

Exercises for “Theoretical Physics (Master)”

Winter 26/27

DR. L. JANSSEN

PROF. DR. M. VOJTA

Exercise 1 (20.-29.10.26)

1. Temperature and entropy in two-level systems

Consider a system with two states of energies ϵ_1 and ϵ_2 , and convince yourself why you can effectively understand it as a spin 1/2. Assume that this system is part of an ensemble of N independent two-level systems with identical properties.

- (a) First assume that the total energy E and the total number of particles N of the ensemble are fixed. To which class does this ensemble belong? Recognize that specifying (E, N) is in general compatible with a multitude of different microstates of the ensemble. Argue that in thermodynamic equilibrium the probabilities p_i of all these compatible microstates must be equal. Now introduce the entropy $S = -\sum_i p_i \ln(p_i)$ and calculate the values of p_i for which S is maximal. Is the entropy a good measure of thermodynamic equilibrium for an isolated ensemble?
- (b) Consider a microcanonical ensemble in which m of the two-level systems are in the state with energy ϵ_1 . How many microstates realize this situation, and what is the expression for the entropy for general N and m in thermodynamic equilibrium? Calculate the entropy explicitly for a single spin 1/2 for $\epsilon_1 = \epsilon_2$ and $\epsilon_1 \neq \epsilon_2$. Can you give a simple interpretation of your result?
- (c) For the ensemble considered in part (b), calculate, sketch, and discuss the entropy S and temperature T for a fixed large number of particles N as a function of the energy E . Assume that $\epsilon_1 > \epsilon_2$.

Hint: The temperature is defined by $T^{-1} = (\partial S / \partial E)_N$. You may use the approximation $\log(x!) \approx x \log(x) - x$. For simplicity, you may also assume that each energy corresponds to only one value of m .

- (d) Now consider two arbitrary microcanonical ensembles A and B with energies $E_{A,B}$ and particle numbers $N_{A,B}$. Let ensemble $i = A, B$ have $\mathcal{N}_i$ microstates that are compatible with the specification of E_i and N_i . If the ensembles are now brought into contact and can exchange energy and particles, a new thermodynamic equilibrium is established. How is this defined for the total system? In the following, restrict yourself to the case where the subsystems can exchange energy only, and express the total entropy as a sum over microstates that realize a given partition of the total energy $E_A + E_B$ between the subsystems. Approximate the sum by its largest contribution and show that this contribution can be obtained by maximizing the total entropy of the two subsystems, each at a given energy E_i . What does this imply for the temperatures of subsystems A and B in equilibrium?
- (e) Now consider a general canonical ensemble of two-level systems. By which quantities is it specified? Is entropy maximization alone still a good criterion for reaching thermodynamic equilibrium? Use the definition of the chemical potential μ ,

$$\mu = -T \left(\frac{\partial S}{\partial N} \right)_E, \quad (1)$$

- to identify, if appropriate, another quantity that is extremized in equilibrium instead of the entropy. Is equilibrium reached at the maximum or minimum of this quantity?
- (f) Now consider specifically the ensemble of N two-level systems from part (b), with the difference that they now form a canonical ensemble. What is the probability p_i of a given microstate with energy E_i in thermodynamic equilibrium? Starting from the p_i , calculate the entropy and express it in terms of the mean energy E and the quantity introduced in the last part, whose extremization defines thermal equilibrium in the canonical ensemble. How can this quantity therefore be calculated from the canonical partition function?
- (g) Now sketch and discuss the behavior of the entropy of the canonical ensemble by calculating the quantity introduced in part (d) for $\epsilon_2 < \epsilon_1$ and taking the appropriate derivatives. Also calculate and discuss the behavior of the specific heat $C(T) = T (\partial S / \partial T)_N$.

2. Quantum-statistical entropy

Consider a quantum-mechanical canonical ensemble, and give the expression for the quantum-statistical entropy $S[\hat{\rho}]$ as a functional of the density-matrix operator. Why can the density matrix of a canonical ensemble in equilibrium be derived by maximizing the entropy subject to the constraint of fixed mean energy (and one additional constraint)? Carry out this maximization and compare your result with the familiar expression for the density matrix in the canonical ensemble.