ . Find the power spectrum using the procedure outlined in Problem ??a.

2. Apply an external force  $F_e = 0.3 \sin \omega_e t$  to each particle, and find the normal modes as outlined in Problem ??b.

3. Repeat parts (a) and (b) for another set of random spring constants. If you have sufficient computer resources, consider  $L = 40$ . Discuss the nature of the localized modes in terms of the specific values of the spring constants. For example, is the edge of a localized mode at a spring that has a relatively large or small spring constant?
4. Repeat parts (a) and (b) for uniform spring constants, but random masses between 0.5 and 1.5. Is there a qualitative difference between the two types of disorder?

In 1955 Fermi, Pasta, and Ulam used the Maniac I computer at Los Alamos to study a chain of oscillators. Their surprising discovery might have been the first time a qualitatively new result, instead of a more precise number, was found from a computer simulation. To understand their results (known as the FPU problem), we need to discuss an idea from statistical mechanics that was mentioned briefly in Project 8.19. Some of the ideas of statistical mechanics are introduced in greater depth in later chapters.

A fundamental assumption of statistical mechanics is that an isolated system of particles is ergodic, that is, the system will evolve through all configurations consistent with the conservation of energy. Clearly, a set of linearly coupled oscillators is not ergodic, because if the system is initially in a normal mode, it stays in that normal mode forever. Before 1955 it was believed that if the interaction between the particles is slightly nonlinear (and the number of particles is sufficiently large), the system would be ergodic and evolve through the different normal modes of the linear system. In Problem ?? we will find, as did Fermi, Pasta, and Ulam, that the behavior of the system is much more complicated.

*Problem 9.11.* Nonlinear oscillators

1. Modify `Program oscillators` so that cubic forces between the particles are added to the linear spring forces, i.e., let the force on particle  $i$  due to particle  $j$  be

$$F_{ij} = -(u_i - u_j) - \alpha(u_i - u_j)^3, \quad (9.37)$$

where  $\alpha$  is the amplitude of the nonlinear term. Choose the masses of the particles to be unity. Consider  $L = 10$  and choose initial displacements corresponding to a normal mode of the linear ( $\alpha = 0$ ) system. Compute the power spectrum over a time interval of 51.2 with  $\Delta = 0.1$  for  $\alpha = 0, 0.1, 0.2$ , and  $0.3$ . For what value of  $\alpha$  does the system become ergodic, i.e., the heights of all the normal mode peaks are approximately the same?

2. Repeat part (a) for the case where the displacements of the particles are initially random. Make sure the same set of random displacements are used for each value of  $\alpha$ .
3. We now know that the number of oscillators is not as important as the magnitude of the nonlinear interaction. Repeat parts (a) and (b) for  $L = 20$  and  $40$  and discuss the effect of increasing the number of particles.

*\*Problem 9.12.* Spatial Fourier transforms

1. So far we have considered Fourier transforms in time and frequency. Spatial Fourier transforms are of interest in many contexts. The main difference is that spatial transforms usually

involve positive and negative values of  $x$ , whereas we have considered only nonnegative values of  $t$ . Modify `Program analyze` so that it computes the real and imaginary parts of the Fourier transform  $\phi(k)$  of a complex function  $\psi(x)$ , where both  $x$  and  $k$  can have negative values. That is, instead of doing the integral (??) from 0 to  $T$ , integrate from  $-L/2$  to  $L/2$ , where  $\psi(x+L) = \psi(x)$ .

2. Compute the Fourier transform of the Gaussian function  $\psi(x) = Ae^{-bx^2}$ . Plot  $\psi(x)$  and  $\phi(k)$  for at least three values of  $b$ . Does  $\phi(k)$  appear to be a Gaussian? Choose a reasonable criterion for the half-width of  $\psi(x)$  and measure its value. Use the same criterion to measure the half-width of  $\phi(k)$ . How do these widths depend on  $b$ ? How does the width of  $\phi(k)$  change as the width of  $\psi(x)$  increases?
3. Repeat part (b) with the function  $\psi(x) = Ae^{-bx^2} e^{ik_0x}$  for various values of  $k_0$ .

### 9.3 Wave Motion

Our simulations of coupled oscillators have shown that the microscopic motion of the individual oscillators leads to macroscopic wave phenomena. To understand the transition between microscopic and macroscopic phenomena, we reconsider the oscillations of a linear chain of  $L$  particles with equal spring constants  $K$  and equal masses  $M$ . As we found in Section 9.1, the equations of motion of the particles can be written as (see (9.1))

$$\frac{d^2 u_j(t)}{dt^2} = -\frac{K}{M} [2u_j(t) - u_{j+1}(t) - u_{j-1}(t)]. \quad (i = 1, \dots, L). \quad (9.38)$$

We consider the limits  $L \rightarrow \infty$  and  $a \rightarrow 0$  with the length of the chain  $La$  fixed. We will find that the discrete equations of motion (??) can be replaced by the continuous *wave equation*

$$\frac{\partial^2 u(x, t)}{\partial t^2} = c^2 \frac{\partial^2 u(x, t)}{\partial x^2}, \quad (9.39)$$

where  $c$  has the dimension of velocity.

