

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 .

$$F = \int -p \, dA \quad (1)$$

$$= - \int \underbrace{- \left(\frac{\partial E}{\partial V} \right)_{\tau}}_{=p} dA$$

$$= \int \partial_V \underbrace{(-\tau \ln(Z))}_{=E} dA$$

$$= -\tau \int \partial_V \ln(Z) dA$$

$$F = -\tau \partial_L \ln(Z) \quad (2)$$

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 .

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

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

The reason for $\partial_L \alpha = 0$ is, that due to the thermal equilibrium the energy ϵ_ν stays constant for different L . N_ν is also constant for each probability density P , and μ and τ are definitely constant here.

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

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

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.

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`.

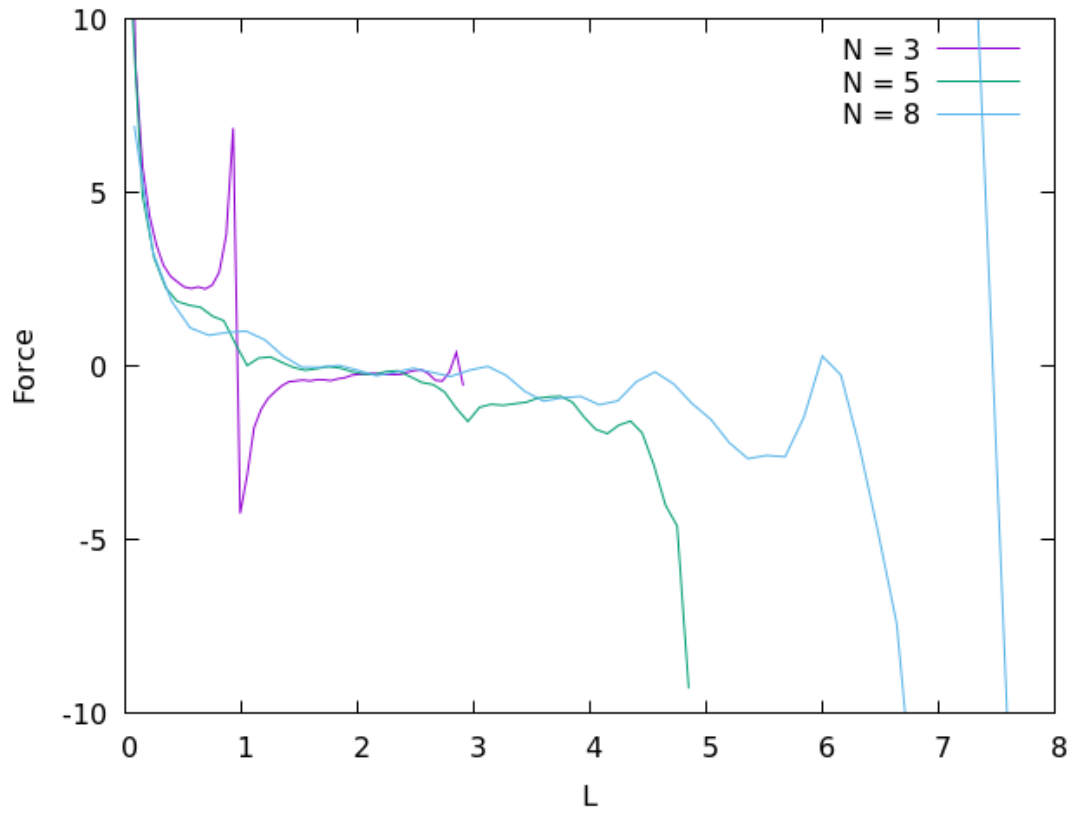


Figure 1: Plot of the calculated force F in relation to the distance L