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Saarbrücken, den 26.01.2024

Blatt 12 zur Theoretischen Physik IV, WS 2023/2024

(Abgabe bis 02.02.2024, 8:30 Uhr)

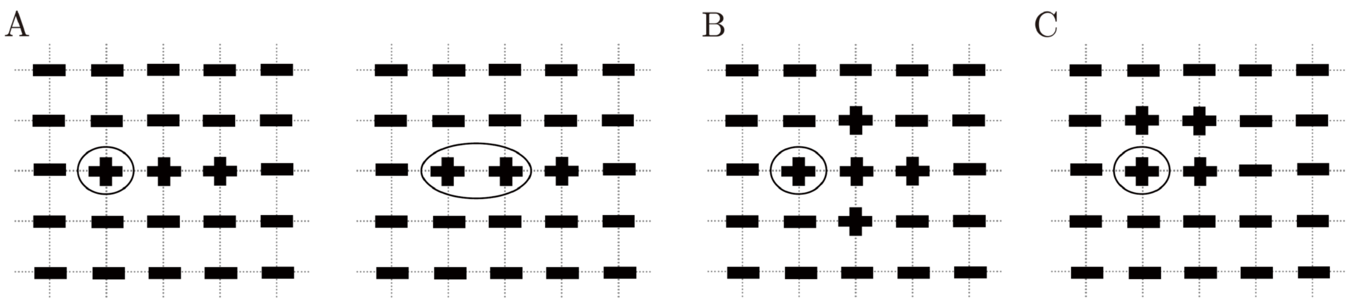
Exercise 1: Wolff algorithm

Consider the two-dimensional Ising model ($s_i = \pm 1$) with periodic boundary conditions. The energy of a configuration is given by

$$E = -\sum_{\langle i,j \rangle} s_i s_j,$$

where the sum runs over all pairs (i, j) of neighboring spins.

The Wolff algorithm is divided into the following steps:
(i) Select a random spin as the initial cluster.
(ii) If the spins inside and outside the cluster are nearest neighbors and aligned in parallel (i.e. $++$ or $--$), then the outer spin will be added to the cluster with probability $1 - \exp(-2\beta)$. This step is repeated until all possible connections have been checked.
(iii) Flip all spins within the cluster.
(iv) Go back to step (i).
As an example, consider panel A of the following figure. Starting with the left configuration with the cluster indicated by the circle, step (ii) can lead to the cluster on the right with probability $\big(1 - \exp(-2\beta)\big) \times \exp(-2\beta)$.



a) Find all the possibilities of cluster formation and the associated probabilities in the two examples B and C. The randomly selected spins from step (i) are marked.

b) Show that this algorithm satisfies the detailed balance condition.

c) Show that magnetic susceptibility can be measured by the cluster size.

[3+5+4= 12 Points]

Exercise 2: One-dimensional Ising model

The one-dimensional Ising model for N spins with nearest neighbor interaction is given by the Hamiltonian function

$$H = -\frac{J}{2}\sum_{j=1}^{N}\sigma_j\sigma_{j+1} - h\sum_{j=1}^{N}\sigma_j$$

where h denotes an external magnetic field. The spin variables σ_j take on the values $+1$ and -1. In the following, periodic boundary conditions are used, i.e. $\sigma_{N+1} = \sigma_1$.

a) Show that the partition function of this Ising model is given by $Z_N = Tr(\tau^N)$, where the transfer matrix is

$$\tau = \begin{pmatrix} \exp(\frac{\beta J}{2} + \beta h) & \exp(-\frac{\beta J}{2}) \\ \exp(-\frac{\beta J}{2}) & \exp(\frac{\beta J}{2} - \beta h) \end{pmatrix},$$

with $\beta = 1/k_B T$.

b) Show that in the thermodynamic limit $N \to \infty$, the free energy per spin is given by

$$f(T,h) = -k_B T \ln \lambda_1,$$

where λ_1 denotes the larger eigenvalue of τ. Calculate the eigenvalues of τ.

c) Calculate the magnetization $m = -\frac{\partial f}{\partial h}$.

[3.5+4.5+4= 12 Points]

Exercise 3: Three-spin interaction

In some materials, a three-spin interaction term may be essential. Consider a one-dimensional model given by the Hamiltonian

$$H = -J\sum_{i=2}^{N-1} s_{i-1}s_i s_{i+1},$$

with $s_i = \pm 1$.

a) Calculate the partition function.

b) Calculate the free energy F.

c) Determine the entropy in the limit $T \to \infty$.

[4+1+3= 8 Points]

Exercise 4: Potts model

The Potts model is closely related to the Ising model. In the following we will discuss the one-dimensional Potts model

$$H = -J\sum_{i=1}^{N-1} \delta_{s_i s_{i+1}},$$

where the spins s_i take the values 0 or 1 and δ represents the Kronecker delta.

a) Calculate the partition function.

b) Determine the thermal average of the Hamiltonian $\langle H\rangle = \frac{\sum H\,\mathrm{e}^{-\beta H}}{Z_N}$ in the limit of a very long chain. Hint: Assume open boundary conditions.

c) Test your answer for part (b) in the limit $\beta \to \infty$.

[4+3+1= 8 Points]