We can obtain the wave equation (??) as follows. First we replace  $u_j(t)$ , where  $j$  is a discrete variable, by the function  $u(x, t)$ , where  $x$  is a *continuous* variable, and rewrite (??) in the form

$$\frac{\partial^2 u(x, t)}{\partial t^2} = \frac{Ka^2}{M} \frac{1}{a^2} [u(x+a, t) - 2u(x, t) + u(x-a, t)]. \quad (9.40)$$

We have written the time derivative as a partial derivative because the function  $u$  depends on two variables. If we use the Taylor series expansion

$$u(x \pm a) = u(x) \pm a \frac{\partial u}{\partial x} + \frac{a^2}{2} \frac{\partial^2 u}{\partial x^2} + \dots, \quad (9.41)$$

it is easy to show that as  $a \rightarrow 0$ , the quantity

$$\frac{1}{a^2} [u(x+a, t) - 2u(x, t) + u(x-a, t)] \rightarrow \frac{\partial^2 u(x, t)}{\partial x^2}. \quad (9.42)$$

The wave equation (??) is obtained by substituting (??) into (??) with  $c^2 = Ka^2/M$ . If we introduce the linear mass density  $\mu = M/a$  and the tension  $T = Ka$ , we can express  $c$  in terms of  $\mu$  and  $T$  and obtain the familiar result  $c^2 = T/\mu$ .

It is straightforward to show that any function of the form  $f(x \pm ct)$  is a solution to (??). Among these many solutions to the wave equation are the familiar forms:

$$u(x, t) = A \cos \frac{2\pi}{\lambda}(x \pm ct) \quad (9.43a)$$

$$u(x, t) = A \sin \frac{2\pi}{\lambda}(x \pm ct). \quad (9.43b)$$

Because the wave equation is linear, and hence satisfies a superposition principle, we can understand the behavior of a wave of arbitrary shape by representing its shape as a sum of sinusoidal waves.

One way to solve the wave equation numerically is to retrace our steps back to the discrete equations (??) to find a discrete form of the wave equation that is convenient for numerical calculations. This procedure of converting a continuum equation to a physically motivated discrete form frequently leads to useful numerical algorithms. From (??) we see how to approximate the second derivative by a finite difference. If we replace  $a$  by  $\Delta x$  and take  $\Delta t$  to be the time step, we can rewrite (??) by

$$\begin{aligned} \frac{1}{(\Delta t)^2} [u(x, t + \Delta t) - 2u(x, t) + u(x, t - \Delta t)] = \\ \frac{c^2}{(\Delta x)^2} [u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)]. \end{aligned} \quad (9.44)$$

The quantity  $\Delta x$  is the spatial interval. The result of solving (??) for  $u(x, t + \Delta t)$  is

$$\begin{aligned} u(x, t + \Delta t) = & 2[1 - b]u(x, t) \\ & + b[u(x + \Delta x, t) + u(x - \Delta x, t)] - u(x, t - \Delta t), \end{aligned} \quad (9.45)$$

where  $b \equiv (c\Delta t/\Delta x)^2$ . Equation (??) expresses the displacements at time  $t + \Delta t$  in terms of the displacements at the current time  $t$  and at the previous time  $t - \Delta t$ .

*Problem 9.13.* Solution of the discrete wave equation

1. Write a program to compute the numerical solutions of the discrete wave equation (??). Three spatial arrays corresponding to  $u(x)$  at times  $t + \Delta t$ ,  $t$ , and  $t - \Delta t$  are needed, where  $\Delta t$  is the time step. We denote the displacement  $u(j\Delta x)$  by the array element  $u(j)$ , where  $\Delta x$  is the size of the spatial grid. Use periodic boundary conditions so that  $u(0) = u(L)$  and  $u(L+1) = u(1)$ , where  $L$  is the total number of spatial intervals. Draw lines between the displacements at neighboring values of  $x$ . Note that the initial conditions require the specification of the array  $u$  at  $t = 0$  and at  $t = -\Delta t$ . Let the waveform at  $t = 0$  and  $t = -\Delta t$  be  $u(x, t = 0) = \exp(-(x - 10)^2)$  and  $u(x, t = -\Delta t) = \exp(-(x - 10 + c\Delta t)^2)$ , respectively. What is the direction of motion implied by these initial conditions?
2. Our first task is to determine the optimum value of the parameter  $b$ . Let  $\Delta x = 1$  and  $L \geq 100$ , and try the following combinations of  $c$  and  $\Delta t$ :  $c = 1, \Delta t = 0.1$ ;  $c = 1, \Delta t = 0.5$ ;  $c = 1, \Delta t = 1$ ;  $c = 1, \Delta t = 1.5$ ;  $c = 2, \Delta t = 0.5$ ; and  $c = 2, \Delta t = 1$ . Verify that the value  $b = (c\Delta t)^2 = 1$  leads to the best results, that is, for this value of  $b$ , the initial form of the wave is preserved.

