



**Figure 8.6** Initial configuration for the model of friction discussed in Problem 8.12. The atoms in the sliding object are placed in two rows of a triangular lattice with seven atoms in the bottom row and six atoms in the top row. There is a damping force on the left-most atom in the bottom row (the atom is shaded differently than the other atoms), and there is an external horizontal spring attached to the right-most atom in the bottom row.

+40. To what does a negative load correspond? Determine the coefficient of static friction from the slope of  $f_s$  versus  $W$ .

- (d) Reduce the surface area by eliminating 4 atoms, 2 from each row. Rerun your simulations and discuss the results. Repeat for an increased size of 17 atoms and fit your results to the form

$$f_s = \mu_s W + cA, \quad (8.14)$$

where  $A$  is the number of atoms in the bottom row, and  $c$  is a constant. The area dependence in (8.14) is different from what is usually assumed for sliding friction in introductory physics textbooks. The surfaces of macroscopic objects are typically rough at the microscopic level, and thus the effective area of contact is much smaller than the surface area. The effective area can be proportional to the load, and thus both terms in (8.14) can be proportional to the load, which is consistent with the usual assumption made in introductory physics texts. ■

## 8.8 ■ RADIAL DISTRIBUTION FUNCTION

We can gain more insight into the structure of a many-body system by looking at how the positions of the particles are correlated with one another due to their interactions. The *radial distribution function*  $g(r)$  is a measure of this correlation and has the following properties. Suppose that  $N$  particles are in a region of volume  $V$  with number density  $\rho = N/V$ . Choose one of the particles to be the origin. Then the mean number of other particles between  $\mathbf{r}$  and  $\mathbf{r} + d\mathbf{r}$  is defined to be  $\rho g(\mathbf{r}) d\mathbf{r}$ . If the interparticle interaction is spherically symmetric and the system is a gas or a liquid, then  $g(\mathbf{r})$  depends only on the separation  $r = |\mathbf{r}|$ . The normalization condition for  $g(r)$  is

$$\rho \int g(r) d\mathbf{r} = N - 1 \approx N, \quad (8.15)$$

where the volume element  $d\mathbf{r} = 4\pi r^2 dr$  ( $d = 3$ ),  $2\pi r dr$  ( $d = 2$ ), and  $2 dr$  ( $d = 1$ ). Equation (8.15) implies that if we choose one particle as the origin and count all the other particles in the system, we obtain  $N - 1$  particles.

For an ideal gas, there are no correlations between the particles, and the normalization condition (8.15) implies that  $g(r) = 1$  for all  $r$ . For the Lennard-Jones interaction, we expect that  $g(r) \rightarrow 0$  as  $r \rightarrow 0$ , because the repulsive force between particles increases rapidly as  $r \rightarrow 0$ . We also expect that  $g(r) \rightarrow 1$  as  $r \rightarrow \infty$ , because the correlation of a given particle with the other particles decreases as their separation increases.

Several thermodynamic properties can be obtained from  $g(r)$ . Because  $\rho g(r)$  can be interpreted as the local density of particles about a given particle, the potential energy of interaction between this particle and all other particles between  $r$  and  $r + dr$  is  $u(r)\rho g(r) d\mathbf{r}$ , if we assume that only two-body interactions are present. The total potential energy is found by integrating over all  $r$  and multiplying by  $N/2$ . The factor of  $N$  is included because any of the  $N$  particles could be chosen as the particle at the origin, and the factor of  $1/2$  is included so that each pair interaction is counted only once. The result is that the mean potential energy per particle can be expressed as

$$\frac{U}{N} = \frac{\rho}{2} \int g(r) u(r) d\mathbf{r}. \quad (8.16)$$

It can also be shown that the relation (8.9) for the mean pressure can be rewritten in terms of  $g(r)$  so that the equation of state can be expressed as

$$\frac{PV}{NkT} = 1 - \frac{\rho}{2kTd} \int g(r) r \frac{du(r)}{dr} d\mathbf{r}. \quad (8.17)$$

To determine  $g(r)$  for a particular configuration of particles, we first compute  $n(r, \Delta r)$ , the number of particles in a spherical (circular) shell of radius  $r$  and a small, but nonzero width  $\Delta r$ , with the center of the shell centered about each particle. A method for computing  $n(r)$  is given in Listing 8.14.

**Listing 8.14** Method to compute  $n(r)$ .

```
public void computeRDF() {
    // accumulate data for n(r)
    for (int i = 0; i < N-1; i++) {
        for (int j = i+1; j < N; j++) {
            double dx = PBC.separation(x[i] - x[j], Lx);
            double dy = PBC.separation(y[i] - y[j], Ly);
            double dy = (dy + Ly) % 0.5*Ly;
            double r2 = dx*dx + dy*dy;
            double r = Math.sqrt(r2);
            int bin = (int)(r/dr); // dr = shell width
            RDFAccumulator[bin]++;
        }
    }
    numberRDFMeasurements++;
}
```

The use of periodic boundary conditions in `computeRDF` implies that the maximum separation between any two particles in the  $x$  and  $y$  directions is  $L_x/2$  and  $L_y/2$ , respectively. Hence, we can determine  $g(r)$  only for  $r \leq \frac{1}{2} \min(L_x, L_y)$ .

To obtain  $g(r)$  from  $n(r)$ , we note that for a given particle  $i$ , we consider only those particles whose index  $j$  is greater than the index  $i$  (see `computeRDF`). Hence, there are a total of  $\frac{1}{2}N(N-1)$  separations that are considered. In two dimensions we compute  $n(r, \Delta r)$  for