Theorie der Wärme – Statistical Physics (Prof. E. Frey)

Problem set 4

Problem 4.1 Paramagnet (5 pts)

The Hamilton operator for a paramagnet of N particles in an external magnetic field H is

$$\mathcal{H} = -H \sum_{i=1}^{N} \sigma_i, \qquad \sigma_i = \pm 1$$

Calculate the partition sum Z and the free energy F of the system. Discuss the mean energy, entropy, and the heat capacity as a function of temperature. Evaluate the mean magnetization $M = -\partial F/\partial H$ and the magnetic susceptibility $\chi = \partial M/\partial H$. Compare the entropy to the result of the microcanonical ensemble.

Problem 4.2 Harmonic oscillators (5 pts)

For a system of N identical uncoupled oscillators the energy eigenvalues read

$$E = \sum_{k=1}^{N} \hbar \omega (n_k + \frac{1}{2}), \qquad n_k = 0, 1, 2, \dots$$

Evaluate the partition sum and the free energy. Discuss the mean energy, entropy and the heat capacity. For what temperatures can the quantization of the levels be neglected?

Problem 4.3 *typical states* (4 pts)

Consider a thermodynamic system with discrete energy levels. The canonical ensemble assigns probabilities for the microstates k with corresponding energy E_k according to

$$p_k = Z^{-1} \exp\left(\frac{-E_k}{k_B T}\right), \qquad Z = \sum_k \exp\left(\frac{-E_k}{k_B T}\right)$$

Use the thermodynamic identity $F = -k_BT \ln Z = \langle E \rangle - TS$ to eliminate the partition sum Z in favor of the mean energy $\langle E \rangle$ and the entropy S. Show that the probability for a *typical state* k, i.e. a state with an energy close to the mean one, $|E_k - \langle E \rangle| \leq N\epsilon$, fulfills the bounds

$$e^{-S/k_B}e^{-N\epsilon/k_BT} \le p_k \le e^{-S/k_B}e^{N\epsilon/k_BT}$$

Use the extensivity of the heat capacity

$$C_V = \frac{1}{k_B T^2} \langle (E - \langle E \rangle)^2 = \frac{1}{k_B T^2} \sum_k (E_k - \langle E \rangle)^2 p_k$$

to show that in the thermodynamic limit, $N \to \infty$ the *atypical states* have negligible weight, i.e. $\sum' p_k \to 0$, where the prime indicates that the sum is restricted to atypical states. Argue that in the thermodynamic limit all typical microstates are essentially equiprobable, and that the entropy is a measure for the number of these typical states.

Problem 4.4 free energy (3 pts)

Consider the probabilities for microstates k

$$p_k(\beta) = Z(\beta)^{-1} \exp(-\beta E_k), \qquad \beta = 1/k_B T$$

of some thermodynamic system as a function of inverse temperature. Use probabilistic arguments to show

$$Z(\beta) = Z(\beta_0) \langle e^{(\beta_0 - \beta)E} \rangle_0,$$

where $\langle \cdot \rangle_0$ denotes canonical averaging at inverse temperature $\beta_0 = 1/k_B T_0$. Use the definition of the cumulants to show that the corresponding free energies satisfy

$$-\beta F(\beta) = -\beta_0 F(\beta_0) + \sum_{n=1}^{\infty} \kappa_n \frac{(\beta_0 - \beta)^n}{n!}$$

where κ_n are the cumulants of the energy with respect to the probability distribution at β_0 .

Termine für Übungsgruppen: Do 12-14 in T3, 1.3.48 (Franosch) Do 16-18 in T1, 1.3.21 (Parmeggiani, Lattanzi) in englischer Sprache Fr 12-14 in E2, 1.1.53 (Falcke) **Abgabe:** In der Vorlesung vom 22.5.02