3. It is possible to show that the discrete form of the wave equation with  $b = 1$  is exact up to numerical roundoff error (cf. DeVries). Hence, we can replace (??) by the simpler algorithm

$$u(x, t + \Delta t) = u(x + \Delta x, t) + u(x - \Delta x, t) - u(x, t - \Delta t). \quad (9.46)$$

That is, the solutions of (??) are equivalent to the solutions of the original partial differential equation (??). Try several different initial waveforms, and show that if the displacements have the form  $f(x \pm ct)$ , then the waveform maintains its shape with time. For the remaining problems we use (??) corresponding to  $b = 1$ . Unless otherwise specified, choose  $c = 1$ ,  $\Delta x = \Delta t = 1$ , and  $L \geq 100$  in the following problems.

*Problem 9.14. Velocity of waves*

1. Use the waveform given in Problem ??a and measure the speed of the wave by determining the distance traveled on the screen in a given amount of time. Add tick marks to the  $x$  axis. Because we have set  $\Delta x = \Delta t = 1$  and  $b = 1$ , the speed  $c = 1$ . (A way of incorporating different values of  $c$  is discussed in Problem ??d.)
2. Replace the waveform considered in part (a) by a sinusoidal wave that fits exactly, i.e., choose  $u(x, t) = \sin(qx - \omega t)$  such that  $\sin q(L + 1) = 0$ . Measure the period  $T$  of the wave by measuring the time it takes for successive maxima to pass a given point. What is the wavelength  $\lambda$  of your wave? Does it depend on the value of  $q$ ? The frequency of the wave is given by  $f = 1/T$ . Verify that  $\lambda f = c$ .

*Problem 9.15. Reflection of waves*

1. Consider a wave of the form  $u(x, t) = e^{-(x-10-ct)^2}$ . Use fixed boundary conditions so that  $u(0) = u(L+1) = 0$ . What happens to the reflected wave?
2. Modify your program so that free boundary conditions are incorporated:  $u(0) = u(1)$  and  $u(L+1) = u(L)$ . Compare the phase of the reflected wave to your result from part (a).
3. Modify your program so that a “sluggish” boundary condition, e.g.,  $u(0) = \frac{1}{2}u(1)$  and  $u(L+1) = \frac{1}{2}u(L)$ , is used. What do you expect the reflected wave to look like? What do you find from your numerical solution?
4. What happens to a pulse at the boundary between two media? Set  $c = 1$  and  $\Delta t = 1$  on the left side of your grid and  $c = 2$  and  $\Delta t = 0.5$  on the right side. These choices of  $c$  and  $\Delta t$  imply that  $b = 1$  on both sides, but that the right side is updated twice as often as the left side. What happens to a pulse that begins on the left side and moves to the right? Is there both a reflected and transmitted wave at the boundary between the two media? What is their relative phase? Find a relation between the amplitude of the incident pulse and the amplitudes of the reflected and transmitted pulses. Repeat for a pulse starting from the right side.

*Problem 9.16. Superposition of waves*

1. Consider the propagation of the wave determined by  $u(x, t = 0) = \sin(4\pi x/L)$ . What must  $u(x, -\Delta t)$  be such that the wave moves in the positive  $x$  direction? Test your answer by doing the simulation. Use periodic boundary conditions. Repeat for a wave moving in the negative  $x$  direction.

2. Simulate two waves moving in opposite directions each with the same spatial dependence given by  $u(x, 0) = \sin 4\pi x/L$ . Describe the resultant wave pattern. Repeat the simulation for  $u(x, 0) = \sin 8\pi x/L$ .
3. Assume that  $u(x, 0) = \sin q_1 x + \sin q_2 x$ , with  $\omega_1 = cq_1 = 10\pi/L$ ,  $\omega_2 = cq_2 = 12\pi/L$ , and  $c = 1$ . Describe the qualitative form of  $u(x, t)$  for fixed  $t$ . What is the distance between modulations of the amplitude? Estimate the wavelength associated with the fine ripples of the amplitude. Estimate the wavelength of the *envelope* of the wave. Find a simple relationship for these two wavelengths in terms of the wavelengths of the two sinusoidal terms. This phenomena is known as *beats*.
4. Consider the motion of the wave described by  $u(x, 0) = e^{-(x-10)^2} + e^{-(x-90)^2}$ ; the two Gaussian pulses move in opposite directions. What happens to the two pulses as they travel through each other? Do they maintain their shape? While they are going through each other, is the displacement  $u(x, t)$  given by the sum of the displacements of the individual pulses?

*Problem 9.17. Standing waves*

1. In Problem ??c we considered a *standing wave*, the continuum analog of a normal mode of a system of coupled oscillators. As is the case for normal modes, each point of the wave has the same time dependence. For fixed boundary conditions, the displacement is given by  $u(x, t) = \sin qx \cos \omega t$ , where  $\omega = cq$  and  $q$  is chosen so that  $\sin qL = 0$ . Choose an initial condition corresponding to a standing wave for  $L = 100$ . Describe the motion of the particles, and compare it with your observations of standing waves on a rope.
2. Establish a standing wave by displacing one end of a system periodically. The other end is fixed. Let  $u(x, 0) = u(x, -\Delta t) = 0$ , and  $u(x = 0, t) = A \sin \omega t$  with  $A = 0.1$ .

