FYS4130: Obligatory Assignment 2

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Abstract

The following sections attempt to give answers to Assignment 2 in the UiO course FYS4130: Statistical Mechanics. Exercise 1 addresses the 1 dimensional Ising Model, whereas exercise 2 solves the Ising model numerically with Monte Carlo (MC) simulations. The numerical results replicate the analytical solutions. All relevant code can be found at my Github page [1].

Problem 1: 1 Dimensional Ising Model

In this problem a 1 dimensional Ising model is explored, with periodic boundary conditions (PBC). A spin can take on the values

$$\sigma_i = \begin{cases} 1, \\ -1, \end{cases} \tag{1}$$

where the index belongs to a spin along the 1D chain of L spins, $i \in [0, L-1]$. Due to PBC, $\sigma_0 = \sigma_L$. One can think of the Ising model as a ferromagnetic model, of interacting electrons in a metal, hence the spin up/down configurations. The Hamiltonian then becomes

$$H = -J \sum_{i=0}^{L-1} \sigma_i \sigma_{i+1}, \tag{2}$$

in which $J > 0$ is the coupling constant between two spins. See [2] for more details.

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a) Finding <m>

The magnetization per site is defined as

$$m = \frac{1}{L}\sum_{i=0}^{L-1}\sigma_i. \tag{3}$$

Thus one can write the *average* magnetization per site $< m >$ as

$$< m >= \frac{1}{L}\sum_{i=0}^{L-1} < \sigma_i > . \tag{4}$$

Since the Hamiltonian (eq. 2) is translationally invariant, the average spin $< \sigma_i >$ should be the same. As a result

$$< m >= \frac{1}{L} < \sigma_i > \sum_{i=0}^{L-1} 1 =< \sigma_i > . \tag{5}$$

Thus, to find the average magnetization per site, we need to find the average spin per site. This can be done Boltzmann statistics, and the per site partition function Z_i. For a 1D chain, spin i has two neighbours, so that the over energy contribution is

$$H_i = -J(\sigma_{i-1}\sigma_i + \sigma_i\sigma_{i+1}). \tag{6}$$

All the possible configurations for these three particles, due to spin up/down (eq. 1), are

$$Z_i = \sum_{\sigma_{i-1}=\pm 1}\sum_{\sigma_i=\pm 1}\sum_{\sigma_{i+1}=\pm 1}\exp(-\beta H_i) \tag{7}$$

Hence, the magnetization per site, should be independet of index i, and

$$< \sigma_i >= \frac{1}{Z_i}\sum_{\sigma_{i-1}=\pm 1}\sum_{\sigma_i=\pm 1}\sum_{\sigma_{i+1}=\pm 1}\sigma_i \exp(-\beta H_i). \tag{8}$$

As a function of T/J set $\beta = 1/T$, and J and $k_b$to 1. For the three spins, there is one configuration each of all spins up and down, respectively. In addition there is a total of four ways to $H_i = 0$. Thus

$$Z_i = 1\cdot e^{\beta(1+1)} + 2\cdot e\beta(-1+1) + 1\cdot e^{\beta(-1-1)} + 2\cdot e^{\beta(+1-1)} \tag{9}$$

$$= e^{2\beta} + 4e^0 + e^{-2\beta} = 4 + 2\cosh 2\beta. \tag{10}$$

Summing up all the different spin up/down configurations in the nominator, yields

$$< \sigma_i >= \frac{1}{4+2\cosh 2\beta}\left[(+1)\left(e^{-2\beta}+2e^{0}+e^{2\beta}\right)+(-1)\left(e^{-2\beta}+2e^{0}+e^{2\beta}\right)\right]=0. \tag{11}$$

Hence, the per site average magnetization should be 0.

b) Finding the correlation function C(r)

