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Problem 8.1: **Radial Distribution Function**

The radial distribution function, $g(r)$, represents the probability density of finding a particle i at a given distance r from another particle j. For a two-dimensional system of area $L \times L$ containing N particles this function is given by

$$2\pi r \rho g(r) = \frac{1}{N} \left\langle \sum_i \sum_{j \neq i} \delta(r - r_{ij}) \right\rangle , \tag{1}$$

where $\langle \cdot \rangle$ denotes a time or ensemble average. $r_{ij} = |\mathbf{r_i} - \mathbf{r_j}|$ is the distance between particles i and j, and $\rho = N/L^2$ is the number density.

a) What do you expect in the limits $r \to 0$ and $r \to \infty$?

b) Develop a code which calculates $g(r)$ for a two-dimensional system with periodic boundary conditions.

c) Test your code as follows:

   i) Use your code to calculate $g(r)$ for a system of randomly distributed particles. In this case, $g(r) = 1$ for all r, why?

   ii) Use your code to compute $g(r)$ for a system where particles are placed on a square lattice. The $g(r)$ should have some peaks and be zero elsewhere. Find the positions of the first few peaks analytically and compare it to the peaks of the calculated $g(r)$. They should match.

d) Use your code to calculate $g(r)$ for the system described in Exercise Sheet 7 (Nosé-Hoover thermostat) at its *equilibrium*. Observe the kinetic and potential energy of the system to find out when you reach equilibrium. After reaching equilibrium you can measure $g(r)$ and you might need to measure it many times and average these measurements to obtain good statistics.

Problem 8.2: **Mean Squared Displacement**

The mean squared displacement is the second moment of the self part of the van Hove correlation function. In the MD simulation of N particles system, it can be defined as follows:

$$MSD(t) = \left\langle \delta\vec{r}^2(t) \right\rangle = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{n_{tor}}\sum_{\alpha=1}^{n_{tor}}\left(\vec{r}_i(t+t_\alpha) - \vec{r}_i(t_\alpha)\right)^2 , \tag{2}$$

where r_i is the position of the i-th particle. The second sum in Eq.(2) is an average over n_{tor} time origins at $t_\alpha\,(\alpha = 1, \cdots, n_{tor})$. Following these steps develop a code to calculate MSD for the system of Exercise 7:

a) In addition to an array for saving the current position of particles you need some more memory. Save the initial positions of particles in an additional array. Allocate this array and save the initial positions.

b) Another array is also needed to save the unfolded positions; the folded positions are the positions of the particles mapped back into the simulation box. To calculate the MSD you need the unfolded positions.

c) Write a function to calculate the MSD using the unfolded coordinates and the initial coordinates.

d) At short times the calculated MSD should be proportional to t^2 and at long times it should be proportional to t. Now divide the obtained MSD by t^2 and locate the time associated with the ballistic regime.

e) Using the MSD to find the Einstein frequency and the diffusion coefficient.