compute $P_{n=0}(t)$ for a number of different times and lengths such that t/L^2 has the same value, you should obtain the same value of $P_{n=0}$. ■

Project 15.42 The inverse power law potential
Consider the inverse power law potential

$$V(r) = V_0 \left(\frac{\sigma}{r}\right)^n, \tag{15.96}$$

with $V_0 > 0$. One reason for the interest in potentials of this form is that thermodynamic quantities such as the mean energy E do not depend on V_0 and σ separately, but depend on a single dimensionless parameter, which is defined as (see Project 8.25)

$$\Gamma = \frac{V_0}{kT}\frac{\sigma}{a}, \tag{15.97}$$

where a is defined in three and two dimensions by $4\pi a^3\rho/3 = 1$ and $\pi a^2 \rho = 1$, respectively. The length a is proportional to the mean distance between particles. A Coulomb interaction corresponds to $n = 1$, and a hard sphere system corresponds to $n \to \infty$. What phases do you expect to occur for arbitrary n?

(a) Compare the qualitative features of $g(r)$ for a "soft" potential with $n = 4$ to a system of hard disks at the same density.
(b) Let $n = 12$ and compute the mean energy E as a function of Γ for a three-dimensional system with $N = 16$, 32, 64, and 128. Does E depend on N? Can you extrapolate your results for the N-dependence of E to $N \to \infty$? Do you see any evidence of a fluid-solid phase transition? If so, estimate the value of Γ at which it occurs. What is the nature of the transition if it exists? What is the symmetry of the ground state?
(c) Let $n = 4$ and determine the symmetry of the ground state. For this value of n, there is a solid-to-solid phase transition at which the solid changes symmetry. To determine the value of Γ at which this phase transition exists and the symmetry of the smaller Γ solid phase (see Dubin and Dewitt), it is necessary to use a Monte Carlo method in which the shape of the simulation cell changes to accomodate the different symmetry (the Rahman–Parrinello method), an interesting project. An alternative is to prepare a bcc lattice at $\Gamma \approx 105$ (for example, $T = 0.06$ and $\rho = 0.95$). Then instantaneously change the potential from $n = 4$ to $n = 12$; the new value of Γ is ≈ 4180, and the new stable phase is fcc. The transition can be observed by watching the evolution of $g(r)$. ■

Project 15.43 Rare gas clusters
There has been much recent interest in structures that contain many particles but that are not macroscopic. An example is the unusual structure of sixty carbon atoms known as a "buckeyball." A less unusual structure is a cluster of argon atoms. Questions of interest include the structure of the clusters, the existence of "magic" numbers of particles for which the cluster is particularly stable, the temperature dependence of the quantities, and the possibility of different phases. This latter question has been subject to some controversy because transitions between different kinds of behavior in finite systems are not well defined, as they are for infinite systems.

(a) Write a Monte Carlo program to simulate a three-dimensional system of particles interacting via the Lennard–Jones potential. Use open boundary conditions; that is, do not enclose the system in a box. The number of particles N and the temperature T should be input parameters.
(b) Find the ground state energy E_0 as a function of N. For each value of N begin with a random initial configuration and accept any trial displacement that lowers the energy. Repeat for at least ten different initial configurations. Plot E_0/N versus N for $N = 2$ to 20 and describe the qualitative dependence of E_0/N on N. Is there any evidence of magic numbers, that is, value(s) of N for which E_0/N is a minimum? For each value of N save the final configuration. Plot the positions of the atoms. Does the cluster look like a part of a crystalline solid?
(c) Repeat part (b) using simulated annealing. The initial temperature should be sufficiently low so that the particles do not move far away from each other. Slowly lower the temperature according to some annealing schedule. Are your results for E_0/N lower than those you obtained in part (b)?
(d) To gain more insight into the structure of the clusters, compute the mean number of neighbors per particle for each value of N. What is a reasonable criteria for two particles to be neighbors? Also compute the mean distance between each pair of particles. Plot both quantities as a function of N and compare their dependence on N with your plot of E_0/N.
(e) Do you find any evidence for a "melting" transition? Begin with the configuration that has the minimum value of E_0/N and slowly increase the temperature T. Compute the energy per particle and the mean square displacement of the particles from their initial positions. Plot your results for these quantities versus T. ■

Project 15.44 The hard disk fluid-solid transition
Although we have mentioned (see Section 15.10) that there is much evidence for a fluid-solid transition in a hard disk system, the nature of the transition still is a problem of current research. In this project we follow the work of Lee and Strandburg and apply the constant pressure Monte Carlo method (see Section 15.12) and the Lee–Kosterlitz method (see Section 15.11) to investigate the nature of the transition. Consider $N = L^2$ hard disks of diameter $\sigma = 1$ in a two-dimensional box of volume $V = \sqrt{3}L^2 v/2$ with periodic boundary conditions. The quantity $v \geq 1$ is the reduced volume and is related to the density ρ by $\rho = N/V = 2/(\sqrt{3}v)$; $v = 1$ corresponds to maximum packing. The aspect ratio of $2/\sqrt{3}$ is used to match the perfect triangular lattice. Do a constant pressure (actually constant $p^* = P/kT$) Monte Carlo simulation. The trial displacement of each disk is implemented as discussed in Section 15.10. Lee and Strandburg find that a maximum displacement of 0.09 gives a 45% acceptance probability. The other type of move is a random isotropic change of the volume of the system. If the change of the volume leads to an overlap of the disks, the change is rejected. Otherwise, if the trial volume $\tilde{V}$ is less than the current volume V, the change is accepted. A larger trial volume is accepted with probability

$$e^{-p^*(\tilde{V}-V)+N\ln(\tilde{V}/V)}. \tag{15.98}$$

Volume changes are attempted 40–200 times for each set of individual disk moves. The quantity of interest is $N(v)$, the distribution of the reduced volume v. Because we need to store information about $N(v)$ in an array, it is convenient to discretize the volume in advance