$\boxed{\text{II}}$

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.

1 ~~0)~~ Definitions/formulas:

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

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

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

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

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

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 ΔW performed by the system in one cycle?
c) What is the heat ΔQ_{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 $T_I,\ldots,T_{IV}$ and $v = V_{II}/V_I$.

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

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 μ in terms of a derivative of $F(T,N)$. Using the formula $F(\beta,N) = -\beta^{-1}\log Z_N(\beta)$ [where $\beta^{-1} = k_BT$], calculate μ for the present system.

4). Lagrange mult. →

4 ~~3~~ A system has N states occupied with probabilities p_n, $n = 1,\dots,N$. 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 $\nu = \sum_n n p_n$. Using the method of Lagrange multipliers, determine the probability distribution which maximizes S for fixed U, ν, and show that it is given by

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

for some β, μ, Y.

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0) Definitions/formulas:

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

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

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d) What is the efficiency?

State your answers in $b), c), d)$ in terms of the temperatures $T_I, \ldots, T_{IV}$ 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 $n = 0, 1, 2, \ldots$.

a) Calculate the *canonical partition function* for one oscillator $Z_1(\beta) = \sum_n e^{-\beta E_n}$.
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3) A system has N states occupied with probabilities p_n, $n = 1, \ldots, N$. 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 $\nu = \sum_n n p_n$. Using the method of Lagrange multipliers, determine the probability distribution which maximizes S for fixed U, ν, and show that it is given by

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

for some β, μ, Y.

VI

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

$$\left.\frac{\partial N}{\partial E}\right|_{V,S} = \frac{1}{\mu}\,, \quad \left.\frac{\partial N}{\partial S}\right|_{V,E} = -\frac{T}{\mu}\,, \quad \left.\frac{\partial N}{\partial V}\right|_{E,S} = \frac{P}{\mu}\,, \tag{2}$$

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 $dS = \ldots$. Applying the exterior differential d to the resulting equation and using $d(dS) = 0$, derive the relation

$$\left.\frac{\partial T}{\partial V}\right|_{E,N} - P\left.\frac{\partial T}{\partial E}\right|_{V,N} + T\left.\frac{\partial P}{\partial E}\right|_{V,N} = 0\,. \tag{3}$$

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

2) (25 points) Consider the following cyclic process:

- $I \to II$: Adiabatic (constant S) expansion
- $II \to III$: Isochoric (constant V) cooling
- $III \to IV$: Adiabatic (constant S) compression
- $IV \to I$: 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:

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

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 ΔW performed by the system in one cycle?

d) What is the heat ΔQ_{in} injected into the system in one cycle?

e) What is the efficiency $\eta = \frac{\Delta W}{\Delta Q_{\text{in}}}$?

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

3) (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

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

where $n_+, n_- \geq 0$ 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

$$\rho = \sum_{n_+,n_- \geq 0} p_{n_+,n_-}|n_+, n_-\rangle\langle n_+, n_-| \tag{6}$$

where $\mathrm{Tr}\rho = 1$ is required as usual, and where expectation values are defined as usual by $\langle A \rangle = \mathrm{Tr}(A\rho)$. The information entropy is defined by $S(\rho) = -k_B \mathrm{Tr}\rho \log \rho$, 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 $p_{n_+,n_-} = \frac{1}{Y}\exp(-\beta[\varepsilon_{n_+,n_-} + \Phi q(n_+ - n_-)])$, or equivalently $\rho = \frac{1}{Y}\exp[-\beta(\hat{H} + \Phi\hat{Q})]$. (Here β, Φ, Y are constants.)

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

$$S = -\left.\frac{\partial G}{\partial T}\right|_\Phi\ , \quad Q = -\left.\frac{\partial G}{\partial \Phi}\right|_T\ , \tag{7}$$

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 Φ? 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 $dG = -SdT - Qd\Phi$.

1 2 3 . . . N+1

4) (25 points) A directed polymer consists of atoms $i = 0, 1, 2, \ldots, N$ at positions $(x_i, y_i) \in \mathbb{Z}^2$ of a square lattice. The atom at the origin is fixed at the $\boxed{\text{position } x_0 = y_0 = 0}$ 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.

a) 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 $i = 1, \ldots, N$, and then in terms of the number ν of $+1$'s in $\{\sigma_i\}$.

$\sum^{N} \sigma_i$

$\sim n_+$

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 β-derivative(s) of $Z(\beta)$.

$|y_1 - y_0| = 1 \Rightarrow y_1 - y_0 = \begin{matrix} 1 \\ -1 \end{matrix}$

V

PROBEKLAUSUR (MOCK EXAM) 16/17.

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b) Derive the relations

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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.

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

2) (25 points) Consider the following cyclic process:

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d) What is the heat ΔQ_{in} injected into the system in one cycle?

e) What is the efficiency $\eta = \frac{\Delta W}{\Delta Q_{\text{in}}}$?

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 $n_+, n_- \geq 0$ 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 β, Φ, Y are constants.)

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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

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

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

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

Perform first the q_i-integrals.

b) Next, perform the p_i-integrals assuming that ΔE is small compared to E. You may use that the volume of a layer of thickness $\delta \ll R$ surrounding the surface of an N-dimensional hyper-pyramid (the set defined by $x_i \geq 0, \sum_{i=1}^N x_i \leq R$) is given by $\sim \delta \cdot \sqrt{N}R^{N-1}/(N-1)!$. Do not forget to take into account that each p_i can be negative or positive!

c) How does the 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

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

up to subleading terms in the large N limit. (Hint: Use Stirling's approximation $N! \sim N^N e^{-N}$.)

e) Use the result of item 2d) and the first law of thermodynamics to derive

$$P = \frac{Nk_B T}{L} \tag{11}$$

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

f) 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

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

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

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

(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))