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

WiSe 2016/17

10. Problem Set
Advanced Statistical Physics

Due Date: Thursday, January 12, 10am

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

Problem 28 *Schematic Models* **12 Punkte**

Consider the Debye-Waller factors $f = \phi(t \to \infty)$ for two schematic models. Determine and plot the physically relevant solutions f of the schematic models and sketch the phase diagram spanned by the model parameters.

a) The F_{12}-model, where

$$\mathcal{F}[\phi](t) = v_1\phi(t) + v_2\phi^2(t)$$

is parametrized by v_1 and v_2

b) The F_{13}-model, where

$$\mathcal{F}[\phi](t) = v_1\phi(t) + v_3\phi^3(t)$$

is paramterized by v_1 and v_3.

Problem 29 *Cumulants* **6 Punkte**

For a random variable X the moment-generating function $M(t)$ and the cumulant-generating function $K(t)$ are defined as follows

$$M(t) := \langle \exp(tX) \rangle \equiv 1 + \sum_{n=1}^{\infty} \frac{t^n}{n!} \langle X^n \rangle$$

$$K(t) := \ln\langle \exp(tX) \rangle =: \sum_{n=1}^{\infty} \frac{t^n}{n!} \kappa_n$$

where κ_n are the *cumulants* of X.

Show that

$$\langle X \rangle = \kappa_1 \qquad \langle X^2 \rangle = \kappa_2 + \kappa_1^2$$

$$\langle X^3 \rangle = \kappa_3 + 3\kappa_2\kappa_1 + \kappa_1^3 \qquad \langle X^4 \rangle = \kappa_4 + 4\kappa_3\kappa_1 + 3\kappa_2^2 + 6\kappa_2\kappa_1^2 + \kappa_1^4$$

Problem 30 *Stochastic Copolymerization* **12 Punkte**

A linear, binary copolymer is a chain of segments comprised of the chemical species A and B (e.g., ●●○●○ $\cdots$). The synthesis of such a sequence can often be modelled as a *Markov process*: The species of a newly added segment only depends on the species of the last segment in the chain and not on any of the previous segments.

Let $p_A(s), p_B(s) = 1 - p_A(s)$ be the probability that segment s is of species A or B, respectively. Using the vector $\boldsymbol{v}(s) := \big(p_A(s), p_B(s)\big)$, we can relate the probabilities of segement $s+1$ to the probabilities of segment s

$$\boldsymbol{v}(s+1) = \mathsf{M} \cdot \boldsymbol{v}(s)$$

via the matrix

$$\mathsf{M} := \begin{pmatrix} 1 - p(B|A) & p(A|B) \\ p(B|A) & 1 - p(A|B) \end{pmatrix}$$

where $p(A|B)$ is the conditional probability for a segment of species A to bind to a chain-end of species B.

Remark: You can also use this approach to generate mathematically well defined (Christmas) decoration.

a) Determine the stationary probability vector $\boldsymbol{v}^* = (p, 1-p)$ that is independent of the segment index s. Argue why under stationary reaction conditions (i.e., the concentrations of the free A and B segments are kept constant throughout the polymerization), p is also the global probability for a segment of species A, including both free and bound segments.

b) Calculate the other eigenvalue λ of M and determine its range. In which limit do we obtain strictly alternating copolymers, ○●○●○ $\cdots$?

c) Rewrite M in terms of p and λ and complete the diagonalization of M for $\lambda \neq -1$. Use powers of M to calculate the conditional probabilities $q_{\Delta s}(A|B)$ to find a segment of species A at segement s, given that the segment at $s \pm \Delta s$ is of species B.