FYS3150 Computational Physics - Project 4

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This is an abstract

INTRODUCTION

THEORY, ALGORITHMS AND METHODS

The Ising Model

In its simplest case, a paramagnet is described as a lattice of noninteracting dipole moments, each in a state up or down. Where the energy of the system is proportional to the sum of the spins, up or down of each noninteracting constituent.

The Ising model is a natural extension to this, by adding local interaction between directly neighboring spins (See fig. 1), such that the energy of the system is instead proportional to the sum of each spin coupled with its nearest neighbors, which gives a much more accurate description of the system compared to the simple case of an ideal paramagnet.

Or more precisely, the energy is given by Eqn. 1, where $s_i \in \{-1, 1\}$ and J is a coupling constant.

$$E = -J \sum_{<kl>} s_k s_l \tag{1}$$

In this summation, the notation $< kl >$ means that for each k, we take the sum over each direct neighbor. However, in this project the lattice will be treated as pseudo-continuous where any spin-sites located at an edge, will also interact with the spin-site on the opposing edge, illustrated in Fig. 2, which strictly speaking constitutes having periodic boundary conditions.

We also have the magnetization, $\mathcal{M}$, which is simply the sum of all spins

$$\mathcal{M} = \sum_i s_i$$

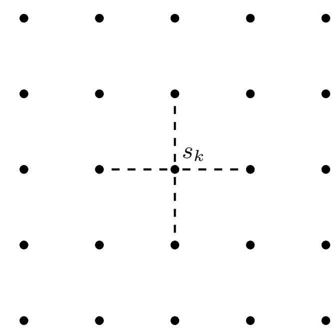

FIG. 1: Section of a 2D lattice, where each spin-site is represented by a dot. In the Ising model, spin-site k will only interact with its directly neighbouring spin-sites, connected by dotted lines in this diagram

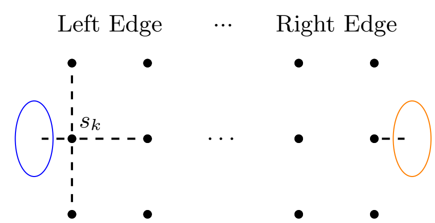

FIG. 2: Spin-site k, located at the left edge of the lattice interacting with its direct neighbors, as well as the spin site on the opposite edge of the lattice

Boltzmann Statistics

From Eqn. 1 we can derive many thermodynamic quantities using Boltzmann statistics, where we have the probability of the system being in some specific macro-state[1]

$$\mathcal{P}(E_s) = \frac{1}{Z} e^{-\beta E_s} \tag{2}$$

With $\beta \equiv \frac{1}{k_B T}$, the thermodynamic beta and Z, the partition function, acting as a normalization factor given by[2]

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[1] Macroscopic states being characterized by their energy, meaning i could just as well have written "... the probability of the system having some speciffic energy"

[2] Strictly speaking, this is the partition function for a system with discrete macro-states. In the continuous case, simply replace sums with integrals.

$$Z = \sum_s e^{-\beta E_s} \tag{3}$$

From this, the expectation value of some quantity X, with a set of known macrostates X_s can be computed by

$$\langle X \rangle = \sum_s X_s \mathcal{P}(E_s) = \frac{1}{Z} \sum_s X_s e^{-\beta E_s} \tag{4}$$

Using this, we can compute the specific heat capacity, C_V by computing the expectation values of E, E^2 [1], related by the following expression

$$C_V = \frac{\left\langle E^2 \right\rangle - \left\langle E \right\rangle^2}{k_B T^2} \tag{5}$$

Where $\left\langle X^2 \right\rangle - \left\langle X \right\rangle^2$ is recognized as the square of the standard deviation in the normal distribution, σ_X^2.

In a similar fashion, the magnetic susceptibility, χ, is calculated from $\sigma_{\mathcal{M}}^2$ [1]

$$\chi = \frac{\sigma_{\mathcal{M}}^2}{k_B T} \tag{6}$$

For more details on the Ising model, or Boltzmann statistics refer to Schroeder [2, Chapters 6, 8.2], Hjorth-Jensen [1], or similar introductory texts on the topic.

Analytic solution of 2x2 Lattice

Consider now a 2x2 lattice, each with spin ± 1. The energy of the system for a particular micro-state is given by Eqn. 1.

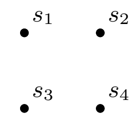

FIG. 3: A 2×2 lattice of spin-sites

The Metropolis Algorithm

RESULTS AND DISCUSSIONS

CONCLUSIONS

[1] M. Hjorth-Jensen, “Computational physics lectures: Statistical physics and the ising model,” (2017).

[2] D. V. Schroeder, *An Introduction to Thermal Physics*, 1st ed. (Pearson, 1999).