# Übungen zur

## **Computational Nanoscience**

- Blatt 9 -

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 $zum \ 22.06.2016$ 

### Aufgabe 1) Ising Model

What is the difference between the Ising and Heisenberg model? Which model is more suitable for magnetic phase transitions?

### Aufgabe 2) Partition Function

Find the partition function, free energy and magnetization for canonical ensemble of one spin in magnetic field at temperature T. Discuss the difference between the quantum and classical problem.

#### Aufgabe 3) Metropolis algorithm

Proof that the Metropolis algorithm for calculating probability  $W_{ij}$  of going from state i to state j:

$$W_{ij} = min(1, \frac{P_j}{P_i}),$$

where the  $P_i = e^{-\beta E_i}$  and  $E_i$  is the energy of state *i*, satisfied the detailed balance condition:

$$P_i W_{ij} = P_j W_{ji}.$$

What is the physical meaning of this condition?