

Übung zur Vorlesung Struktur und Simulation.

Aufgabe 1

Gegeben $S = -k \sum p_i \log(p_i)$. Für $p_i = \frac{1}{N}$ zeigen dass $S = k \log(N)$

Loesung: $S = -k \sum_{i=0}^N \frac{1}{N} \log\left(\frac{1}{N}\right) \Rightarrow S = k \sum_{i=0}^N \frac{1}{N} \log(N) \Rightarrow S = \frac{k}{N} \log(N) \sum_{i=0}^N 1 \Rightarrow$

$$S = \frac{Nk}{N} \log(N) \Rightarrow S = k \log(N)$$

Aufgabe 2

aufgabe2.py

State	E	$e^{(-E/RT)}$	p	$p \cdot \log(p)$
T= 3K				
1	0	1.0	1.5051660576620003e-35	-1.2068658517805181e-33
2	-1	2.577554114851961e+17	3.879646965462193e-18	-1.5553810211655957e-16
3	-2	6.643785214990277e+34	1.0	0.0
Z: 6.643785214990277e+34				S: 1.5553810211655957e-16
T= 300K				
1	0	1.0	0.21174035343869668	-0.32870456071133425
2	-1	1.4931797031726477	0.31616639809726466	-0.3640613795467765
3	-2	2.229585625966756	0.47209324846403866	-0.35434316154485274
Z: 4.722765329139404				S: 1.0471091018029635
T= 300000K				
1	0	1.0	0.33319970630782186	-0.3661908921680369
2	-1	1.0004009882494296	0.3333333154747647	-0.3662040944616284
3	-2	1.0008021372904352	0.3334669782174134	-0.3662172484627384
Z: 3.001203125539865				S: 1.0986122350924037

State	E	$e^{(-E/RT)}$	p	$p \cdot \log(p)$
T=300K				
(1, 1)	-5	7.422674044658944	0.09900260169200192	-0.22895432249481829
(1, 2)	-1	1.4931797031726477	0.019915824744339252	-0.07799516244171611
(1, 3)	-2	2.229585625966756	0.02973790528019095	-0.10453863308702062
(2, 1)	-1	1.4931797031726477	0.019915824744339252	-0.07799516244171611
(2, 2)	-7	16.549487356208104	0.22073477766579955	-0.3334846450762381
(2, 3)	-3	3.3291720031790426	0.044404036579251835	-0.1382930371709111
(3, 1)	-2	2.229585625966756	0.02973790528019095	-0.10453863308702062
(3, 2)	-3	3.3291720031790426	0.044404036579251835	-0.1382930371709111
(3, 3)	-9	36.898499126520164	0.4921470874346344	-0.34892128499607766
Z: 74.9745351920241				S: 1.5530139179664297