For a canonical ensemble (NVT held fixed), the partition function Z for the 1D Hamiltonian H (eq. 2), becomes

$$Z=\sum_{\{\sigma\}}\exp\left(-\beta H(\{\sigma\})\right)\overset{\text{exp. prop.}}{=}\sum_{\{\sigma\}}\prod_{i=0}^{L-1}\exp\left(\beta\sigma_i\sigma i+1\right). \tag{12}$$

The right hand side of eq. 12 can be written in terms of the transfer matrix $T(\sigma_i,\sigma_{i+1})$. With this notation

$$Z=\sum_{\{\sigma\}}\prod_{i=0}^{L-1}T(\sigma_i,\sigma_{i+1}), \tag{13}$$

in which T contains all possible values of the exponent,

$$T(\sigma_i,\sigma_{i+1})=\begin{bmatrix}\exp(\beta) & \exp(-\beta)\\ \exp(-\beta) & \exp(\beta)\end{bmatrix}. \tag{14}$$

Eq. 14 is a product of all transfer matrices. Due to symmetries in the Hamiltonian (eq. 2), the T matrices are all the same. After L multiplications, by enforcing PBCs, $T^L(\sigma_0,\sigma_L)=^L(\sigma_0,\sigma_0)$. As a result

$$Z=\sum_{\sigma=\pm1}T^L(\sigma_0,\sigma_0). \tag{15}$$

Since T is a square matrix with linearly independent column vectors, one can decompose the matrix into its eigenvalue decomposition $T=R^{-1}DR$, where $D=diag(\{\lambda_i\})$ and $RR^{-1}=R^{-1}R=I_2$. Thus

$$T^L=R^{-1}DR\cdot R^{-1}DR\cdots R\cdot R^{-1}RDR \tag{16}$$

$$=R^{-1}D^LR, \tag{17}$$

and the trace of $T^L(\sigma_0,\sigma_0)$ becomes

$$Z = Tr\left(T^L(\sigma_0,\sigma_0)\right) = Tr(D^L) = \lambda_+^L + \lambda_-^L, \tag{18}$$

since the trace is invariant under cyclic permutation of matrices and $R^{-1}R = I_2$.
Finding the eigenvalues of T involves solving

$$\begin{vmatrix} \exp(\beta) & \exp(-\beta) \\ \exp(-\beta) & \exp(\beta) \end{vmatrix} = 0, \tag{19}$$

and using the ABC formula to find the roots $\lambda_\pm$. The results are

$$\lambda_+ = 2\cosh\beta \tag{20}$$
$$\lambda_- = 2\sinh\beta, \tag{21}$$

so that the partition function for the 1D Ising model becomes

$$Z = \lambda_+^L + \lambda_-^L = 2^L\left(\cosh^L\beta + \sinh^L\beta\right). \tag{22}$$

The correlation function $C(r)$ is defined as

$$C(r) = <\sigma_0\sigma_r> - <\sigma_0><\sigma_r>. \tag{23}$$

It is the covariance of per site magnetization between spin 0 and a given spin $r \in [1, L-1]$. From eq. 11 $<\sigma_0> = <\sigma_r> = 0$, thus C(r) reduces to

$$C(r) = <\sigma_0\sigma_r> = \frac{1}{Z}\sum_{\{\sigma\}} \sigma_i\sigma_j \exp(-\beta H(\{\sigma\})). \tag{24}$$

To find this quantity, it's easier to use the bra-ket notation, so that Z can be written as

$$Z = \sum_{\sigma_0}\sum_{\sigma_1}\cdots\sum_{\sigma_{L-1}} \langle\sigma_0|T|\sigma_1\rangle\langle\sigma_1|T|\sigma_2\rangle\cdots\langle\sigma_0|T|\sigma_{L-1}\rangle \tag{25}$$
$$= \sum_{\sigma_0}\langle\sigma_0|T^L|\sigma_0\rangle = Tr(T^L), \tag{26}$$

