Firstly, a few words about this exercise course. You can forms groups up to 3 persons. The solutions should be uploaded to StudIP in form of a PDF file or a Mathematica notebook into the corresponding folder. I will look at the latest version uploaded before 12:00 on the submission day. The solutions should contain the code, its output and comments describing what you do and why.

The preferred program is Mathematica. You can use other tools and languages (e.g. Python), but support is not guaranteed.

There is no strict grading system as these exercises are not about following a recipe. There are several ways to approach the problem, and many ways to shape your approach into a code. The exercises are not extensive: if you know what you're doing, you can solve them in a few lines.

If you have questions about this exercise, or if you're stuck, you can contact me via zhilin@math.uni-hannover.de.

[H7] Thermodynamics of a chain

(12 points)

Imagine a chain (see picture) built from N absolutely rigid rods of equal length ℓ (in our units $\ell = 1$) which connect at freely moving joints. The endpoints of the chain are held in place, separated by distance L. Suppose that the chain is confined to a plane (lives in 2d space), and is in thermal equilibrium with temperature τ . Compute the force that the chain exerts at the endpoints (also note its direction). Plot this force as a function of length L in the cases when N = 3, 5, 8.



A chain with N = 5 links. Endpoints are fixed, inner joints can move freely (save for constraints from rigid rods). The rods are allowed to overlap, the joints have zero size. The chain is thermalized, you can imagine that the it twitches chaotically under thermal fluctuations.

Hint 1 You can compute the force in the same manner you derive the pressure of a gas from its partition function. You will find that the temperature τ will enter the formula in a very simple way, so for numerical computations you can set $\tau = 1$.

Please turn

- Hint 2 One way to do the computation (other approaches are very much welcome) is to think of the chain as of a result of a random walk with N steps. In such a walk each step has fixed length $\ell = 1$ and random direction, and for a moment we let one of the chain's endpoints move freely. The position of this free endpoint is random, described by some probability density $p_N(x, y)$. Careful thought reveals that the partition function $Z_N(L, \tau)$ is given, up to an irrelevant factor, by $p_N(L, 0)$. If you use this approach, explain why the last statement is correct.
- *Hint 3* If you choose to simulate a random walk, note that $p_N(x, y)$ is rotationally symmetric (no preferred direction). So instead of counting walks that end in the vicinity of (x, y) = (L, 0) you can use the vicinity of the whole $x^2 + y^2 = L^2$ ring.

Remark The pressure of a gas can be deduced from the amount of work the gas does when it expands. In our case expansion means increase of the distance L between the endpoints of the chain.