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SoSe 05

Set 6
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T IV: Thermodynamik und Statistik
(Prof. E. Frey)

Problem set 6

Problem 6.1 *Brillouin function*

Generalize the spin 1/2 paramagnet to spin J, i.e. for the Hamilton operator of N spins in an external magnetic field H

$$\mathcal{H} = -gH\sum_{i=1}^{N} s_i\,, \qquad s_i = -J, -(J-1), .., (J-1), J\,.$$

Use the canonical ensemble to evaluate the partition sum and free energy. Discuss the mean energy, magnetization, entropy, the heat capacity and the magnetic susceptibility as a function of temperature. Compare with a model of classical spins

$$\mathcal{H} = -\mu H\sum_{i=1}^{N} \cos\theta_i\,, \qquad Z = \int \left[\prod_{i=1}^{N} \frac{(2J+1)d\varphi_i d\cos\theta_i}{4\pi}\right] \exp\left(\frac{-\mathcal{H}}{k_B T}\right)$$

where each spin is characterized by its polar angles (φ_i, θ_i) and averaging is performed over a sphere.

Problem 6.2 *Legendre transformation*

Evaluate the free energy density $f = \mathrm{e} - Ts$ for the spin 1/2 paramagnet as the Legendre transform of the energy density $\mathrm{e}(s)$. Here the entropy density in the microcanonical ensemble reads

$$s(\mathrm{e}) = -k_B \frac{1-\mathrm{e}/H}{2} \ln \frac{1-\mathrm{e}/H}{2} - k_B \frac{1+\mathrm{e}/H}{2} \ln \frac{1+\mathrm{e}/H}{2}\,,$$

and the temperature is defined as $1/T = (\partial s/\partial \mathrm{e})$. Eliminate e and s from the free energy density and express f in terms of the temperature.

Problem 6.3 *Harmonic oscillators*

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

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

Use the canonical ensemble to 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 6.4 *Specific heat*

Starting from the expansion of the free energy F in powers of the inverse temperature $\beta = 1/k_B T$ (Problem 4.4) derive the following relations for the specific heat $C_V = -T(\partial^2 F/\partial T^2)$

$$\begin{aligned}
\langle(\delta E)^2\rangle &= k_B T^2 C_V \\
\langle(\delta E)^3\rangle &= k_B^2 T^2 \frac{\partial}{\partial T}\left[T^2 C_V\right] \\
\langle(\delta E)^4\rangle - 3\langle(\delta E)^2\rangle^2 &= k_B^3 T^3 \frac{\partial}{\partial T^2}\left[T^3 C_V\right] \\
\langle(\delta E)^5\rangle - 10\langle(\delta E)^3\rangle\langle(\delta E)^2\rangle &= k_B^4 T^4 \frac{\partial}{\partial T^3}\left[T^4 C_V\right]
\end{aligned}$$

Here $\delta E = E - \langle E\rangle$ denotes the energy fluctuation. Check your results for the ideal monatomic gas. In what sense can the energy fluctuations be considered as gaussian?