

Exercise 1. Random walk in 2D

Goal: In this exercise we learn how to simulate simple random walks in two dimensions.

Task 1: Generate a two dimensional random walk consisting of N positions (i.e. $N-1$ segments) and measure the square of the end to end difference \mathbf{R} . The step size is fixed. Only the angle has to be chosen at random.

Task 2: Generate several configurations $k \in \{1, \dots, M\}$ (random walks of same N , but different sequence of random numbers) and compute the average of \mathbf{R}^2 as well as the estimated error Δ :

$$\langle \mathbf{R}^2 \rangle \simeq \frac{1}{M} \sum_{k=1}^M \mathbf{R}_k^2, \quad \Delta = \sqrt{\langle (\mathbf{R}^2)^2 \rangle - \langle \mathbf{R}^2 \rangle^2}, \quad \left(\langle (\mathbf{R}^2)^2 \rangle \simeq \frac{1}{M} \sum_{k=1}^M (\mathbf{R}_k^2)^2 \right)$$

Choose the number M of configurations such that the estimated error is below 1% of the average value.

Task 3: Vary the number N of positions and check your result by comparing it to the analytical result (see lecture notes).

Exercise 2. Chains of spherical particles

Goal: Here, we learn how to simulate self-avoiding random walks in two dimensions.

Now, consider chains consisting of N hard spherical particles of radius r in 2 dimensions (disks). The particles are not allowed to overlap and neighboring particles in a chain touch each other (self-avoiding random walk).

Task 1: Measure $\langle \mathbf{R}^2 \rangle$ and Δ (same as in Exercise 1).

Task 2: Vary the number of particles N and compare the behavior to the results obtained in Exercise 1.

Please consider the following points:

- \mathbf{R}^2 , $\langle \mathbf{R}^2 \rangle$, etc. depend on the number of particles N .
- The chain of non-overlapping particles is created in a way similar to the simple random walk (Exercise 1), but it has to be checked that there is no overlap with other particles. If the new particle overlaps with any other in the chain it is rejected.