11. About entropy (I)

Let us consider two sets a and b of paramagnetic ions. The Hamiltonian function of a set is

$$H_i = \mu_B B_i \sum_{j=1}^{N_i} \sigma_j,\ i = a, b; \tag{1}$$

where $\sigma_j = \pm 1$. The macrostate of each system is characterised by three variables: the energy, the magnetic field and the number of paramagnetic ions. These variables will be denoted hereafter as (U_a, B_a, N_a) for the system a, and (U_b, B_b, N_b) for the system b. Both systems are in contact: their magnetic dipoles interact weakly with each other, whereby an energy exchange between both systems is possible. Here U_a and U_b can vary, but the total energy $U = U_a + U_b$ remains constant within a boundary ΔU, since the total system is closed. We assume that the system is in thermal equilibrium and is described by a microcanonical distribution. The probability of system a to have the energy E_a is

$$p(E_a) = \frac{A_a A_b e^{(S_a+S_b)/k}}{\int A_a A_b e^{(S_a+S_b)/k} \mathrm{d}E_a}, \tag{2}$$

where k is a constant and

$$S_i(U_i, B_i, N_i) = kN_i \left[\frac{1}{2}(1+\rho_i)\ln\frac{2}{1+\rho_i} + \frac{1}{2}(1-\rho_i)\ln\frac{2}{1-\rho_i}\right], \tag{3a}$$

$$A_i = \frac{1}{\mu_B B_i \sqrt{2\pi N_i(1-\rho_i^2)}}, \tag{3b}$$

$$\rho_i = \frac{U_i}{N_i \mu_B B_i}, \tag{3c}$$

with $i = a, b$. Consider the extensive quantity $x = E_a/N_a$. For given values of B_a, B_b, N_b/N_a and U/N_a, in the limit $N_a \to \infty$ the dominant contribution to equation (2) is

$$\ln p(x) \sim N_a f(x), \tag{4}$$

where $f(x)$ is an extensive quantity.

(a) Determine the function $f(x)$. (1 point)

(b) Show that $f(x)$ is concave.

(2 points)

(c) Determine the Taylor expansion of f around the maximum of $f(x)$. Under what conditions is it justified to truncate the Taylor series after the second order?

(2 points)

12. About entropy (II)

We consider a system of paramagnetic ions with the internal energy

$$U = -N\mu_B B \frac{e^{2\mu_B B/kT} - 1}{e^{2\mu_B B/kT} + 1}. \tag{5}$$

(a) How do the parameter β defined as

$$\beta = \frac{1}{k}\frac{\partial S}{\partial U}, \tag{6}$$

the entropy S and the temperature T change, when the internal energy U (from equation 5) changes continuously from the minimum value $-N\mu_B B$ to the maximum value $+N\mu_B B$?
Hint: the temperature $T = \pm\infty$ should be considered identical, while $T = 0^+$ belongs to the ground state and $T = 0^-$ to the highest state. (2 points)

(b) Exploit the fact that entropy is a concave function of energy to show that two types of systems can be distinguished. The first type has an energy spectrum that is only truncated from below and β varies from $+\infty$ to 0^+. The second type has both an upward and downward curved spectrum and β varies from $+\infty$ to $-\infty$.

(2 points)

(c) Consider two systems of both types with initial temperatures β_a and $\beta_b > \beta_a$. Show that when both systems are brought into thermal contact, in equilibrium the mean temperature β, with $\beta_a < \beta < \beta_b$ is reached. Discuss this result for each of the three possible combinations of the different signs of the temperatures.

Hint: Consider the curves $S_a(U_a)$ and $S_b(U_b)$; starting from the final equilibrium state, where $\beta_a = \beta_b = \beta$, examine the change in temperatures as energy is transferred from one system to the other.

(2 Punkte)