

Project 4 FYS4150

Vilde Mari Reinertsen

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Abstract

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1 Introduction

The energy:

2 Theory

2.1 Introduction to statistics

$$P(a \leq X \leq b) = \int_b^a p(x) dx \quad (1)$$

$$\langle h \rangle_X = \int h(x) p(x) dx \quad (2)$$

$$\langle x^n \rangle = \int x^n p(x) dx \quad (3)$$

$$\langle x \rangle = \int x p(x) dx \quad (4)$$

2.2 Magnet - properties

Energy, magnetic moment, susceptibility, heat capacity.

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

Boltzman Markhow chain - convergence

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:

$$\begin{aligned} Z &= \sum_i^M e^{-\beta E_i} = e^{-\beta 8J} + e^{-\beta 8J} + e^{\beta 8J} e^{\beta 8J} + 12 \\ &= 2e^{-\beta 8J} + 2e^{\beta 8J} + 12 = 4 \left(\frac{e^{-\beta 8J} + e^{\beta 8J}}{2} \right) + 12 \\ &= 4 \cosh(\beta 8J) + 12 \end{aligned}$$

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

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

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

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

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

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

Following the same method, we found that:

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

$$\langle M \rangle = 0$$

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

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

We can use these to calculate the rest:

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

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

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
$\langle M \rangle$	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.

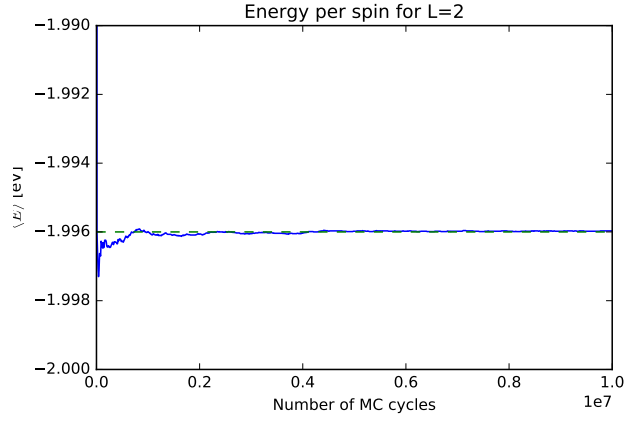


Figure 4.1: This is a plot of the expectation value of the energy per spin versus number of Monte Carlo cycles. The plot shows that at least $9 \cdot 10^5$ MC cycles are necessary for a good agreement.

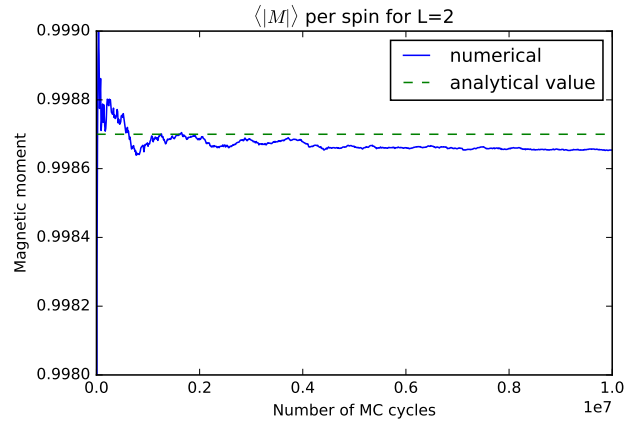


Figure 4.2: This is a plot of the expectation value of the mean absolute value of the magnetic moment per spin versus number of Monte Carlo cycles. The plot shows that at least $8 \cdot 10^5$ MC cycles are necessary for a good agreement, but all the way to 10^6 the value is a bit low.

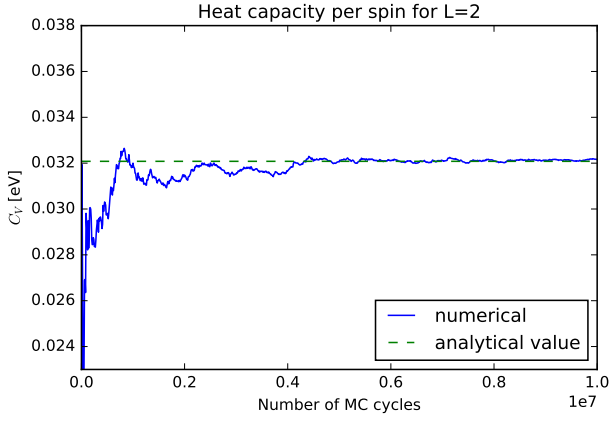


Figure 4.3: This is a plot of the heat capacity per spin versus number of Monte Carlo cycles. The plot shows that at least $6 \cdot 10^5$ MC cycles are necessary for a good agreement.