where the identity $\sum_{\sigma_i}|\sigma_i\rangle\langle\sigma_i| = I$ is used. Note that the trace can be written in terms of the eigenbasis $|\pm\rangle$. In a similar way, eq. 24 can be rewritten as

$$C(r) = < \sigma_{i=0}\sigma_{j=r} > = \frac{1}{Z} Tr\left(T^0 \sigma_k T^{r-0} \sigma_k T^{L-r}\right) \tag{27}$$

$$= Tr\left(\sigma_k T^r \sigma_k T^{L-r}\right). \tag{28}$$

In the equation above σ_k is an operator which picks out the possible up(+)/down(-) configurations of σ_0 and σ_r, with the effect $\sigma_k |\pm\rangle = -|\mp\rangle$. As a result, by writing the trace in terms of eigenstates, C(r) becomes

$$Z \cdot C(r) = \langle +| \sigma_k T^r \sigma_k T^{L-r} |+\rangle + \langle -| \sigma_k T^r \sigma_k T^{L-r} |-\rangle \tag{29}$$

$$= \lambda_+^{L-r} \langle +| \sigma_k T^r \sigma_k |+\rangle + \lambda_-^{L-r} \langle -| \sigma_k T^r \sigma_k |-\rangle \tag{30}$$

$$= (-1)\cdot(-1)\cdot\lambda_+^{L-r} \langle -| T^r |-\rangle + (-1)\cdot(-1)\cdot\lambda_-^{L-r} \langle +| T^r |+\rangle \tag{31}$$

$$= \lambda_+^{L-r}\lambda_-^r + \lambda_-^{L-r}\lambda_+^r. \tag{32}$$

Thus, inserting for Z from eq. 22, for a 1D Ising chain,

$$C(r) = \frac{1}{\lambda_+^L + \lambda_-^L}\left(\lambda_+^{L-r}\lambda_-^r + \lambda_-^{L-r}\lambda_+^r\right). \tag{33}$$

For $L \to \infty$, then $\lambda_-^{L-r} \approx \lambda_-^L$ and $\lambda_+^{L-r} \approx \lambda_+^L$, assuming $L >> r$. In addition since $\lambda_- < \lambda_+$, as $L \to \infty$, the ratio $(\lambda_-/\lambda_+)^L \to 0$. As a result, C(r) in the thermodynamic limit becomes

$$C(r) = \lim_{L\to\infty} \frac{1}{\lambda_+^L(1 + (\lambda_-/\lambda_+)^L)}\left(\lambda_+^{L-r}\lambda_-^r + \lambda_-^{L-r}\lambda_+^r\right) \tag{34}$$

$$\approx \frac{1}{\lambda_+^L}\left(\lambda_+^{L-r}\lambda_-^r + \lambda_-^{L-r}\lambda_+^r\right) \tag{35}$$

$$= \left(\frac{\lambda_-}{\lambda_+}\right)^r + \left(\frac{\lambda_-}{\lambda_+}\right)^L \left(\frac{\lambda_+}{\lambda_-}\right)^r \approx \left(\frac{\lambda_-}{\lambda_+}\right)^r \tag{36}$$

$$= \tanh(\beta). \tag{37}$$

In the limit $T \to 0$, $\beta \to \infty$ and $C(r) = 1$ in this limit. It means that in the thermodynamic limit, as the temperature approaches zero, spins align. Yet, since this only occurs as $T \to 0$, it can't really be called a phase transition.

