### KLAUSUR (EXAM)

- Answer all questions 0)-3).
- · Put your name on each sheet submitted.
- Illegible scripts might be ignored.
- The duration of the exam is 180 mins.
- Indicate clearly which question (and part) your respective solution is referring to.

# Of Definitions/formulas:

- a) Define the grand canonical ensemble in quantum mechanics.
- b) State the first law of thermodynamics in terms of  $E, S, T, \mu, N, P, V$ .
- c) Define the *efficiency* of a general cyclic process (closed curve  $\gamma$  in (T, S)-diagram).

Consider the following cyclic process in the (P,V)-diagram:

- $I \rightarrow II$ : Isothermal (constant T) expansion.
- $II \rightarrow III$ : Adiabatic expansion.
- $III \rightarrow IV$ : Isobaric (constant P) compression.
- $IV \rightarrow I$ : Adiabatic compression.

You can assume the equations of state of an ideal gas,

$$PV = Nk_BT , \qquad E = \frac{3}{2}PV . \tag{1}$$

- a) Sketch the process in a (P,V)-diagram, and identify where heat is injected/given off by the system.
- b) What is the work  $\Delta W$  performed by the system in one cycle?
- c) What is the heat  $\Delta Q_{in}$  injected into the system in one cycle?
- (d) What is the efficiency? -> finish

State your answers in b), c), d) in terms of the temperatures  $T_I, ..., T_{IV}$  and  $v = V_{II}/V_I$ .

Recall that the energy eigenstates  $|n\rangle$  of a single harmonic oscillator have energy  $E_n = \varepsilon(n + \frac{1}{2})$ , where n = 0, 1, 2, ...

- a) Calculate the canonical partition function for one oscillator  $Z_1(\beta) = \sum_n e^{-\beta E_n}$ .
- b) Calculate the canonical partition function  $Z_N(\beta)$  for a system of N independent harmonic oscillators in terms of that found for the single oscillator.
- c) Calculate the mean energy E.
- d) The free energy is F = E TS. Show that the first law takes the form

$$dF = -SdT + \mu dN \tag{2}$$

in terms of F (noting that dV = 0 in this question). Give a formula for the chemical potential  $\mu$  in terms of a derivative of F(T,N). Using the formula  $F(\beta,N) = -\beta^{-1} \log Z_N(\beta)$  [where  $\beta^{-1} = k_B T$ ], calculate  $\mu$  for the present system.

4). Lagrange unit. ->

43

A system has N states occupied with probabilities  $p_n$ , n = 1, ..., N. The n-th state has energy  $E_n$  and particle number n. The entropy is defined as  $S = -k_B \sum_n p_n \log p_n$ , the average energy is  $U = \sum_n E_n p_n$ , and the average particle number is  $v = \sum_n np_n$ . Using the method of Lagrange multipliers, determine the probability distribution which maximizes S for fixed U, v, and show that it is given by

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$$p_n = \frac{1}{Y} e^{-\beta(E_n - \mu n)} \tag{3}$$

for some  $\beta, \mu, Y$ .

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b) Calculate the canonical partition function \$3 (10) for a system of \$5 in reported functions as calculated for the standard and sugla oscillator.

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- c) Define the efficiency of a general cyclic process (closed curve  $\gamma$  in (T, S)-diagram).

1) Consider the following cyclic process in the (P, V)-diagram:

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State your answers in b), c), d) in terms of the temperatures  $T_I, ..., T_{IV}$  and  $v = V_{II}/V_I$ .

2) Recall that the energy eigenstates  $|n\rangle$  of a single harmonic oscillator have energy  $E_n = \varepsilon(n + \frac{1}{2})$ , where n = 0, 1, 2, ...