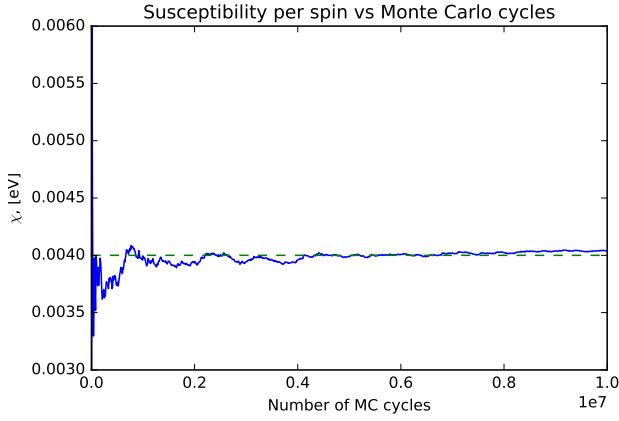


Figure 4.4: This is a plot of the susceptibility per spin versus number of Monte Carlo cycles. The plot shows that at least $6 \cdot 10^5$ MC cycles are necessary for a good agreement.

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

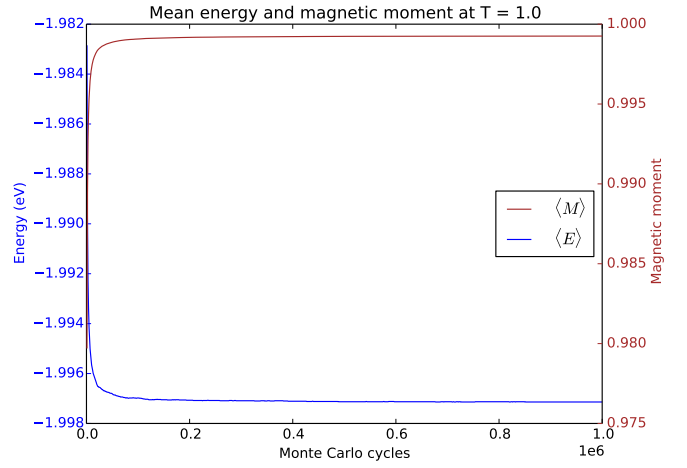


Figure 4.5: This is a plot of both the expectation value of the energy and absolute magnetic moment per spin versus number of Monte Carlo cycles at $T = 1.0$ K. The plot shows that at least $??$ C cycles are necessary to reach equilibrium.

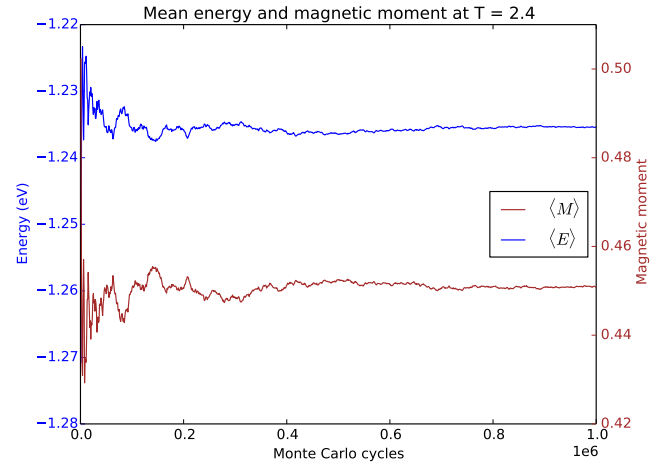


Figure 4.6: This is a plot of both the expectation value of the energy and absolute magnetic moment per spin versus number of Monte Carlo cycles at $T = 2.4$ K. The plot shows that at least $??$ C cycles are necessary to reach equilibrium.