We have seen that the wave equation can support pulses that propagate indefinitely without distortion. In addition, because the wave equation is linear, the sum of any two solutions also is a solution, and the principle of superposition is satisfied. As a consequence, we know that two pulses can pass through each other unchanged. We also have seen that similar phenomena exist in the discrete system of linearly coupled oscillators. What happens if we create a pulse in a system of nonlinear oscillators? As an introduction to nonlinear wave phenomena, we consider a system of  $L$  coupled oscillators with the potential energy of interaction given by

$$V = \frac{1}{2} \sum_{j=1}^L (e^{-(u_j - u_{j-1})} - 1)^2. \quad (9.47)$$

This form of the interaction is known as the Morse potential. All parameters in the potential (such as the overall strength of the potential) have been set to unity. The force on the  $j$ th particle is

$$F_j = -\frac{\partial V}{\partial u_j} = Q_j(1 - Q_j) - Q_{j+1}(1 - Q_{j+1}), \quad (9.48a)$$

where

$$Q_j \equiv e^{-(u_j - u_{j-1})}. \quad (9.48b)$$

In linear systems it is possible to set up a pulse of any shape and maintain the shape of the pulse indefinitely. In a nonlinear system there also exist solutions that maintain their shape, but we will find in Problem ?? that not all pulse shapes do so. The pulses that maintain their shape are called *solitons*.

*Problem 9.18. Solitons*

1. Modify **Program oscillators** so that the force on particle  $j$  is given by (??). Use periodic boundary conditions. Choose  $L \geq 60$  and an initial Gaussian pulse of the form  $u(x, t) = 0.5 e^{-(x-10)^2}$ . You should find that the initial pulse splits into two pulses plus some noise. Describe the motion of the pulses (solitons). Do they maintain their shape, or is this shape modified as they move? Describe the motion of the particles far from the pulse. Are they stationary?
2. Save the displacements of the particles when the peak of one of the solitons is located near the center of your screen. Is it possible to fit the shape of the soliton to a Gaussian? Continue the simulation, and after one of the solitons is relatively isolated, set  $u(j) = 0$  for all  $j$  far from this soliton. Does the soliton maintain its shape?
3. Repeat part (b) with a pulse given by  $u(x, 0) = 0$  everywhere except for  $u(20, 0) = u(21, 0) = 1$ . Do the resulting solitons have the same shape as in part (b)?
4. Begin with the same Gaussian pulse as in part (a), and run until the two solitons are well separated. Then change at random the values of  $u(j)$  for particles in the larger soliton by about 5%, and continue the simulation. Is the soliton destroyed? Increase this perturbation until the soliton is no longer discernible.
5. Begin with a single Gaussian pulse as in part (a). The two resultant solitons will eventually "collide." Do the solitons maintain their shape after the collision? The principle of superposition implies that the displacement of the particles is given by the sum of the displacements due to each pulse. Does the principle of superposition hold for solitons?
6. Compute the speeds, amplitudes, and width of the solitons produced from a single Gaussian pulse. Take the amplitude of a soliton to be the largest value of its displacement and the half-width to correspond to the value of  $x$  at which the displacement is half its maximum value. Repeat these calculations for solitons of different amplitudes by choosing the initial amplitude of the Gaussian pulse to be 0.1, 0.3, 0.5, 0.7, and 0.9. Plot the soliton speed and width versus the corresponding soliton amplitude.
7. Change the boundary conditions to free boundary conditions and describe the behavior of the soliton as it reaches a boundary. Compare this behavior with that of a pulse in a system of linear oscillators.
8. Begin with an initial sinusoidal disturbance that would be a normal mode for a linear system. Does the sinusoidal mode maintain its shape? Compare the behavior of the nonlinear and linear systems.

## 9.4 Interference and Diffraction

Interference is one of the most fundamental characteristics of all wave phenomena. The term *interference* is used when relatively few sources of waves separately derived from the same source are brought together. The term *diffraction* has a similar meaning and is commonly used if there are many sources. Because it is relatively easy to observe interference and diffraction phenomena with light, we discuss these phenomena in this context.

The classic example of interference is Young's double slit experiment (see Figure ??). Imagine two narrow parallel slits separated by a distance  $a$  and illuminated by a light source that emits light of only one frequency (monochromatic light). If the light source is placed on the line bisecting the two slits and the slit opening is very narrow, the two slits become coherent light sources with equal phases. We first assume that the slits act as point sources, e.g., pinholes. A screen that displays the intensity of the light from the two sources is placed a distance  $L$  away. What do we see on the screen?

The electric field at position  $\mathbf{r}$  associated with the light emitted from a monochromatic point source at  $\mathbf{r}_1$  has the form

$$E(\mathbf{r}, t) = \frac{A}{|\mathbf{r} - \mathbf{r}_1|} \cos(q|\mathbf{r} - \mathbf{r}_1| - \omega t), \quad (9.49)$$

where  $|\mathbf{r} - \mathbf{r}_1|$  is the distance between the source and the point of observation. The superposition principle implies that the total electric field at  $\mathbf{r}$  from  $N$  point sources at  $\mathbf{r}_i$  is

$$E(\mathbf{r}, t) = \sum_{i=1}^N \frac{A}{|\mathbf{r} - \mathbf{r}_i|} \cos(q|\mathbf{r} - \mathbf{r}_i| - \omega t). \quad (9.50)$$

Equation ?? assumes that the amplitude of each source is the same. The observed intensity is proportional to the time-averaged value of  $|E|^2$ .