- a) Calculate the *canonical partition function* for one oscillator  $Z_1(\beta) = \sum_n e^{-\beta E_n}$ .
- b) Calculate the canonical partition function  $Z_N(\beta)$  for a system of N independent harmonic oscillators in terms of that found for the single oscillator.
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2

3) A system has N states occupied with probabilities  $p_n$ , n = 1, ..., N. The *n*-th state has energy  $E_n$  and particle number *n*. The entropy is defined as  $S = -k_B \sum_n p_n \log p_n$ , the average energy is  $U = \sum_n E_n p_n$ , and the average particle number is  $v = \sum_n np_n$ . Using the method of Lagrange multipliers, determine the probability distribution which maximizes S for fixed U, v, and show that it is given by

$$p_n = \frac{1}{\gamma} e^{-\beta(E_n - \mu n)}$$
(3)

for some  $\beta, \mu, Y$ .

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## All - -- Self + p. d.

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### PROBEKLAUSUR (MOCK EXAM)

- You need at least 50 points to pass this exam
- · Put your name on each sheet submitted.
- Illegible scripts might be ignored.
- The duration of the exam is 180 mins.
- Indicate clearly which question (and part) your respective solution is referring to.

1) (25 points) Recall the first law of thermodynamics:

$$TdS = dE + PdV - \mu dN . \tag{1}$$

- a) State the "microscopic" (i.e. statistical mechanics-) definition of the entropy S in the context of the classical micro canonical ensemble. State what it means for S to be an "extensive quantity".
- b) Derive the relations

$$\frac{\partial N}{\partial E}\Big|_{VS} = \frac{1}{\mu}, \quad \frac{\partial N}{\partial S}\Big|_{VE} = -\frac{T}{\mu}, \quad \frac{\partial N}{\partial V}\Big|_{ES} = \frac{P}{\mu}, \quad (2)$$

- from the first law (Hint: rewrite the first law in terms of the differentials dE, dV, dS.).
  c) Introduce the free energy by F = E TS, viewed as a function of T, N, V. Write the first law in terms of F instead of E.
- d) Write the first law (1) as  $dS = \dots$  Applying the exterior differential d to the resulting equation and using d(dS) = 0, derive the relation

$$\frac{\partial T}{\partial V}\Big|_{E,N} - P\frac{\partial T}{\partial E}\Big|_{V,N} + T\frac{\partial P}{\partial E}\Big|_{V,N} = 0.$$
(3)

(Hint: Keep in mind that dEdV = -dVdE.)

- 2) (25 points) Consider the following cyclic process:
  - $I \rightarrow II$ : Adiabatic (constant S) expansion
  - $II \rightarrow III$ : Isochoric (constant V) cooling
  - $III \rightarrow IV$ : Adiabatic (constant S) compression
  - $IV \rightarrow I$ : Isothermal (constant T) expansion

Throughout it is assumed that the particle number N remains constant (so that dN = 0 in the entire process), and we assume that the equations of state of an ideal gas hold:

$$PV = Nk_BT , \qquad E = \frac{3}{2}PV . \tag{4}$$

- a) Show that PV = cst. on isotherms and  $PV^{5/3} = cst$ . on adiabatics using the equation(s) of state and the first law TdS = dE + PdV. (If you cannot do this, carry on with b) e) assuming these results.)
- b) Sketch the process in a (P,V)-diagram, and identify where heat is injected/given off by the system.
- c) What is the work  $\Delta W$  performed by the system in one cycle?
- d) What is the heat  $\Delta Q_{in}$  injected into the system in one cycle?
- e) What is the efficiency  $\eta = \frac{\Delta W}{\Delta Q_{in}}$ ?

State your answers in c) – e) in terms of  $N, T_I, V_I, V_{II} (= V_{III}), V_{IV}$ .

