a circular shell whose area is $2\pi r \Delta r$. These considerations imply that $g(r)$ is related to $n(r)$ by

$$\rho g(r) = \frac{\overline{n(r, \Delta r)}}{\frac{1}{2} N \, 2\pi r \Delta r} \qquad \text{(two dimensions)}. \tag{8.18}$$

Note the factor of $N/2$ in the denominator of (8.18). Method `normalizeRDF` normalizes the array `RDFAccumulator` and yields $g(r)$.

Listing 8.15 Method for obtaining $g(r)$ from $n(r)$.

```
public void normalizeRDF(PlotFrame dataRDF) {
   double density = N/(Lx*Ly);
   double L = Math.min(Lx,Ly);
   // maximum index is one less than binMax
   int binMax = (int)(L/(2*dr));
   double normalization = density*numberRDFMeasurements*N/2;
   for (int bin = 0; bin < binMax; bin++) {
      shellArea = Math.PI*(Math.pow(bin+dr,2) - Math.pow(bin,2));
      double RDF = RDFAccumulator[bin]/(normalization*shellArea);
      dataRDF.append(0,dr*(bin+0.5),g);   // adds results to be plotted
   }
}
```

The shell thickness Δr needs to be sufficiently small so that the important features of $g(r)$ are found, but large enough so that each bin has a reasonable number of contributions. The value of Δr should be a class variable. A reasonable choice for its magnitude is $\Delta r = 0.025$.

Problem 8.13 The structure of $g(r)$ for a dense liquid and a solid

(a) Write a test program that incorporates `computeRDF` and `normalizeRDF` and compute $g(r)$ for a system of $N = 64$ particles that are fixed on a triangular lattice with $L_x = 8$ and $L_y = \sqrt{3}L_x/2$. What is the density of the system? What is the nearest neighbor distance between sites? At what value of r does the first maximum of $g(r)$ occur? What is the next nearest distance between sites? Does your calculated $g(r)$ have any other peaks? If so, relate these peaks to the structure of the triangular lattice.

(b) Modify your molecular dynamics program and compute $g(r)$ for a dense fluid ($\rho > 0.6$, $T \approx 1.0$) with $N \geq 64$. How many peaks in $g(r)$ can you observe? In what ways do they change as the density is increased? How does the behavior of $g(r)$ for a dense liquid compare to that of a dilute gas and a solid? ■

8.9 ■ HARD DISKS

How can we understand the temperature and density dependence of the equation of state and the structure of a dense liquid? One way to gain more insight into this dependence is to modify the interaction and see how the properties of the system change. In particular, we would like to understand the relative role of the repulsive and attractive parts of the

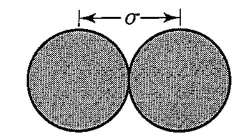

Figure 8.7 The closest distance between two hard disks is σ. The disks exert no force on one another unless they touch.

interaction. For this reason, we consider an idealized system of hard disks for which the interaction $u(r)$ is purely repulsive:

$$u(r) = \begin{cases} +\infty & r < \sigma \\ 0 & r \geq \sigma. \end{cases} \tag{8.19}$$

The length σ is the diameter of the hard disks (see Figure 8.7). In three dimensions the interaction (8.19) describes the interaction of hard spheres (billiard balls); in one dimension (8.19) describes the interaction of hard rods.

Because the interaction $u(r)$ between hard disks is a discontinuous function of r, the dynamics of hard disks is qualitatively different than it is for a continuous interaction, such as the Lennard–Jones potential. For hard disks the particles move in straight lines at constant speed between collisions and change their velocities instantaneously when a collision occurs. Hence, the problem becomes finding the next collision and computing the change in the velocities of the colliding pair. The dynamics is *event driven* and can be computed exactly in principle; in practice, it is limited only by roundoff errors.

The dynamics of a system of hard disks can be treated as a sequence of two-body elastic collisions. The idea is to consider all pairs of particles i and j and to find the collision time t_{ij} for their next collision, ignoring the presence of all other particles. In many cases the particles will be going away from each other and the collision time is infinite. From the collection of collision times for all pairs of particles, we find the minimum collision time. We then move all the particles forward in time until the collision occurs and calculate the postcollision velocities of the colliding pair. The main problem is dealing with the large number of possible collision events.

We first determine the particle velocities of the colliding pair. Consider a collision between particles i and j. Let $\mathbf{v}_i$ and $\mathbf{v}_j$ be their velocities before the collision and $\mathbf{v}'_i$ and $\mathbf{v}'_j$ be their velocities after the collision. Because the particles have equal mass, it follows from conservation of energy and linear momentum that

$$v'^2_i + v'^2_j = v^2_i + v^2_j \tag{8.20}$$

$$\mathbf{v}'_i + \mathbf{v}'_j = \mathbf{v}_i + \mathbf{v}_j. \tag{8.21}$$

From (8.21) we have

$$\Delta \mathbf{v}_i = \mathbf{v}'_i - \mathbf{v}_i = -(\mathbf{v}'_j - \mathbf{v}_j) = -\Delta \mathbf{v}_j. \tag{8.22}$$

When two hard disks collide, the force is exerted along the line connecting their centers, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. Hence, the components of the velocities parallel to $\mathbf{r}_{ij}$ are exchanged, and the perpendicular components of the velocities are unchanged. It is convenient to write the