In Problem ?? we discuss writing a program to determine the intensity of light that is observed on a screen due to an arrangement of point sources. The wavelength of the light sources, the positions of the sources  $\mathbf{r}_i$ , and the observation points on the screen need to be specified. The program sums the fields due to all the sources for a given observation point, and computes  $|E|^2$ . The part of the program that is not straightforward is the calculation of the time average of  $|E|^2$ . One way of obtaining the time average is to compute the integral

$$\overline{E^2} = \frac{1}{T} \int_0^T |E|^2 dt, \quad (9.51)$$

where  $T = 1/f$  is the period, and  $f$  is the frequency of the light sources. We now show that such a calculation is not necessary if the sources are much closer to each other than they are to the screen. In this case (the *far field condition*), we can ignore the slow  $r$  dependence of  $|\mathbf{r} - \mathbf{r}_i|^{-1}$  and write the field in the form

$$E(\mathbf{r}) = E_0 \cos(\phi - \omega t). \quad (9.52)$$

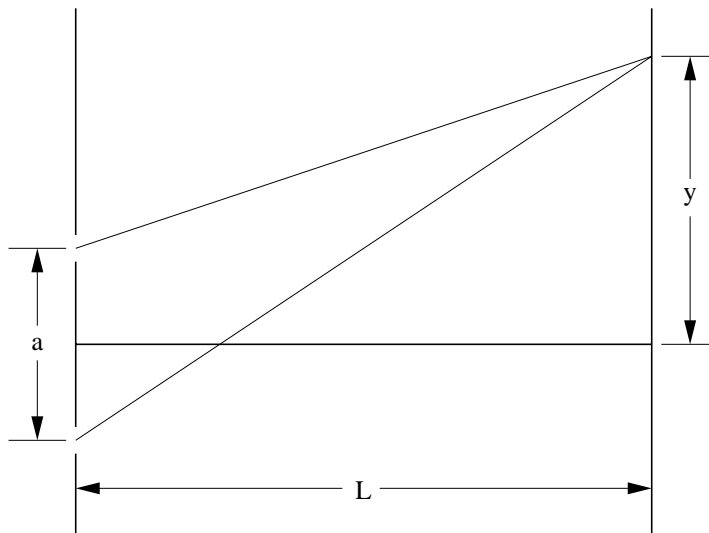


Figure 9.2: Young's double slit experiment. The figure defines the quantities  $a$ ,  $L$ , and  $y$  that are used in Problem ??.

We have absorbed the factors of  $|\mathbf{r} - \mathbf{r}_i|^{-1}$  into  $E_0$ . The phase  $\phi$  is a function of the source positions and  $\mathbf{r}$ . The form of (??) allows us to write

$$\frac{1}{T} \int_0^T \cos^2(\phi - \omega t) dt = \frac{1}{M} \sum_{m=1}^M \cos^2(\phi - \frac{2\pi m}{M}) = \frac{1}{2}. \quad (M > 2) \quad (9.53)$$

The result (??) is independent of  $\phi$  and allows us to perform the time average by using the summation in (??) with  $M = 3$ .

In the following problems we discuss a variety of geometries. The main part of your program that must be changed is the specification of the source positions.

*Problem 9.19.* Double slit interference

1. Verify (??) by finding an analytical expression for  $E$  from two and three point sources. Explain why the form (??) is valid for an arbitrary number of sources. Then write a program to verify the result (??) for  $M = 3, 4, 5$ , and  $10$ . What is the value of the sum in (??) for  $M = 2$ ?
2. Write a program to plot the intensity of light on a screen due to two slits. Calculate  $E$  using (??) and do the time average using the relation (??). Let  $a$  be the distance between the slits and  $y$  be the vertical position along the screen as measured from the central maximum. Set  $L = 200$  mm,  $a = 0.1$  mm, the wavelength of light  $\lambda = 5000 \text{ \AA}$  ( $1 \text{ \AA} = 10^{-7}$  mm), and consider  $-5.0 \text{ mm} \leq y \leq 5.0 \text{ mm}$  (see Figure ??). Describe the interference pattern you observe with  $M = 3$ . Identify the locations of the intensity maxima, and plot the intensity of the maxima as a function of  $y$ .

- Repeat part (b) for  $L = 0.5 \text{ mm}$  and  $1.0 \text{ mm} \leq y \leq 1.0 \text{ mm}$ . Do your results change as you vary  $M$  from 3 to 5? Note that in this case  $L$  is not much greater than  $a$ , and hence we cannot ignore the  $r$  dependence of  $|\mathbf{r} - \mathbf{r}_i|^{-1}$  in (??). How large must  $M$  be so that your results are approximately independent of  $M$ ?

