Introduction

Prussian Blue Analogues

Monte Carlo Method

In order to get a macroscopic view of a system, of which we know all possible states and the hamiltonian of each state $\mathcal{H}(\sigma)$, we make the following observation. For this report we start from the observation that the probability of a state occuring $\rho(\sigma)$ at some temperature T is proportional to $\exp\left(-\frac{\mathcal{H}(\sigma)}{k_b T}\right)$ Additional we know that the sum of all probabilities must be 1.

$$1 = \sum_{\sigma\in\Omega} \frac{\exp\left(-\frac{\mathcal{H}(\sigma)}{k_b T}\right)}{Z} = \frac{1}{Z}\sum_{\sigma\in\Omega} \exp\left(-\frac{\mathcal{H}(\sigma)}{k_b T}\right)$$

$$\Rightarrow Z = \sum_{\sigma\in\Omega} \exp\left(-\frac{\mathcal{H}(\sigma)}{k_b T}\right)$$

Methods

Results

Discussion

Appendix

Considerations about the parameter space

From statistical mechanics we know that the partition function Z describes the system completely. Lets consider a system where the hamiltonian $\mathcal{H}$ can be described by the sum of two energies multiplied by the functions c_1 and c_2 on the state of the system σ.

$$\mathcal{H}(\sigma) = J_1 c_1(\sigma) + J_2 c_2(\sigma)$$

Lets define two new variables J' and T' such that $J_2 J' = J_1$ and $J_2 T' = k_b T$.

$$\begin{aligned} Z &= \sum_{\sigma} \exp\left(-\frac{\mathcal{H}(\sigma)}{k_b T}\right) \\ &= \sum_{\sigma} \exp\left(-\frac{J_1 c_1(\sigma) + J_2 c_2(\sigma)}{k_b T}\right) \\ &= \sum_{\sigma} \exp\left(-\frac{\cancel{J_2} J' c_1(\sigma) + \cancel{J_2} c_2(\sigma)}{\cancel{J_2} T'}\right) \\ &= \sum_{\sigma} \exp\left(-\frac{J' c_1(\sigma) + c_2(\sigma)}{T'}\right) \end{aligned}$$

Thus we see that the system only depends on two parameters.