Problem 2: Monte Carlo Simulation of 1D and 2D Ising Model

Monte Carlo simulations take advantage of the fact that integrals can be interpreted as averages. In this context, Monte Carlo (MC) simulations, or more specifically Markov

chain Monte Carlo simulations, are applied to the 1D and 2D Ising model, with PBC. Instead of finding the observable O analytically

$$< O >= \frac{1}{Z}\sum_{O} O_i \exp(-\beta H), \tag{38}$$

experiments are carried out numerically as

$$\overline{O} = \frac{1}{N}\sum_{i=1}^{N} O_{s_i}. \tag{39}$$

At equilibrium, there must be as many spins going from spin up to down, as vice versa. As a result, the observables O_{s_i} are governed by the detailed balance [2]

$$P(s \to s')W(s) = W(s)P(s' \to s), \tag{40}$$

where P is the probability of transitioning from a state to another, and the W's is the probability density of a state. For a system at equilibrium, the net flux of particles $N_{s\to s'}$ and $N_{s'\to s}$ must be the same. From eq. 40

$$\frac{N_s'}{N_s} = \frac{W(s')}{W(s)}. \tag{41}$$

As result, the MC simulation will reproduce the true distribution, when approaching the equilibrium of the system numerically, by describing the transition probability P correctly. How P is chosen depends on the sampling algorithm chosen. The first-developed algorithm was the Metropolis algorithm, but here the single cluster Wolff algorithm (see [3]) - inspired by Swendsen and Wang clustering - is used, in which

$$P = 1 - e^{-2\beta J}. \tag{42}$$

By applying Markov chains the averages of observables can be obtained numerically, by ensuring ergodicity [2]. The code can be found at [1]. The results are given below. The results are scaled by the system size, to eliminate the extensive L dependency of the magnetization. In addition $J = 1$ and $k_b = 1$.

b) Correlation function 1D Ising Model

The correlation function is regional for temperatures higher than 0.5, which means that as $T \to 0$, more spins align over a larger spin interval (fig. 1).

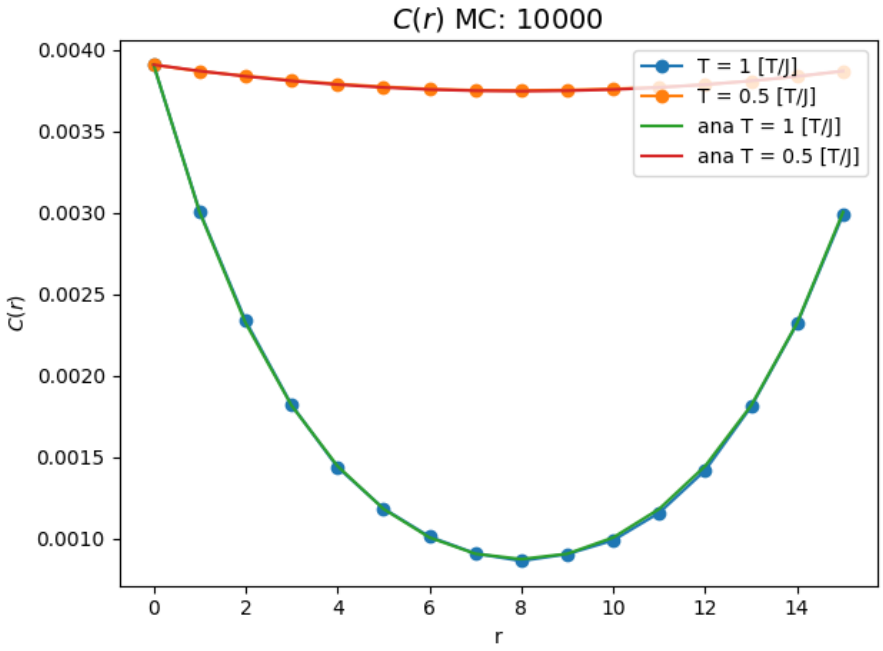

Figure 1: **Correlation function**. $C(r)$ as a function of spin index r for a 16 spin 1D Ising chain.. The correlation function obtained numerically is in agreement with the analytical results found in eq. 24. MC parameters - Nbins:10, MC cycles: 10 000, calibration cycles: 20 000.

c)-d) <m> and <m^2> as a function of temperature

For the 2D Ising model, $< m^2 > \to 1$ as $T \to 0$, and $< m^2 > \to 0$ as $T \to \infty$ fig. 2. This can be explained by the phase transition occuring around $T_c \approx 2.269$. For $T < T_c$, the spins are generally more aligned across MC cycles, so the value of $M_{S_i}^2$, which is collected as the sum of spins values squared for each MC cycle, is high. However, for $T > T_c$, spins are more often anti-aligned and $< m^2 > \to 0$ (fig- 2). The per site magnetization, $< m >$, remains around zero for each temperature, because even though spins are aligned, they have an equal probability of being aligned up(+) or down (-).