*Problem 9.20.* Diffraction grating

High resolution optical spectroscopy is done with multiple slits. In its simplest form, a diffraction grating consists of  $N$  parallel slits made, for example, by ruling with a diamond stylus on aluminum plated glass. Compute the intensity of light for  $N = 3, 4, 5$ , and 10 slits with  $\lambda = 5000 \text{ \AA}$ , slit separation  $a = 0.01 \text{ mm}$ , screen distance  $L = 200 \text{ mm}$ , and  $-15 \text{ mm} \leq y \leq 15 \text{ mm}$ . How does the intensity of the peaks and their separation vary with  $N$ ?

In our analysis of the double slit and the diffraction grating, we assumed that each slit was a pinhole that emits spherical waves. In practice, real slits are much wider than the wavelength of visible light. In Problem ?? we consider the pattern of light produced when a plane wave is incident on an aperture such as a single slit. To do so, we use Huygens' principle and replace the slit by many coherent sources of spherical waves. This equivalence is not exact, but is applicable when the aperture width is large compared to the wavelength.

*Problem 9.21.* Single slit diffraction

- Compute the time averaged intensity of light diffracted from a single slit of width  $0.02 \text{ mm}$  by replacing the slit by  $N = 20$  point sources spaced  $0.001 \text{ mm}$  apart. Choose  $\lambda = 5000 \text{ \AA}$ ,  $L = 200 \text{ mm}$ , and consider  $-30 \text{ mm} \leq y \leq 30 \text{ mm}$ . What is the width of the central peak? How does the width of the central peak compare to the width of the slit? Do your results change if  $N$  is increased?
- Determine the position of the first minimum of the diffraction pattern as a function of wavelength, slit width, and distance to the screen.
- Compute the intensity pattern for  $L = 1 \text{ mm}$  and  $50 \text{ mm}$ . Is the far field condition satisfied in this case? How do the patterns differ?

*Problem 9.22.* A more realistic double slit simulation

Reconsider the intensity distribution for double slit interference using slits of finite width. Modify your program to simulate two "thick" slits by replacing each slit by 20 point sources spaced  $0.001 \text{ mm}$  apart. The centers of the thick slits are  $a = 0.1 \text{ mm}$  apart. How does the intensity pattern change?

\**Problem 9.23.* Diffraction pattern due to a rectangular aperture

We can use a similar approach to determine the diffraction pattern due to an aperture of finite width and height. The simplest approach is to divide the aperture into little squares and to consider each square as a source of spherical waves. Similarly we can divide the screen or photographic plate into small regions or cells and calculate the time averaged intensity at the center of each cell. The calculations are straightforward, but time consuming, because of the necessity of evaluating the cosine function many times. The less straightforward part of the problem is deciding how to plot the different values of the calculated intensity on the screen. One way is to plot "points" at random locations in each cell so that the number of points is proportional to the computed

intensity at the center of the cell. Suggested parameters are  $\lambda = 5000 \text{ \AA}$  and  $L = 200 \text{ mm}$  for an aperture of dimensions  $1 \text{ mm} \times 3 \text{ mm}$ .

## Appendix 9A: Fast Fourier Transform

The fast Fourier transform (FFT) has been discovered independently by many workers in a variety of contexts, and there are a number of variations on the basic algorithm. In the following, we describe a version due to Danielson and Lanczos. The goal is to compute the Fourier transform  $g(\omega_k)$  given the data set  $f(j) \equiv f_j$  of (??). For convenience we rewrite the relation:

$$g_k \equiv g(\omega_k) = \sum_{j=0}^{N-1} f(j\Delta) e^{-i2\pi kj/N}, \quad (9.54)$$

and introduce the complex number  $W$  given by

$$W = e^{-i2\pi/N}. \quad (9.55)$$

The following algorithm works with any complex data set if we require that  $N$  is a power of two. Real data sets can be transformed by setting the array elements corresponding to the imaginary part equal to 0.

To understand the FFT algorithm, we consider the case  $N = 8$ , and rewrite (??) as

$$g_k = \sum_{j=0,2,4,6} f(j\Delta) e^{-i2\pi kj/N} + \sum_{j=1,3,5,7} f(j\Delta) e^{-i2\pi kj/N} \quad (9.56)$$

$$= \sum_{j=0,1,2,3} f(2j\Delta) e^{-i2\pi k2j/N} + \sum_{j=0,1,2,3} f((2j+1)\Delta) e^{-i2\pi k(2j+1)/N} \quad (9.57)$$

$$= \sum_{j=0,1,2,3} f(2j\Delta) e^{-i2\pi kj/(N/2)} + W^k \sum_{j=0,1,2,3} f((2j+1)\Delta) e^{-i2\pi kj/(N/2)} \quad (9.58)$$

$$= g_k^e + W^k g_k^o, \quad (9.59)$$

where  $W^k = e^{-i2\pi k/N}$ . The quantity  $g^e$  is the Fourier transform of length  $N/2$  formed from the even components of the original  $f(j)$ ;  $g^o$  is the Fourier transform of length  $N/2$  formed from the odd components.

