Project 4 FYS4150

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Abstract

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2.1 Introduction to statistics

$$P(a \le X \le b) = \int_b^a p(x)\,dx \tag{1}$$

$$\langle h \rangle_X = \int h(x)\,p(x)\,dx \tag{2}$$

$$\langle x^n \rangle = \int x^n\,p(x)\,dx \tag{3}$$

$$\langle x \rangle = \int x\,p(x)\,dx \tag{4}$$

2.2 Magnet - properties

Energy, magnetic moment, susceptibility, heat capacity.

$$T_C(L) - T_C(L=\infty) = aL^{-1/\nu} \tag{5}$$

Boltzman Markhow chain - convergance

L=2 case:

Table 2.1: text

No spin up	Deg	Energy	Magnetization
0	1	-8J	-4
1	4	0	-2
2	4	0	0
2	2	8J	0
3	4	0	2
4	1	-8J	4

Error Random number

The partition function:

$$Z = \sum_i^M e^{-\beta E_i} = e^{-\beta 8J} + e^{-\beta 8J} + e^{\beta 8J} e^{\beta 8J} + 12$$

$$= 2e^{-\beta 8J} + 2e^{\beta 8J} + 12 = 4\left(\frac{e^{-\beta 8J} + e^{-\beta 8J}}{2}\right) + 12$$

$$= 4\cosh\left(\beta 8J\right) + 12$$

The energy:

$$\langle E \rangle = k_B T^2 \left(\frac{\partial Z}{\partial T}\right)_{V,N}$$

$$= k_B T^2 \frac{\partial}{\partial T}\left[\ln\left(4\cosh\left(\frac{8J}{k_B T}\right) + 12\right)\right]$$

$$\frac{\partial \ln Z}{\partial T} = \frac{\partial Z}{\partial \beta}\frac{\partial \beta}{\partial T} = \frac{\partial \ln Z}{\partial \beta}\left(\frac{-1}{k_B T^2}\right)$$

$$\langle E \rangle = -\left(\frac{\partial Z}{\partial \beta}\right)_{V,N} = -\frac{\partial}{\partial \beta}\ln\left[4\cosh\left(8J\beta\right) + 12\right]$$

$$= \frac{-1}{4\cosh(8J\beta) + 12} 4\sinh(8J\beta) 8J\beta$$

$$= \frac{-8J\sinh(8J\beta)}{3\cosh((J\beta) + 4}$$

Following the same method, we found that:

$$\langle |M| \rangle = \frac{1}{Z}\sum_i^M M_i e^{\beta E_i} = \frac{(8J)^2\cosh(8J\beta)}{\cosh(8J\beta) + 3}$$

$$\langle M \rangle = 0$$

$$\langle E^2 \rangle = \frac{8\left(e^{8J\beta} + 1\right)}{\cosh(8J\beta) + 3}$$

$$\langle M^2 \rangle = \frac{1}{Z}\left(\sum_i^M M_i^2 e^{\beta E_i}\right) = \frac{2\left(e^{8J\beta} + 2\right)}{\cosh(8J\beta) + 3}$$

We can use these to calculate the rest:

$$C_V = k\beta^2\left(\langle E^2 \rangle - \langle E \rangle^2\right)$$

$$\chi = \beta\left(\langle M^2 \rangle - \langle M \rangle^2\right)$$

3 Method

In this project we tried out many new concepts in our algorithm. We used Monte Carlo method.

Table 4.1: This table compares the analytical values for L=2 with the numerical ones after 10^6 Monte Carlo cycles. The values are in units per spin.

	Numerical:	Analytical:
$\langle E \rangle$	-1.9958	-1.9960
$\langle E^2 \rangle$	15.9664	15.9679
$\langle M \rangle$	0.0451	0
$\langle M^2 \rangle$	3.9930	3.9933
$\langle \lvert M \rvert \rangle$	0.9986	0.9987
χ	3.9849	3.9933
C_V	0.0335	0.0321

3.1 Monte Carlo cycles

In Monte Carlo methods, the goal is to

3.2 Metropolis algorithm

3.3 Random number generator

3.4 Parallelizing

Metropolis (T,A,...) Stochastic matrix - convergences (forhold eigenvalue).

Hvilken random number engine

MPI:

- Develop codes locally, run with some few processes and test your codes. Do benchmarking, timing and so forth on local nodes, for example your laptop or PC. - When you are convinced that your codes run correctly, you can start your production runs on available supercomputers.

MPI functions:

4 Result

4.1 Matrix dimension L=2

OBS! Need an number of MC cycles necessary!

