D. Thirumalai and Raymond D. Mountain, "Ergodic convergence properties of supercooled liquids and glasses," Phys. Rev. A **42**, 4574–4587 (1990).

Shan-Ho Tsai, H. K. Lee, and D. P. Landau, "Molecular and spin dynamics simulations using modern integration methods," Am. J. Phys., to be published.

James H. Williams and Glenn Joyce, "Equilibrium properties of a one-dimensional kinetic system," J. Chem. Phys. **59**, 741–750 (1973). Simulations in one dimension are even easier than in two.

Zoran Slanič, Harvey Gould, and Jan Tobochnik, "Dynamics of the classical Heisenberg chain," Computers in Physics **5** (6), 630–635 (1991).

CHAPTER 9 Normal Modes and Waves

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 waves and oscillatory motion, 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 first consider a one-dimensional chain of N 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 9.1). For many purposes the most realistic boundary conditions are to attach particles $j = 1$ and $j = N$ to springs which are attached to fixed walls. We denote the walls by $j = 0$ and $j = N + 1$ and require that $u_0(t) = u_{N+1}(t) = 0$.

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

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

Equation (9.1) couples the motion of particle j to its two nearest neighbors and describes *longitudinal* oscillations, that is, motion along the length of the system. It is straightforward to show that identical equations hold for the *transverse* oscillations of N identical mass points equally spaced on a stretched massless string (cf. French).

Because 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). We first discuss these solutions because they will help us interpret the nature of the numerical solutions. To find the *normal modes*, we look for oscillatory solutions for which the displacement of each particle is proportional to $\sin \omega t$ or $\cos \omega t$. We write