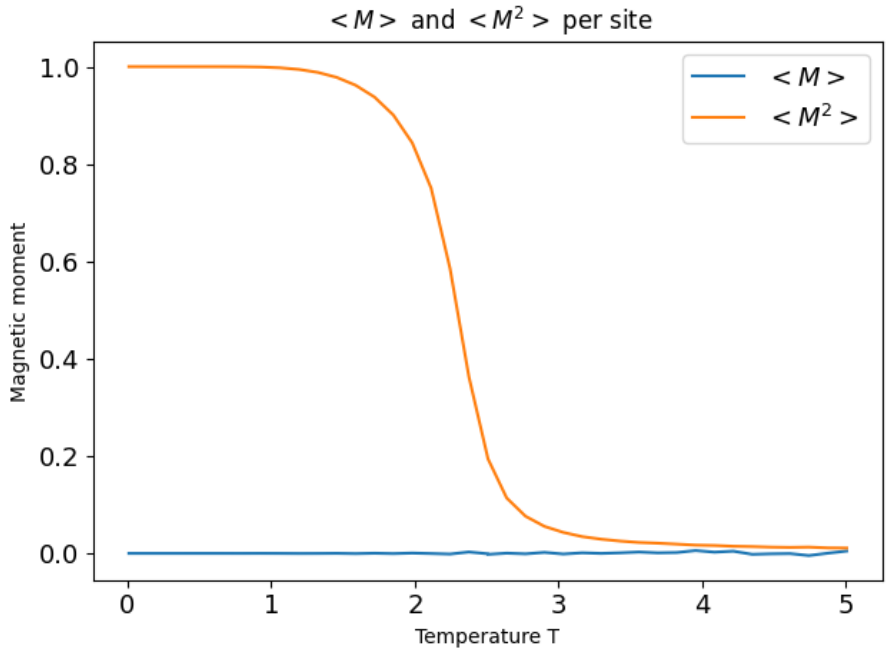

Figure 2: **Per site magnetization for a 16×16 grid**. $< m >$ and $< m^2 >$ as a function of temperature (T/J). 4 OpenMP ranks were used. Per temperature MC parameters - Nbins:10, MC cycles: 10 000, calibration cycles: 20 000.

e) Finite size scaling arguments for obtaining T_c

The finite size scaling arguments used in obtaining T_c by plotting averages of m as a function of temperature, with $L = \{8, 16, 32\}$ is described by Binder [4].

The basic idea is that when the the system size is changed, i.e. the microscopic properties of the system is not the same, the macroscopic properties remain the same up to some constant factor. This factor can depend on the dimensionality d of the system, s.t. some property $\tilde{Q}$ as a function of a set of variables$\{K\}$ is scalable

$$\tilde{Q}(\{K\}) = S^{-d}\tilde{Q}(\{KS^{y_k}\}), \tag{43}$$

where S and $y_k \in \mathbb{R}$. This is a result of renormalization group (RG) theory. For $\Gamma(t, L^{-1})$, then we can use the argument that

$$\Gamma(t, L^{-1}) = S\Gamma(tS^{y_t}, L^{-1}S), \tag{44}$$

where L is the linear system size, and if T_c is the critical temperature

$$t = \frac{T - T_c}{T_c}. \tag{45}$$

By choosing $S = L$, one gets a function of 1 variable

$$\Gamma(t, L^{-1}) = L\Gamma(tL^{y_t}, 1). \tag{46}$$

For temperatures close to T_c, t is close to zero. Thus, one can Taylor expand $\Gamma(tL^{y_t}, 1) = g(tL^{y_t})$, so that

$$\Gamma(t, L^{-1}) = L\left(g(0) + tL^{y_t}Lg'(0) + \mathcal{O}(t^2)\right), \tag{47}$$

or

$$\frac{\Gamma(t, L^{-1})}{L} = \left(g(0) + tL^{y_t}Lg'(0) + \mathcal{O}(t^2)\right). \tag{48}$$