All calculations in this subsection are at T = 1.0 K.

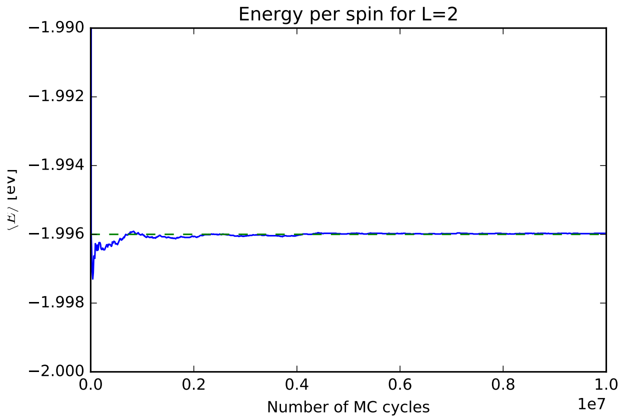

Figure 4.1: This is a plot of the expectation value of the energy per spin verus number of Monte Carlo cycles. The plot shows that at least $9 \cdot 10^5$ MC cycles are necessary for a good argeement.

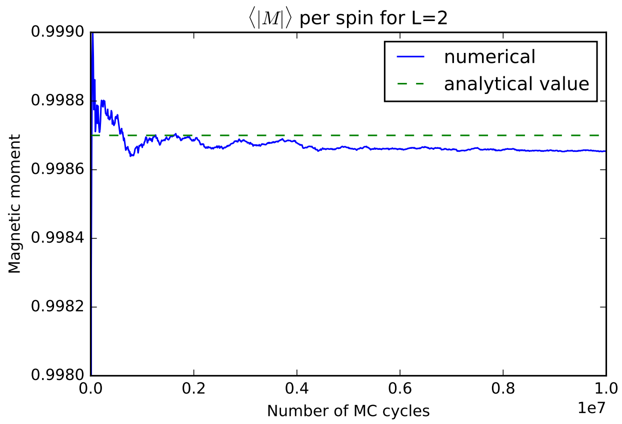

Figure 4.2: This is a plot of the expectation value of the mean absolute value of the magnetic moment per spin verus number of Monte Carlo cycles. The plot shows that at least $8 \cdot 10^5$ MC cycles are necessary for a good argeement, but all the way to 10^6 the value is a bit low.

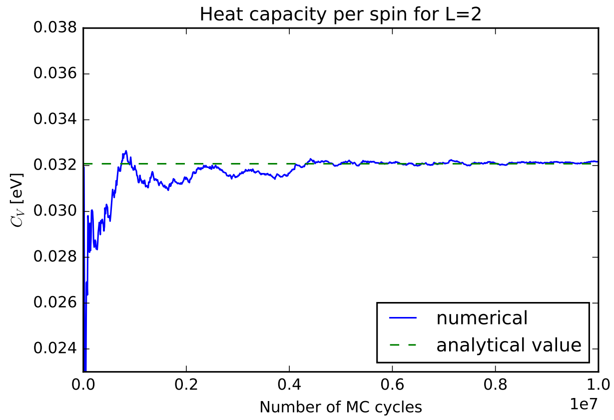

Figure 4.3: This is a plot of the heat capacity per spin verus number of Monte Carlo cycles. The plot shows that at least $6 \cdot 10^5$ MC cycles are necessary for a good argeement.

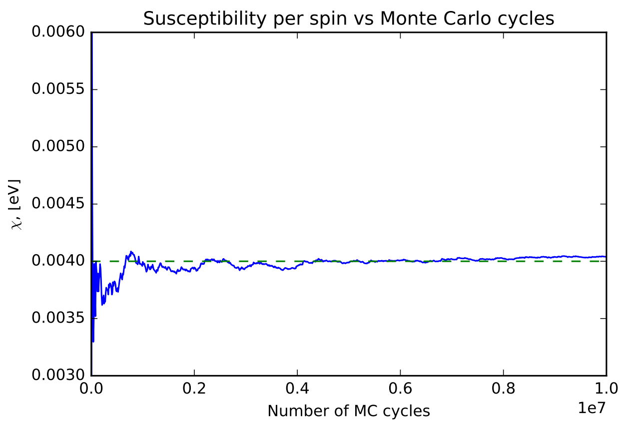

Figure 4.4: This is a plot of the susceptibility per spin verus number of Monte Carlo cycles. The plot shows that at least $6 \cdot 10^5$ MC cycles are necessary for a good argeement.

