Exercise 03

NAME:	MATRICULATION NUMBER:
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RESULTS:

3.1		OF 6 P
3.2		OF 3 P
3.3		OF 2 P
3.4		OF 4 P
TOTAL		OF 15 P

GENERAL INSTRUCTIONS

- SUBMIT YOUR SOLUTION TO OLIVER LEMKE (R. 35.17) BEFORE **THURSDAY 19. MAY AT 8.15 AM.**
- FILL OUT THIS COVER SHEET AND SUBMIT IT ALONG WITH YOUR SOLUTION.
- SHOW HOW YOU ARRIVED AT YOUR ANSWER.

3.1 Partition function for equidistant energy levels (6 P)

If we consider a system with n equidistant energy levels (e.g the harmonic oscillator)

$$E_0, E_1 = 2E_0, ..., E_{n-1} = nE_0$$

The partition function for a canonical ensemble is defined as

$$Z = \sum_{i=0}^{n} e^{-i\beta E_0} \tag{1}$$

with β being the Langrange multiplier.

(a) Show that for this case the partition fuction can be written as

$$Z = \frac{1}{1 - e^{-\beta E_0}}$$

(b) Calculate the propability to populate a specific energy level (general expression)

(c) To calculate the partition function consider that only the first 10 energy levels are accessible. Calculate the partition function for rising T:

1.) $\beta E_0 = 3.0$
2.) $\beta E_0 = 1.0$
3.) $\beta E_0 = 0.7$
4.) $\beta E_0 = 0.3$

(d) What do you observe? Explain your observations.

(e) Plot the occupancy of the single energy levels for the cases 1.) to 4.) in an energy diagram.

(f) What do you observe?

3.2 Temperature dependency of the partition function (3 P)

In general the partition function can be expressed as:

$$Z(T) = \sum_{i=0}^{\infty} g_i e^{-\frac{E_i}{k_b T}} \tag{2}$$

where g_i denotes the degeneracy factor of energy level i.

(a) What do you observe for $T \to 0$? Explain your results and calculate the partition function.

(b) Repeat (a) for $T \to \infty$.

(c) For which case does the partition function for $T \to \infty$ have a finite limit?

3.3 Additivity of the entropy (2 P)

From classical thermodynamics we know that the entropy of a combined system $S_{A,B}$ can be calculated as the sum of the entropy of the subsystems S_A and S_B.

$$S_{A,B} = S_A + S_B \tag{3}$$

In terms of statistical thermodynamics the (Gibbs) entropy is defined as:

$$S_{A,B} = -k_b \sum_{i,j} p_{ij} \log p_{ij} \tag{4}$$

where p_{ij} denotes the probability that subsystem A is in state i and subsystem B is in state j. Show that the entropy in terms of statistical thermodynamics is additive. The entropy of the single subsystem is defined as:

$$S_A = -k_b \sum_{i} p_i \log p_i \tag{5}$$

where p_i is the probability that subsystem A is in state i.

3.4 Calculation of energy levels (4 P)

Consider a system at 25 °C with 4 accessible energy levels. Now assume that the energy levels are populated with

$$p_0 = 0.8, p_1 = 0.1, p_2 = 0.05, p_3 = 0.05.$$

(a) Calculate the energy of the first 4 energy levels as well as the energy difference between them if $E_0 = 10^{-20}$ J.

(b) Draw an energy scheme. What do you observe?

(c) Consider E_2 and E_3 as a single energy level E_2' with $g_2 = 2$. At which temperature are the energy levels E_2' and E_1 equally populated? At which temperature E_2' and E_0?

(d) Is there a finite temperature at which E_0 and E_1 are populated equally? Justify your answer.