Statistical Physics

Homework, Sheet 4

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If you have trouble understanding the program I would be happy to explain it. Contact me via `stud.IP` or e-Mail (`felixspringer149@gmail.com`).

1 Thermodynamics of a chain [H7]

In my solution I am using the approach that is shown in the hints. I am calculating the probability density P in form of a histogram and then try to derive the force F directly from there.

1.1 Theoretical background

First I use the relation (1) of force F and pressure p, in which I then insert the free Energy E, which leads to the partition function Z.

$$\begin{aligned} F &= \int p \, \mathrm{d}A \qquad (1)\\ &= \int \underbrace{-\left(\frac{\partial E}{\partial V}\right)_\tau}_{=p} \mathrm{d}A \\ &= \int -\partial_V \underbrace{(-\tau \ln(Z))}_{=E} \, \mathrm{d}A \\ &= \tau \int \partial_V \ln(Z) \, \mathrm{d}A \\ F &= \tau \, \partial_L \ln(Z) \qquad (2) \end{aligned}$$

Now with equation (2) I only need to be able to calculate the partition function Z. In this case there is a relation (3) to the probability density P.

$$P(N_\nu, \epsilon_\nu) = \frac{1}{Z} \underbrace{\exp\left(\frac{\mu N_\nu - \epsilon_\nu}{\tau}\right)}_{=:\alpha} \qquad (3)$$

$$\implies \quad Z = \frac{\alpha}{P} \tag{4}$$

Now I can use equation (4) to further simplify equation (2).

$$\begin{aligned} F &= \tau \partial_L \ln\left(\frac{\alpha}{P}\right) \\ &= \tau(\underbrace{\partial_L \ln(\alpha)}_{=0} - \partial_L \ln(P)) \\ F &= -\tau\ \partial_L \ln(P) \end{aligned} \tag{5}$$

With equation (5) I can directly compute the force F from the probability density $P(L)$ which I am simulating with a distribution of "randomwalks".

2 Result

The end result of the computation can be found in Figure 1.

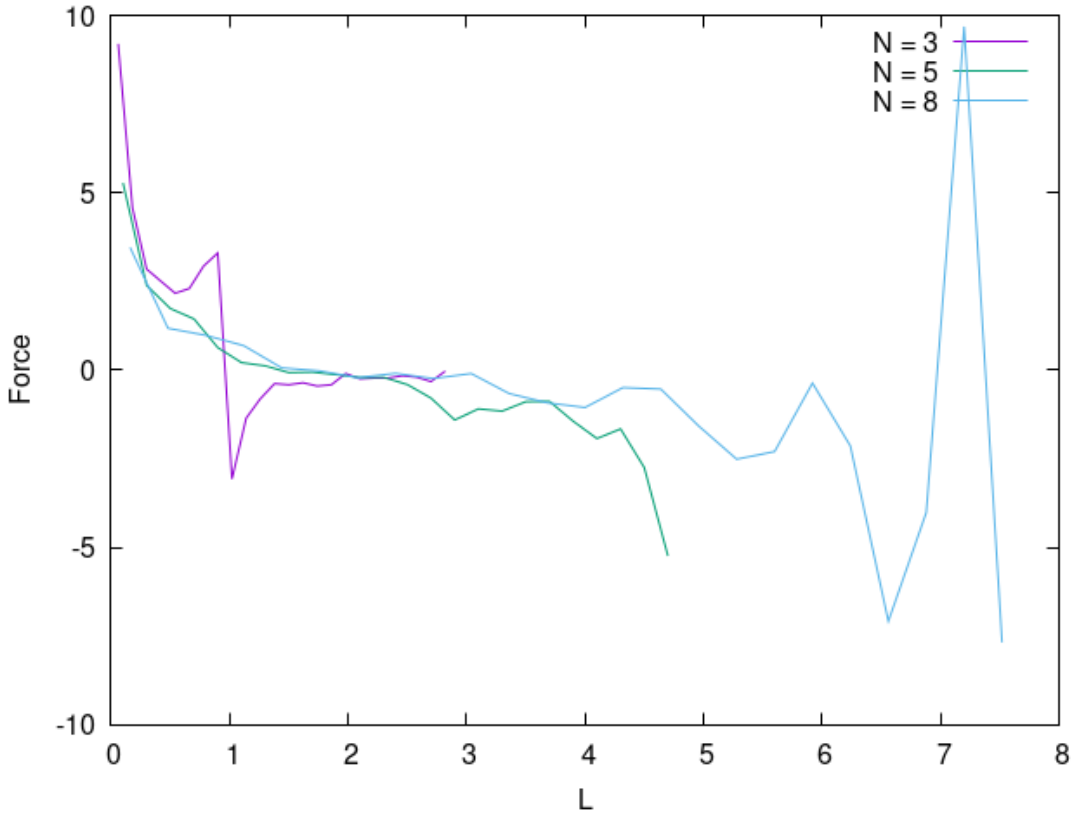

Figure 1: Plot of the calculated force F in relation to the distance L

To look into the details of the computation check out `calc-force.ss`. It is executed with "Chez-Scheme 9.5.1". The plot is created with "gnuplot" in `plot-L-force.gp`.

To completely execute everything there is `main.sh`.