4.2 Matrix dimension L = 20

HMM: Should define an area that is enough for equilibrium!

OBS: Need the number of MC cycles to reach equilibrium!

OBS: Need equilibration time! (5 1e5?)

OBS: Comment accepted configs T dependency

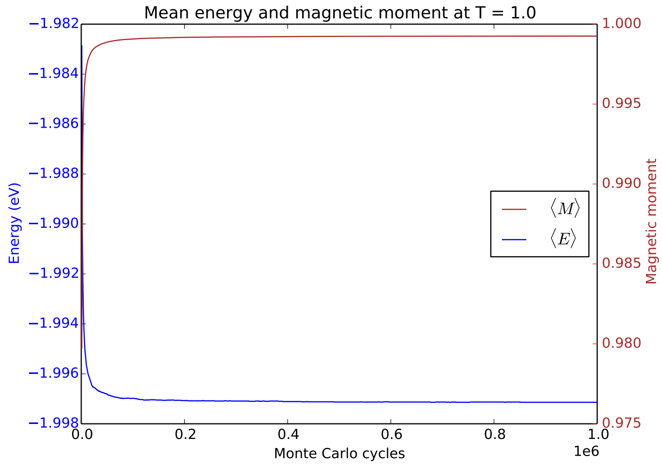

Figure 4.5: This is a plot of both the expectation value of the energy and absolute magnetic moment per spin verus number of Monte Carlo cycles at T = 1.0 K. The plot shows that at least **??**C cycles are necessary to reach equilibrium.

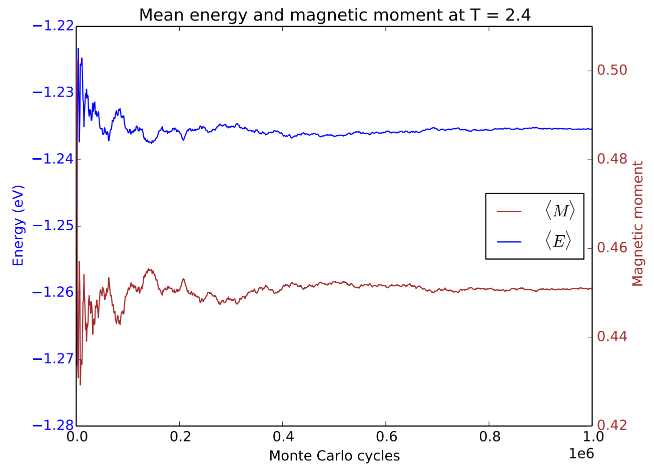

Figure 4.6: This is a plot of both the expectation value of the energy and absolute magnetic moment per spin verus number of Monte Carlo cycles at T = 2.4 K. The plot shows that at least **??**C cycles are necessary to reach equilibrium.

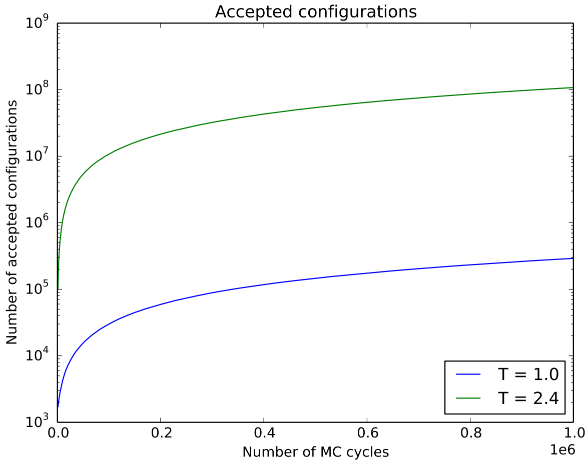

Figure 4.7: This is a plot of the total number of accepted configurations versus number of Monte Carlo cycles with random initial state.

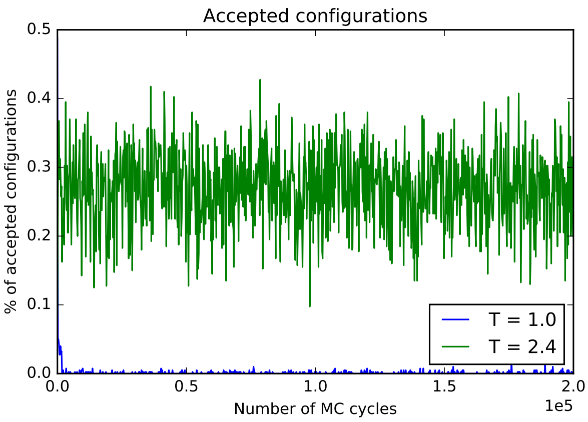

Figure 4.8: This is a plot of the percentage accepted of attempted configurations versus Monte Carlo cycles with random initial state.

