

1. Self-avoiding random walk

The files *mainpivot.m* and *fpivot.m* contain a Monte Carlo program for self-avoiding random walks in two dimensions.

- (a) Open the files *mainpivot.m* and *fpivot.m* in the editor and familiarize yourself with their contents. In the first part of the problem, we will focus on the generation of new chain configurations by the pivot algorithm. Set the `illustration` flag to 1 and set the `evaluation` flag to 0 in the program *mainpivot.m*, choose a chain length of $N = 21$ and a small number (`MCsteps` = 5) of Monte Carlo steps, and set the equilibration time to zero for now (`MCequilib` = 0). Run the program and observe how the chain loses its original straight conformation over time. The actual moves are performed in the file *fpivot.m*. Study the section where rotations about 90, -90, and 180 degrees are performed and explain, why the center of the chain stays in place during the simulation.
- (b) In this part of the problem, you will study the chain length dependence of the mean-square end-to-end distance, R_e^2 . The variation of R_e^2 with bond number $n = N - 1$ (in the limit of very long chains) follows a power law

$$R_e^2(n) \propto n^{2\nu} \text{ with } \nu = 0.75 \text{ for dimension } d = 2. \quad (1)$$

You will determine a value for the exponent ν from your data. To begin, set the `illustration` flag to 0 and set the `evaluation` flag to 1 in the program *mainpivot.m*. Start with a short chain length, e.g. $N = 11$, and set the number of Monte Carlo steps to 10000 and the equilibration time to `MCequilib` = `MCsteps`/10. Run the program and describe and save Fig. 2. Perform simulations for chain lengths $N = 11, 21, 31, 51, 101$ that is bond numbers of $n = 10, 20, 30, 50, 100$ and store the results of $R_e^2(n)$ and $\sigma(n)$ (note, in the program, $\sigma = \text{stdResq}$) in row vectors. Use the Matlab plotting function `errorbar` to plot the results for R_e^2 along with its errors. Calculate the logarithms of n and $R_e^2(n)$, plot them in a second graph, and determine the slope of the graph. What is your value for the exponent ν and how does it compare to $\nu = 0.75$?