Of course, we do not have to stop here, and we can continue this decomposition if  $N$  is a power of two. That is, we can decompose  $g^e$  into its  $N/4$  even and  $N/4$  odd components,  $g^{ee}$  and  $g^{eo}$ , and decompose  $g^o$  into its  $N/4$  even and  $N/4$  odd components,  $g^{oe}$  and  $g^{oo}$ . We find

$$g_k = g_k^{ee} + W^{2k} g_k^{eo} + W^k g_k^{oe} + W^{3k} g_k^{oo}. \quad (9.60)$$

One more decomposition leads to

$$g_k = g_k^{eee} + W^{4k} g_k^{eoo} + W^{2k} g_k^{eoe} + W^{6k} g_k^{eoo} \\ + W^k g_k^{oee} + W^{5k} g_k^{oee} + W^{3k} g_k^{oeo} + W^{7k} g_k^{ooo}. \quad (9.61)$$

At this stage each of the Fourier transforms in (??) use only one data point. We see from (??) with  $N = 1$ , that the value of each of these Fourier transforms,  $g_k^{eee}, g_k^{eeo}, \dots$ , is equal to the value of  $f$  at the corresponding data point. Note that for  $N = 8$ , we have performed  $3 = \log_2 N$  decompositions. In general, we would perform  $\log_2 N$  decompositions.

There are two steps to the FFT. First, we reorder the components so that they appear in the order given in (??). This step makes the subsequent calculations easier to organize. To see how to do the reordering, we rewrite (??) using the values of  $f$ :

$$g_k = f(0) + W^{4k} f(4\Delta) + W^{2k} f(2\Delta) + W^{6k} f(6\Delta) \\ + W^k f(\Delta) + W^{5k} f(5\Delta) + W^{3k} f(3\Delta) + W^{7k} f(7\Delta). \quad (9.62)$$

We use a trick to obtain the ordering in (??) from the original order  $f(0\Delta), f(1\Delta), \dots, f(7\Delta)$ . Part of the trick is to refer to each  $g$  in (??) by a string of ‘e’ and ‘o’ characters. We assign 0 to ‘e’ and 1 to ‘o’ so that each string represents the binary representation of a number. If we reverse the order of the representation, i.e., set 110 to 011, we obtain the value of  $f$  we want. For example, the fifth term in (??) contains  $g^{oee}$  corresponding to the binary number 100. The reverse of this number is 001 which equals 1 in decimal notation, and hence the fifth term in (??) contains the function  $f(1)$ . Convince yourself that this bit reversal procedure works for the other seven terms.

The first step in the FFT algorithm is to use this bit reversal procedure on the original array representing the data. In the next step this array is replaced by its Fourier transform. If you want to save your original data, it is necessary to first copy the data to another array before passing the array to a FFT subroutine. The Danielson-Lanczos algorithm involves three loops. The outer loop runs over  $\log_2 N$  steps. For each of these steps,  $N$  calculations are performed in the two inner loops. As can be seen in SUB FFT, in each pass through the innermost loop each element of the array **g** is updated once by the quantity **temp** formed from a power of  $W$  multiplied by the current value of an appropriate element of **g**. The power of  $W$  used in **temp** is changed after each pass through the innermost loop. The power of the FFT algorithm is that we do not separately multiply each  $f(j\Delta)$  by the appropriate power of  $W$ . Instead, we first take pairs of  $f(j)$  and multiply them by an appropriate power of  $W$  to create new values for the array **g**. Then we repeat this process for pairs of the new array elements (each array element now contains four of the  $f(j\Delta)$ ). We repeat this process until each array element contains a sum of all  $N$  values of  $f(j)$  with the correct powers of  $W$  multiplying each term to form the Fourier transform.

```
SUB FFT(g(,),p)
! fast Fourier transform of complex input data set g
! transform returned in g
DIM Wp(2),factor(2),temp(2)
LET N = 2^p                ! number of data points
LET N2 = N/2
! rearrange input data according to bit reversal
LET j = 1
FOR i = 1 to N-1
! g(i,1) is real part of f((i-1)*del_t)
! g(i,2) is imaginary part of f((i-1)*del_t)
! set g(i,2) = 0 if data real
IF i < j then             ! swap values
```

```

        LET temp(1) = g(j,1)
        LET temp(2) = g(j,2)
        LET g(j,1) = g(i,1)
        LET g(j,2) = g(i,2)
        LET g(i,1) = temp(1)
        LET g(i,2) = temp(2)
    END IF
    LET k = N2
    DO while k < j
        LET j = j-k
        LET k = k/2
    LOOP
    LET j = j + k
NEXT i
! begin Danielson-Lanczos algorithm
LET jmax = 1
FOR L = 1 to p
    LET del_i = 2*jmax
    LET Wp(1) = 1           ! Wp initialized at W^0
    LET Wp(2) = 0
    LET angle = pi/jmax
    LET factor(1) = cos(angle) ! ratio of new to old W^p
    LET factor(2) = -sin(angle)
    FOR j = 1 to jmax
        FOR i = j to N step del_i
            ! calculate transforms of length 2^L
            LET ip = i + jmax
            LET temp(1) = g(ip,1)*Wp(1) - g(ip,2)*Wp(2)
            LET temp(2) = g(ip,1)*Wp(2) + g(ip,2)*Wp(1)
            LET g(ip,1) = g(i,1) - temp(1)
            LET g(ip,2) = g(i,2) - temp(2)
            LET g(i,1) = g(i,1) + temp(1)
            LET g(i,2) = g(i,2) + temp(2)
        NEXT i
        ! find new W^p
        LET temp(1) = Wp(1)*factor(1) - Wp(2)*factor(2)
        LET temp(2) = Wp(1)*factor(2) + Wp(2)*factor(1)
        MAT Wp = temp
    NEXT j
    LET jmax = del_i
NEXT L
END SUB