4.3 Energy probability

OBS: Compare result with computed variance!

OBS: Discuss behavior (In Discussion - maybe just merge result and discussion?)

Computed variance (from same dataset?):

$$\sigma_E^2 = \langle E^2 \rangle - \langle E \rangle^2$$

T = 1.0 K:

$$\sigma_E^2 = 638181 - (-798.855)^2 = 11.69$$

$$\sigma = 3.42$$

T = 2.4 K:

$$\sigma_E^2 = 247886 - (-494.628)^2 = 3229.14$$

$$\sigma = 56.8$$

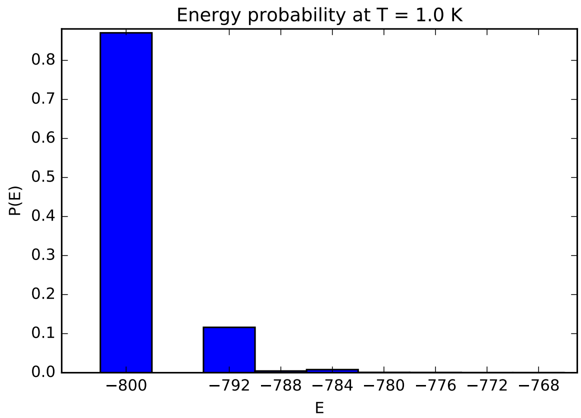

Figure 4.9: This is a plot of the energy probability when T = 1.0 K. The energy is the total energy of the 2D lattice with 20×20 spins.

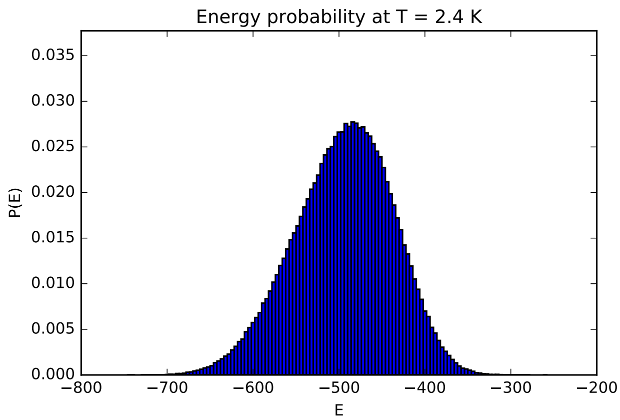

Figure 4.10: This is a plot of the energy probability when T = 2.4 K.The energy is the total energy of the 2D lattice with 20×20 spins.

4.4 Increasing dimensionality/ Critical temperature

OBS: Plot of E, M, Cv, X as functions of T (put L as legend and plot together)

OBS: Indication of phase transition? (Peak - at least for Cv and X)

OBS: Use Equation 5 to extract T_C.

Getting these equations from 5 where $\nu = 1$:

$$T_C(40) - T_C(\infty) = a40^{-1}$$
$$T_C(60) - T_C(\infty) = a60^{-1}$$
$$T_C(80) - T_C(\infty) = a80^{-1}$$
$$T_C(100) - T_C(\infty) = a100^{-1}$$

$$T_C(\infty) = -a40^{-1} + T_C(40)$$
$$T_C(\infty) = -a60^{-1} + T_C(60)$$
$$T_C(\infty) = -a80^{-1} + T_C(80)$$
$$T_C(\infty) = -a100^{-1} + T_C(100)$$

Exact $T_C = kTC/J = 2/\ln(1+\sqrt{2}) \approx 2.269$ [1]

5 Discussion

6 Conclusion

References

[1] Lars Onsager. Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Phys. Rev.*, 65:117–149, Feb 1944.

Appendix

State	Spinn	Energi	Magnetization
0	↓↓↓↓	−8J	−4
1	↓↓↓↑	0	−2
2	↓↓↑↓	0	−2
3	↓↑↓↓	0	−2
4	↑↓↓↓	0	−2
5	↓↓↑↑	0	0
6	↓↑↓↑	0	0
7	↓↑↑↓	8J	0
8	↑↓↓↑	8J	0
9	↑↓↑↓	0	0
10	↑↑↓↓	0	0
11	↓↑↑↑	0	2
12	↑↓↑↑	0	2
13	↑↑↓↑	0	2
14	↑↑↑↓	0	2
15	↑↑↑↑	−8J	4