Prof. Dr. M. Sperl
Dr. T. Kranz

WiSe 2016/17

2. Problem Set
Advanced Statistical Physics

Due Date: Thursday, November 3, 10am

Please indicate your name and the number of your group on the first page!

Problem 4 *Hubbard-Stratonovich-Transformation for a long-range Ising-Model* **14 Punkte**

Consider the Ising-model with a pair interaction of “infinite”-range (introduced in the lecture) in a homogeneous external field H with the Hamiltonian

$$\mathcal{H} = -\frac{J}{2N} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} s_i s_j - H \sum_{i=1}^{N} s_i$$

a) To calculate the canonical partition function $Z = \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} e^{-\beta \mathcal{H}}$, perform a Hubbard-Stratonovich-Transformation with an auxiliary field η and justify that Z can be expressed in the following form

$$Z = e^{-\beta J/2} \sqrt{\frac{N}{2\pi \beta J}} \int d\eta \exp\left\{ -N \left(\frac{1}{2\beta J} \eta^2 - \ln[2\cosh(\eta + \beta H)] \right) \right\}$$

b) Consider the function in the exponent $N f(\eta)$. Use the saddle-point approximation (expansion of f) to determine the free energy F.

c) Show that the magnetization $m = -\partial F / \partial H$ for this model is determined by the following implicit equation

$$m = \tanh(\beta J m + \beta H)$$

d) Determine the susceptibility $\chi_0 := \frac{\partial m}{\partial H}\Big|_{H \to 0}$ at zero field.

Problem 5 *Central Limit Theorem* **6 Punkte**

a) Consider the set $\{Z_j\}, j = 1, \ldots, N$ of independent random variables Z_j which all have the same characteristic function $\varphi(k)$. All Z_j have zero mean and variance σ^2. Determine the characteristic function$\varphi_N(k)$ of the sum $S_N = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} Z_j$

b) Show that $\varphi_N(k)$ for $N \to \infty$ is the characteristic function of a Gaussian distribution. What are the mean and the variance of this distribution?

Hint: Use the results of Problem 2 and remember the definition of Euler’s number.

Problem 6 *A Molecular Zipper Model for DNA* **10 Punkte**

Investigate a simplified model for the 'helix-coil' transition in a polypeptide or in DNA: A linear double chain of N pairs of linking segments may open up (unzip) subject to the following energetic constraints:

i) If the segments $1, 2, \ldots, p$ are already open, unlinking segment $(p + 1)$ costs an energy ϵ.

ii) If segment p is linked, unlinking segment $p + 1$ takes infinite energy.

Each open segment can have g energetically degenerate states (e.g., g energetically equivalent orientations of a free hydrogen bond)

a) Show that the canonical partition function of the molecule is given as

$$Z = \frac{1 - x^{N+1}}{1 - x} \quad \text{with } x := g e^{-\epsilon/k_{\mathrm{B}}T}$$

b) Determine the average number of open segments $\langle S \rangle$ for $N \gg 1$. Discuss the behavior of $\langle S \rangle$ close to $x_c = 1$, or the corresponding critical temperature T_c, respectively. What value does $\langle S \rangle$ assume at x_c, and what is the slope of $\langle S \rangle(x)$ there? What is the behavior of $\langle S \rangle$ for $x \gg 1$ and $x \ll 1$?

c) Make a plot of $\langle S \rangle(x)/N$ for $0.1 \leq x \leq 10$ containing three curves for $N = 4$, $N = 16$, and $N = 64$. Use a logarithmic x-axis. Discuss what you observe.