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CHAPTER

8 The Dynamics of Many-Particle Systems

We simulate the dynamical behavior of many-particle systems, such as dense gases, liquids, and solids, and observe their qualitative features. Some of the basic ideas of equilibrium statistical mechanics and kinetic theory are introduced.

8.1 ■ INTRODUCTION

Given our knowledge of the laws of physics at the microscopic level, how can we understand the behavior of gases, liquids, and solids and more complex systems such as polymers and proteins? For example, consider two cups of water prepared under similar conditions. Each cup contains approximately 10^{25} molecules which mutually interact and, to a good approximation, move according to the laws of classical physics. Although the intermolecular forces produce a complicated trajectory for each molecule, the observable properties of the water in each cup are indistinguishable and are easy to describe. For example, the temperature of the water in each cup is independent of time even though the positions and velocities of the individual molecules are changing continually.

One way to understand the behavior of a classical many-particle system is to simulate the trajectory of each particle. This approach, known as *molecular dynamics*, has been applied to systems of up to 10^9 particles and has given us much insight into a variety of systems in which the particles obey the laws of classical dynamics.

A calculation of the trajectories of many particles would not be very useful unless we knew the right questions to ask. Saving these trajectories would quickly fill up any storage medium, and we do not usually care about the trajectory of any particular particle. What are the useful quantities needed to describe these many particle systems? What are the essential characteristics and regularities they exhibit? Questions such as these are addressed by statistical mechanics, and some of the ideas of statistical mechanics are discussed in this chapter. However, the only background needed for this chapter is a knowledge of Newton's laws of motion.

8.2 ■ THE INTERMOLECULAR POTENTIAL

The first step is to specify the model system we wish to simulate. We assume that the dynamics can be treated classically, the molecules are spherical and chemically inert and their internal structure can be ignored, and the interaction between any pair of particles depends only on the distance between them. In this case the total potential energy U is a