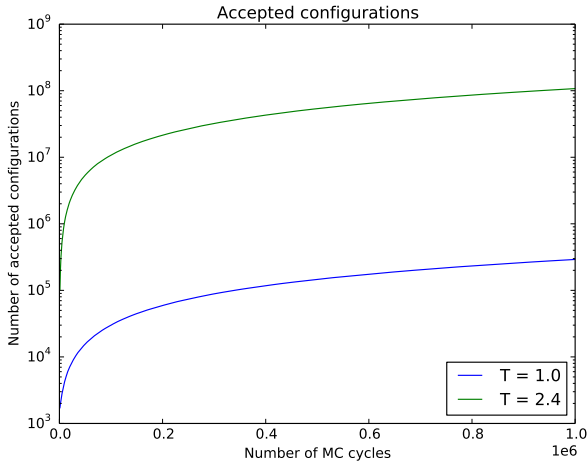


Figure 4.7: This is a plot of the total number of accepted configurations versus number of Monte Carlo cycles with random initial state.

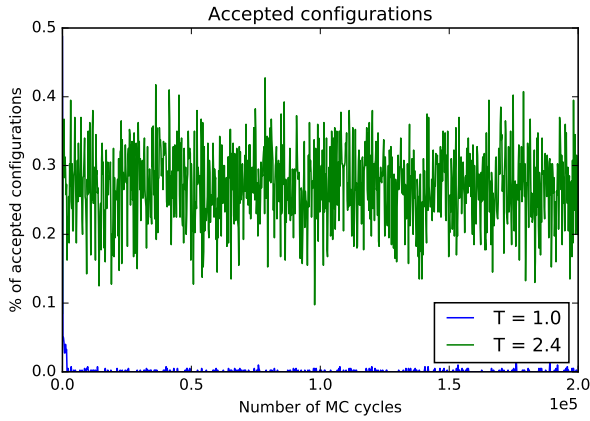


Figure 4.8: This is a plot of the percentage accepted of attempted configurations versus Monte Carlo cycles with random initial state.

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:

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

$$\sigma = 56.8$$

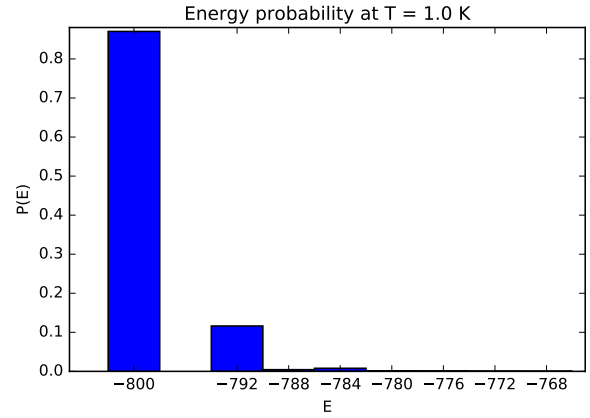


Figure 4.9: This is a plot of the energy probability when T = 1.0 K. The energy is the total energy of the 2D lattice with 20×20 spins.

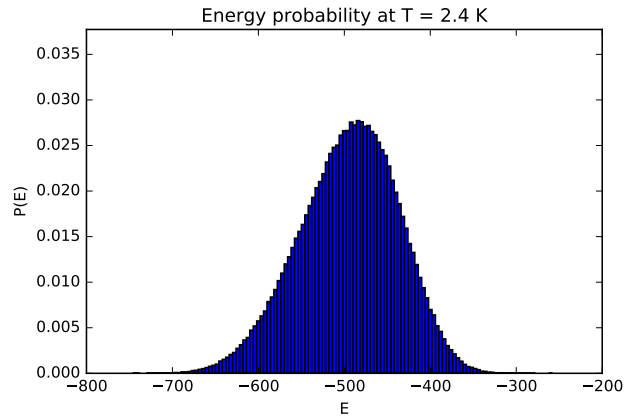


Figure 4.10: This is a plot of the energy probability when T = 2.4 K. The energy is the total energy of the 2D lattice with 20×20 spins.

4.4 Increasing dimensionality/ Critical temperature

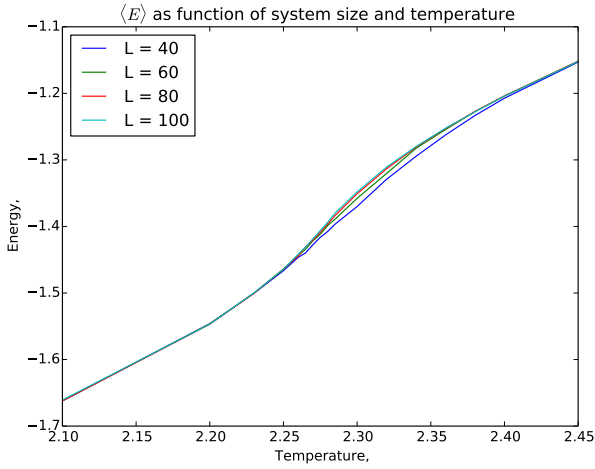


Figure 4.11: This is a plot of the energy versus temperature around the critical temperature for the different lattice sizes with $L = 40$, $L = 60$, $L = 80$ and $L = 100$.