2

(25 points) We consider a gas of charged particles of unit charge  $\pm q$ . The eigenstates of the charge operator  $\hat{Q}$  and Hamiltonian  $\hat{H}$  are  $|n_+, n_-\rangle$  with

$$\hat{H}|n_{+},n_{-}\rangle = \varepsilon_{n_{+},n_{-}}|n_{+},n_{-}\rangle, \quad \hat{Q}|n_{+},n_{-}\rangle = q(n_{+}-n_{-})|n_{+},n_{-}\rangle,$$
(5)

where  $n_+, n_- \ge 0$  are integers that have the interpretation of the number of positively resp. negatively charged particles in the state. We consider a density matrix of the form

$$\rho = \sum_{n_+, n_- \ge 0} p_{n_+, n_-} |n_+, n_-\rangle \langle n_+, n_-|$$
(6)

where  $Tr\rho = 1$  is required as usual, and where expectation values are defined as usual by  $\langle A \rangle =$  $Tr(A\rho)$ . The information entropy is defined by  $S(\rho) = -k_B Tr\rho \log \rho$ , the mean energy by  $E = \langle \hat{H} \rangle$ and the mean charge by  $Q = \langle \hat{Q} \rangle$ .

- a) Using the method of Lagrange multipliers, show that the density matrix which maximizes  $S(\rho)$  for fixed E, Q is of the form  $p_{n_+,n_-} = \frac{1}{V} \exp(-\beta [\varepsilon_{n_+,n_-} + \Phi q(n_+ - n_-)])$ , or equivalently  $\rho = \frac{1}{V} \exp[-\beta(\hat{H} + \Phi \hat{Q})]$ . (Here  $\beta, \Phi, Y$  are constants.)
- b) Define  $G = -k_B T \log Y(T, \Phi)$ , where  $\beta^{-1} = k_B T$ . Using  $Y = \text{Trexp}[-(\hat{H} + \Phi \hat{Q})/(k_B T)]$ , show that

$$S = -\frac{\partial G}{\partial T}\Big|_{\Phi}, \quad Q = -\frac{\partial G}{\partial \Phi}\Big|_{T}, \tag{7}$$

where S, Q are defined as above.

- c) For a charged gas at fixed volume, the first law of thermodynamics is  $TdS = dE \Phi dQ$ . What is the physical meaning of  $\Phi$ ? Show that if we define  $G = E - TS - \Phi Q$ , then  $G = G(T, \Phi)$ satisfies  $dG = -SdT - Qd\Phi$ .
- (d) Verify the relations (7) using  $dG = -SdT Qd\Phi$ .

123 ... Nul (4) (25 points) A directed polymer consists of atoms i = 0, 1, 2, ..., N at positions  $(x_i, y_i) \in \mathbb{Z}^2$  of a square lattice. The atom at the origin is fixed at the position  $x_0 = y_0 = 0$  and the other atoms are chained together such that  $x_i - x_{i-1} = 1$  and  $|y_i - y_{i-1}| = 1$ . This polymer is hence oriented in the *x*-direction and it does not self-intersect. Ner:

- Determine the total number of micro-states of the polymer.
- b) Determine the number of microstates W(y) having the property that  $y_N = y$ . Hint: Write  $y_N$  in terms of  $\sigma_i = y_i - y_{i-1} \in \{\pm 1\}$ , where i = 1, ..., N, and then in terms of the number v of +1's in  $\{\sigma_i\}$ .
- c) Calculate the typical deflection of the chain end,

$$\langle y_N^2 \rangle = \frac{\sum_y y^2 W(y)}{\sum_y W(y)} \,. \tag{8}$$

Hint: Consider the partition function of the canonical ensemble  $Z(\beta) = \sum_{y} e^{\beta y} W(y)$ . Write  $\langle y_N^2 \rangle$  in terms of  $\beta$ -derivative(s) of  $Z(\beta)$ .

$$|y_1 - y_0| - 7 = ) \quad y_1 - y_0 = -1$$

# PROBEKLAUSUR (MOCK EXAM) 16/17

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State your answers in c) – e) in terms of  $N, T_I, V_I, V_{II} (= V_{III}), V_{IV}$ .

