

## Statistical Physics and Thermodynamics (SS 2018)

### Problem sheet 7

Hand in: Friday, June 15 during the lecture

<http://www.physik.fu-berlin.de/en/einrichtungen/ag/ag-netz/lehre/>

#### 1 Ideal gas in the canonical ensemble (12 points)

The canonical partition function of an ideal gas is given by

$$Z = \frac{1}{N!} \left( \frac{V}{\lambda_t^3} \right)^N, \quad \lambda_t = \frac{h}{\sqrt{2\pi m k_B T}}. \quad (1)$$

- a) Obtain the free energy  $F(N, V, T)$  from the canonical partition function. **(1 point)**  
b) Start from the definition  $F = U - TS$  and use the first law of thermodynamics  $dU = TdS - PdV$  to derive the differential relation

$$dF = -PdV - SdT. \quad (2)$$

**(1 point)**

- c) Use your results from a) and b) to construct the entropy  $S(N, V, T)$ . **(2 points)**

*Hint:* Note the  $T$ -dependence of  $\lambda_t$ .

- d) Obtain the caloric equation of state

$$U(N, V, T) = \frac{3}{2} N k_B T \quad (3)$$

from the relation  $F = U - TS$  and by using your results from a) and c). **(1 point)**

- e) Construct an expression for the entropy  $S(U, V, N)$  from your previous results, and compare your result to the Sackur-Tetrode equation derived in the lecture

$$S(N, V, U) = -k_B N \ln \left( \frac{N}{V} \right) + \frac{3}{2} k_B N \ln \left( \frac{U}{N} \right) + k_B N \left( \frac{3}{2} \ln \left( \frac{4\pi m}{3h^2} \right) + \frac{5}{2} \right). \quad (4)$$

**(2 points)**

*Hint:* Start by obtaining  $S(N, V, T)$  and  $T(N, V, U)$ .

- f) Invert eq. (4) to get an expression for  $U(S, V, N)$ . **(1 point)**  
g) Calculate the temperature as a function of  $S, V, N$  by an appropriate derivative of  $U(S, V, N)$ . **(2 points)**  
h) Invert this equation again to obtain a result for  $S(N, V, T)$ . Is it equal to your result from c)? **(1 point)**  
i) As an application, calculate the heat capacity  $C_V$  of the ideal gas from the caloric equation of state eq. (3). **(1 point)**

## 2 Shannon entropy (8 points)

The Shannon entropy for a discrete random variable  $x_i$  is defined as

$$H = - \sum_i p_i \log p_i. \quad (5)$$

a) Consider a binary random variable with  $x_i \in \{0, 1\}$ . Calculate the Shannon entropy for

- (a)  $p_0 = p_1 = 0.5$ ,
- (b)  $p_0 = 0.9, p_1 = 0.1$ ,
- (c)  $p_0 = 1, p_1 = 0$ .

Use your results to explain why the Shannon entropy is a measure for information content. **(1 point)**

*Remark:* If one replaces the logarithms in eq. (5) by base-2 logarithms, the Shannon entropy is a measure for the minimum number of bits required for a lossless compression of the output.

b) Show that  $H \geq 0$ . **(1 point)**

c) Derive the maximal value of  $H$  for a random variable  $N$  possible outcomes  $x_i$ . **(2 points)**

*Hint:* Introduce a Lagrange multiplier to ensure  $\sum_i p_i = 1$  when you maximize  $H$ .

d) Given the definitions

$$H_x = - \sum_i p(x_i) \log p(x_i), \quad (6)$$

$$H_y = - \sum_j p(y_j) \log p(y_j), \quad (7)$$

and

$$H_{xy} = - \sum_{ij} p(x_i, y_j) \log p(x_i, y_j), \quad (8)$$

show that  $H_{xy} \leq H_x + H_y$ , where the equality holds if and only if  $x_i$  and  $y_i$  are independent. **(2 points)**

A related quantity to the Shannon entropy is the so-called Kullback-Leibler divergence for two (discrete) probability distributions  $p, q$ . It is defined by

$$D(p||q) = \sum_i p_i \log \left( \frac{p_i}{q_i} \right). \quad (9)$$

e) Calculate the Kullback-Leibler divergence for the two cases

- (a)  $p_i = q_i$ ,
- (b)  $q_i = 1/N = \text{const.}$

Use your results to argue why the Kullback-Leibler divergence is a measure for the information lost if one approximates a (true) probability distribution  $p$  by a (model) distribution  $q$ . **(1 point)**

The cross entropy of two distributions  $p$  and  $q$  is defined as

$$H_{ce}(p; q) = - \sum_i p_i \log q_i. \quad (10)$$

f) Express the cross entropy in terms of the Shannon entropy and the Kullback-Leibler divergence. **(1 point)**

*Remark:* The cross entropy and the Kullback-Leibler divergence play an important role as objective functions in machine learning.