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Blatt 6 zur Theoretischen Physik IV, WS 2023/2024

(Abgabe bis 15.12.2023, 8:30 Uhr)

Exercise 1: Grand canonical ensemble

a) Consider a system that exchanges energy and particles with its surroundings. The energy and particle number of state i are denoted by E_i and N_i. The average energy and the average particle number are given by

$$U = \sum_i \omega_i E_i \quad \text{and} \quad N = \sum_i \omega_i N_i.$$

The grand canonical ensemble of this system can be obtained by maximizing the entropy

$$S = -k_{\mathrm{B}} \sum_i \omega_i \ln \omega_i \,,$$

where ω_i is the probability of occupation of the state i. Use the method of Lagrange multipliers (see Blatt 4) to find the form of ω_i and the grand canonical partition function Z_g in terms of the energy and particle number of the states. Hint: Note the normalization $\sum_i \omega_i = 1$.

b) Express ω_i in terms of temperature T and chemical potential μ:

$$T = 1 \Big/ \frac{\partial S}{\partial U}, \quad \mu = -T \frac{\partial S}{\partial N}.$$

c) Using the grand canonical potential as

$$\Phi = -k_{\mathrm{B}} T \ln Z_g.$$

show that

$$\Phi = U - ST - \mu N.$$

[4+6+1=11 Points]

Exercise 2: A simplified model of the crystal surface

Consider a system consisting of M discrete sites, such as the surface of a crystal. Each site can be occupied by particles and its energy content is denoted by ϵ_n when it is occupied by n particles.

a) Find the partition function $Z_N(\beta)$ when there are a total of N particles in the system. As usual, $\beta = 1/k_{\mathrm{B}}T$.

b) Find the grand canonical partition function $Z_g(\beta, \mu)$ if the system is in contact with a reservoir and can exchange particles with it. The chemical potential is given by μ.

c) Derive a formula for the average number of particles in the system.

d) Calculate the average number of particles for the following cases:

   i) $\epsilon_n = \epsilon\, n$ (with $\mu < \epsilon$)

   ii) $\epsilon_n = \infty$ for $n \geq 2$ (therefore each site can be occupied by a maximum of one particle)

   iii) $\epsilon_n = \frac{1}{\beta} \ln n!$

[1.5+2.5+2+7=13 Points]

Exercise 3: Computational task (modeling the crystal surface)

Here we calculate the grand canonical partition function of the crystal surface introduced in exercise 2 assuming that $\epsilon_n = 1$ for $0 \geq n \geq N_{\max}$ and $\epsilon_n = \infty$ for $n > N_{\max}$. Set $\beta = \mu = 1$ and $M = 10$ for simplicity. Plot $\ln Z_g$ versus $N_{\max}$ for $N_{\max} \in \{1, 10\}$. As a guide, there is a Python code in the exercise folder (Blatt6-ZgCrystalSurface.py), where Z_g is obtained for a given $N_{\max}$. You can complete it.

[4 Points]

Exercise 4: Ideal gas in a box

Consider a system of N particles in a cube of volume $V = L^3$. Each of the particles of mass m carries the energy

$$\epsilon(n_x, n_y, n_z) = (n_x^2 + n_y^2 + n_z^2)\epsilon_0, \ \ \epsilon_0 = \frac{h^2}{8mL^2},$$

where $n_x, n_y, n_z \in \mathbb{Z}_{\geq 0}$ and h denotes Planck's constant. In the following we assume that the particles are indistinguishable.

a) Find the partition function $Z_N(\beta)$ when there are N particles in the system. Hint: We assume that $\beta\epsilon_0 = \epsilon_0/k_B T \ll 1$, thus, you can approximate the summation by appropriate integration.

b) Find the grand canonical partition function $Z_g(\beta, \mu)$ if the system is in contact with a reservoir and can exchange particles with it. The chemical potential is given by μ.

c) Calculate the pressure $p = \frac{1}{\beta}\frac{\partial}{\partial V} \ln Z_g(\beta, \mu)$ and the average number $\langle N \rangle$ of particles in the system. Then show that $pV = \langle N \rangle k_B T$.

[6+1.5+4.5=12 Points]