At the critical temperature T_c, then $t = 0$, and the right hand side expression is independent of L. As a consequence, by scaling Γ by the system size L, eq. 48 must hold, and $\Gamma(t, L^{-}1)$ curves must have equal values at T_c regardless of system size!

f) Critical temperature for the 2D Ising lattice

The critical temperature can be estimated from the crossing of the function $\Gamma(T)$ at T_c for different lattice sizes, as predicted from finite scaling arguments (eq. 48). The result of fine resolution MC simulations for $L = \{8, 16, 32\}$ is presented in fig. 3. The analytical prediction is replicated by the MC simulation.

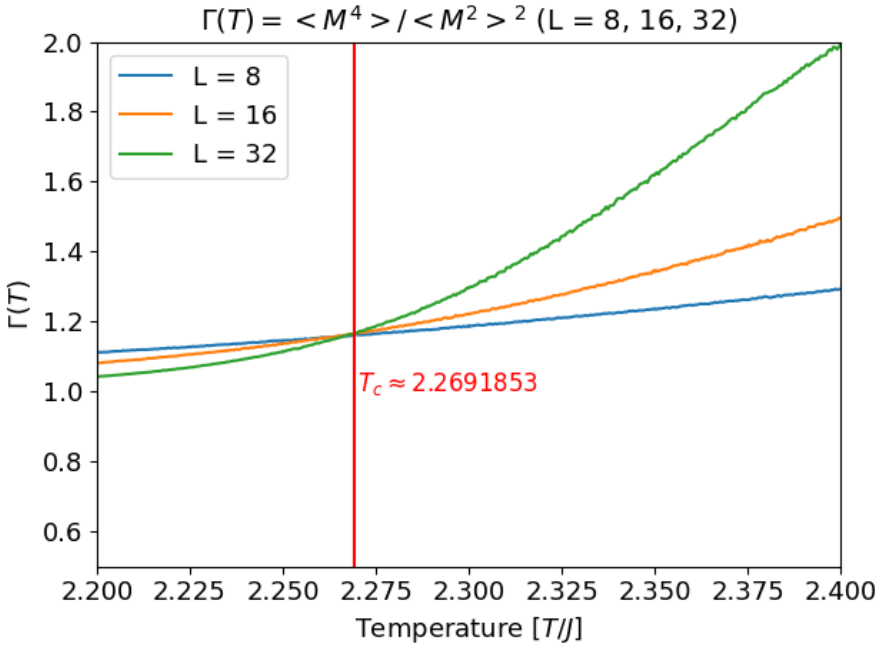

Figure 3: **Critical temperature for the 2D Ising model**. $< m >$ and $< m^2 >$ as a function of temperature (T/J). $T \in [2.20, 2.40]$. 4 OpenMP ranks were used with 100 temperature values per rank. Per temperature MC parameters - Nbins:10, MC cycles: 50 000, calibration cycles: 20 000.

References

[1] Lasse Steinnes. Assignment2-GIT, 2020.

[2] Robert H. Swendsen. *An Introduction to Statistical Mechanics and Thermodynamics, 2nd edition*. Oxford University Press, 2020.

[3] Ulli Wolff. Collective monte carlo updating for spin systems. *Phys. Rev. Lett.*, 62:361–364, Jan 1989.

[4] K. Binder. Finite size scaling analysis of ising model block distribution functions. *Condensed Matter*, pages 119–140, 1981.