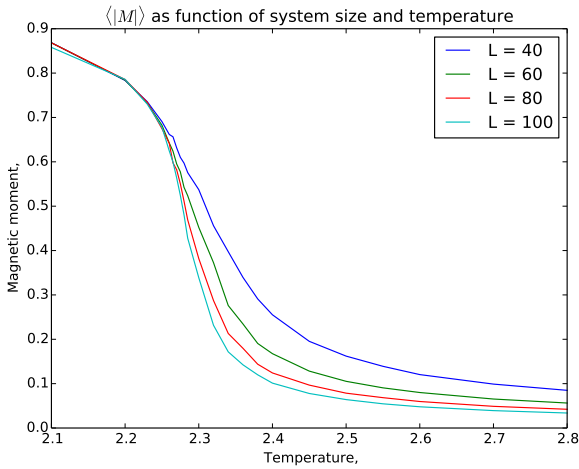


Figure 4.12: This is a plot of the absolute magnetic moment versus temperature around the critical temperature for the different lattice sizes with $L = 40$, $L = 60$, $L = 80$ and $L = 100$.

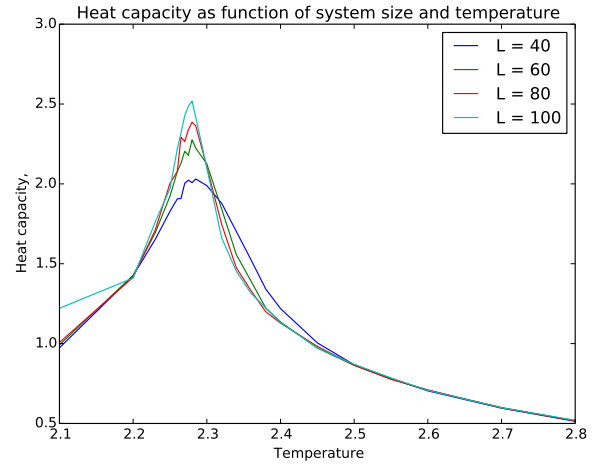


Figure 4.13: This is a plot of the heat capacity versus temperature around the critical temperature for the different lattice sizes with $L = 40$, $L = 60$, $L = 80$ and $L = 100$.

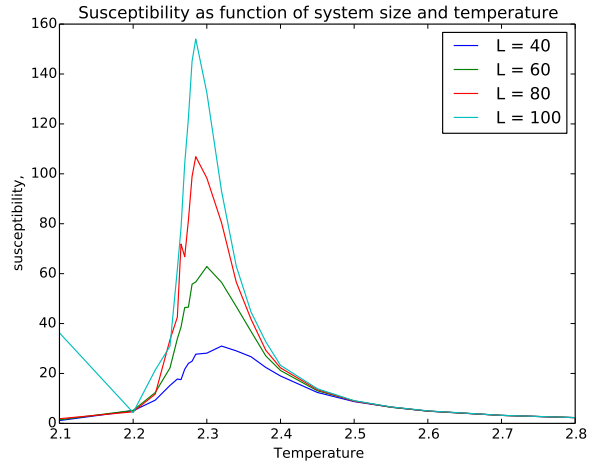


Figure 4.14: This is a plot of the susceptibility versus temperature around the critical temperature for the different lattice sizes with $L = 40$, $L = 60$, $L = 80$ and $L = 100$.

OBS: Indication of phase transition? (Peak - at least for C_v and χ)

OBS: Use Equation 5 to extract T_C .

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

$$\begin{aligned} T_C(40) - T_C(\infty) &= a \cdot 40^{-1} \\ T_C(60) - T_C(\infty) &= a \cdot 60^{-1} \\ T_C(80) - T_C(\infty) &= a \cdot 80^{-1} \\ T_C(100) - T_C(\infty) &= a \cdot 100^{-1} \end{aligned}$$

(Sett inn tall!)

$$T_C(\infty) = -a \cdot 40^{-1} + 2.28$$

$$T_C(\infty) = -a \cdot 60^{-1} + 2.27$$

$$T_C(\infty) = -a \cdot 80^{-1} + 2.28$$

$$T_C(\infty) = -a \cdot 100^{-1} + 2.27$$

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

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