Bray, and Godrèche) for $N = 10^5$ indicate that $f(t)$

$$f(t) \sim t^{-\theta} \tag{17.68}$$

for $t \approx 3$ to $t \approx 10,000$ with $\theta \approx 0.37$. Verify this result and extend your results to the one-dimensional $q$-state Potts model. In the latter model each site is initially given a random integer between 1 and $q$. A site is chosen at random and set equal to either of its two neighbors with equal probability. The value of the exponent $\theta$ is not understood at present, but might be related to analogous behavior in reaction-diffusion models.

*Project 17.29.* The inverse power law potential

from Gould-Tobochnick

Consider the inverse power law potential

$$V(r) = V_0\,(\frac{\sigma}{r})^n \tag{17.69}$$

with $V_0 > 0$. One reason for interest in potentials of this form is that thermodynamic quantities such as the mean energy $E$ do not depend on $V_0$ and $\sigma$ separately, but depend on a single dimensionless parameter. This dimensionless parameter can be defined as

$$\Gamma = \frac{V_0}{kT}\frac{\sigma}{a}, \tag{17.70}$$

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 $T$ for fixed density for a three-dimensional system. Fix $T$ and consider $N = 16, 32, 64$, and 128. Does $E$ depend on $N$? Can you extrapolate your results for the $N$-dependence of $E$ to $N \to \infty$? Fix $N$ and determine $E$ as a function of $\Gamma$. Do you see any evidence of a phase transition? If so, estimate the value of $\Gamma$ at which it occurs. What is the nature of the transition if it exists?

*Project 17.30.* 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 thermodynamic 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 nearly as sharp 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.