Fachbereich Physik
Freie Universität Berlin
Theoretische Physik

SoSe 02
Set 5
5/22/02

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

Problem set 5

Problem 5.1 *Brillouin function* (4 pts)

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

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

Discuss the mean energy, magnitizazion, 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 characterised by its polar angles (φ_i, θ_i) and averaging is performed over a sphere.

Problem 5.2 *Legendre transformation* (3 pts)

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 5.3 *Pressure ensemble* (3 pts)

Use the NPT (constant pressure) ensemble with the phase space density

$$\rho_P = Z_P^{-1}\exp\left(-\beta\mathcal{H} - \beta PV\right)\,, \qquad Z_P(T,P,N) = \int_0^\infty dV \int \frac{d^{3N}r\,d^{3N}p}{N!h^{3N}}\exp\left(-\beta\mathcal{H} - \beta PV\right)$$

and the definition of averages to show that

$$Z_P(T,P,N) = Z_P(T,P_0,N)\langle e^{\beta(P_0-P)V}\rangle_0\,.$$

Here $\langle\cdot\rangle_0$ denotes averaging with respect to ρ_P at pressure P_0. Derive the corresponding expansion of the free enthalpy $G(T,P,N) = -k_B T\ln Z_P(T,P,N)$ in terms of the cumulants of the volume.

Problem 5.4 *Specific heat* (4 pts)

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?

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 29.5.02