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where  $n_+, n_- \ge 0$  are integers that have the interpretation of the number of positively resp. negatively charged particles in the state. We consider a density matrix of the form

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a) Using the method of Lagrange multipliers, show that the density matrix which maximizes  $S(\rho)$  for fixed E, Q is of the form  $p_{n_+,n_-} = \frac{1}{Y} \exp(-\beta[\varepsilon_{n_+,n_-} + \Phi q(n_+ - n_-)])$ , or equivalently  $\rho = \frac{1}{Y} \exp[-\beta(\hat{H} + \Phi \hat{Q})]$ . (Here  $\beta, \Phi, Y$  are constants.)

b) Define  $G = -k_B T \log Y(T, \Phi)$ , where  $\beta^{-1} = k_B T$ . Using  $Y = \text{Trexp}[-(\hat{H} + \Phi \hat{Q})/(k_B T)]$ , show that

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(d) Verify the relations (7) using  $dG = -SdT - Qd\Phi$ .

4) (25 points) The Hamiltonian of a gas of N classical, relativistic particles moving in one dimension is

$$H(q_1, \dots, q_N, p_1, \dots, p_N) = \sum_{i=1}^N \{c | p_i | + U(q_i)\} \,. \tag{8}$$

Here  $(p_1, \ldots, p_N)$  are the momenta of the particles, and  $(q_1, \ldots, q_N)$  the positions (i.e.  $q_i, p_i \in \mathbb{R}$  for all  $i = 1, \ldots, N$ ). The potential U(q) is = 0 if  $q \in [0, L]$  and  $= \infty$  otherwise and effectively restricts the particles to the interval [0, L].

a) The micro-canonical partition function for *distinguishable* particles is

$$W(E,L,N) = h^{-N} \int_{E \le H(\{p_i\},\{q_j\}) \le E + \Delta E} dq_1 \dots dq_N dp_1 \dots dp_N .$$
(9)

Perform first the  $q_i$ -integrals.

- b) Next, perform the p<sub>i</sub>-integrals assuming that ΔE is small compared to E. You may use that the volume of a layer of thickness δ ≪ R surrounding the surface of an N-dimensional hyper-pyramid (the set defined by x<sub>i</sub> ≥ 0, ∑<sub>i=1</sub><sup>N</sup> x<sub>i</sub> ≤ R) is given by ~ δ · √NR<sup>N-1</sup>/(N-1)!. Do not forget to take into account that each p<sub>i</sub> can be negative or positive!
- c) How does the partition function W have to be modified if the particles are indistinguishable?

d) Compute the entropy  $S = k_B \log W$  in the micro canonical ensemble for indistinguishable particles, and verify that

$$S(E,L,N) = Nk_B \log\left(\frac{2e^2LE}{hcN^2}\right)$$
(10)

up to subleading terms in the large N limit. (Hint: Use Stirling's approximation  $N! \sim N^N e^{-N}$ .) (Use the result of item 2d) and the first law of thermodynamics to derive

$$P = \frac{Nk_B}{L}$$
(11)

for the pressure. (Hint: First derive  $P = T \frac{\partial S}{\partial L|_{E,N}}$ .) B Similarly, derive the relation  $1/T = Nk_B/E$ .

g) Argue that the probability density  $\mathscr{P}(p)$  for finding a particle with momentum p is given by

$$\mathscr{P}(p) = \frac{L}{Nh} \cdot \frac{W(E-c|p|,L,N-1)}{W(E,L,N)}$$
(12)

(Hint: If one particle has momentum *p*, what is the energy left for the remaining particles?) From this, derive

$$\mathscr{P}(p) \sim \frac{c}{2k_B T} e^{-c|p|/(k_B T)}.$$
(13)

(Hint: Use the relation  $(1 + a/N)^N \sim e^a$  for large N, and the relation between E and T derived before. For W, use the result of question 2d))