Statistical Physics

Homework, Sheet 4

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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.

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

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

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

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

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”.