```

*Exercise 9.24.* Testing the FFT algorithm

1. Test sub FFT for  $N = 8$  by going through the code by hand and showing that the subroutine reproduces (??).

2. Write a subroutine to do the Fourier transform in the conventional manner based on (??). Make sure that your subroutine has the same arguments as `SUB FFT`, that is, write a subroutine to convert  $f(j\Delta)$  to the two-dimensional array `g`. If the data is real, let  $g(i, 2) = 0$ . The subroutine should consist of two nested loops, one over  $k$  and one over  $j$ . Print the Fourier transform of random real values of  $f(j\Delta)$  for  $N = 8$ , using both `SUB FFT` and the direct computation of the Fourier transform. Compare the two sets of data to insure that there are no errors in `SUB FFT`. Repeat for a random collection of complex data points.
3. Compute the CPU time as a function of  $N$  for  $N = 16, 64, 256$ , and  $1024$  for the FFT algorithm and the direct computation. You can use the `time` function in True BASIC before and after each call to the subroutines. Verify that the dependence on  $N$  is what you expect.
4. Modify `SUB FFT` to compute the inverse Fourier transform defined by (??). The inverse Fourier transform of a Fourier transformed data set should be the original data set.

## References and Suggestions for Further Reading

- E. Oran Brigham, *The Fast Fourier Transform*, Prentice Hall (1988). A classic text on Fourier transform methods.
- David C. Champeney, *Fourier Transforms and Their Physical Applications*, Academic Press (1973).
- James B. Cole, Rudolph A. Krutar, Susan K. Numrich, and Dennis B. Creamer, "Finite-difference time-domain simulations of wave propagation and scattering as a research and educational tool," *Computers in Physics* **9**, 235 (1995).
- Frank S. Crawford, *Waves*, Berkeley Physics Course, Vol. 3, McGraw-Hill (1968). A delightful book on waves of all types. The home experiments are highly recommended. One observation of wave phenomena equals many computer demonstrations.
- Paul DeVries, *A First Course in Computational Physics*, John Wiley & Sons (1994). Part of our discussion of the wave equation is based on Chapter 7. There also are good sections on the numerical solution of other partial differential equations, Fourier transforms, and the FFT.
- N. A. Dodd, "Computer simulation of diffraction patterns," *Phys. Educ.* **18**, 294 (1983).
- P. G. Drazin and R. S. Johnson, *Solitons: an Introduction*, Cambridge (1989). This book focuses on analytical solutions to the Korteweg-de Vries equation which has soliton solutions.
- Richard P. Feynman, Robert B. Leighton, and Matthew Sands, *The Feynman Lectures on Physics*, Vol. 1, Addison-Wesley (1963). Chapters relevant to wave phenomena include Chapters 28–30 and Chapter 33.
- A. P. French, *Vibrations and Waves*, W. W. Norton & Co. (1971). An introductory level text that emphasizes mechanical systems.

- Eugene Hecht, *Optics*, second edition, Addison-Wesley & Sons (1987). An intermediate level optics text that emphasizes wave concepts.
- Akira Hirose and Karl E. Lonngren, *Introduction to Wave Phenomena*, John Wiley & Sons (1985). An intermediate level text that treats the general properties of waves in various contexts.
- Amy Kolan, Barry Cipra, and Bill Titus, "Exploring localization in nonperiodic systems," *Computers in Physics* **9**, to be published (1995). An elementary discussion of how to solve the problem of a chain of coupled oscillators with disorder using transfer matrices.
- William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery, *Numerical Recipes*, second edition, Cambridge University Press (1992). See Chapter 12 for a discussion of the fast Fourier transform.
- Timothy J. Rolfe, Stuart A. Rice, and John Dancz, "A numerical study of large amplitude motion on a chain of coupled nonlinear oscillators," *J. Chem. Phys.* **70**, 26 (1979). Problem ?? is based on this paper.
- Garrison Sposito, *An Introduction to Classical Dynamics*, John Wiley & Sons (1976). A good discussion of the coupled harmonic oscillator problem is given in Chapter 6.
- William J. Thompson, *Computing for Scientists and Engineers*, John Wiley & Sons (1992). See Chapters 9 and 10 for a discussion of Fourier transform methods.
- Michael L. Williams and Humphrey J. Maris, "Numerical study of phonon localization in disordered systems," *Phys. Rev. B* **31**, 4508 (1985). The authors consider the normal modes of a two-dimensional system of coupled oscillators with random masses. The idea of using mechanical resonance to extract the normal modes is the basis of a new numerical method for finding the eigenmodes of large lattices. See Kousuke Yukubo, Tsuneyoshi Nakayama, and Humphrey J. Maris, "Analysis of a new method for finding eigenmodes of very large lattice systems," *J. Phys. Soc. Japan* **60**, 3249 (1991).