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PROJECT 4

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ABSTRACT

Subject headings: computational science: Ising model — methods: Metropolis, Monte Carlo

TABLE 1

Spins up	Degeneracy	Energy	Magnetic moment
4	1	-8J	4
3	4	0	2
2	4	0	0
2	2	8J	0
1	4	0	-2
0	1	-8J	-4

Note. — States of the 2x2 lattice and corresponding values for energy and magnetic moment. Notice that the ground state (the lowest energy) has either all spins pointing up or down.

2. The energy equal to zero has a degeneracy of 12. Expanding the sum of the partition function we get

$$\begin{aligned} z &= 2e^{8J\beta} + 12 + 2e^{-8J\beta} \\ &= 12 + 2\left(e^{8J\beta} + e^{-8J\beta}\right), \end{aligned}$$

where we have inserted $e^0 = 1$. We know that $\cosh(x) = \frac{1}{2}\left(e^{-x} + e^{x}\right)$, inserting this gives

$$Z = 12 + 4\cosh(8J\beta). \tag{3}$$

The mean value of the energy is given by

$$\langle E \rangle = -\frac{\partial}{\partial\beta}\ln Z = -\frac{1}{Z}\frac{\partial Z}{\partial\beta},$$

which is found by inserting the partition function.

$$\begin{aligned} \langle E \rangle &= -\frac{1}{Z}\frac{\partial}{\partial\beta}\left(12 + 4\cosh\left(8J\beta\right)\right) \\ &= -\frac{4}{Z}\left(8J\sinh\left(8J\beta\right)\right), \end{aligned}$$

pulling a factor 4 from the partition function and inserting we are left with a analytical solution to the mean energy of the lattice

$$\langle E \rangle = -\frac{8J\sinh\left(8J\beta\right)}{3 + \cosh(8J\beta}.$$

The heat capacity can be found by

$$C_V = \frac{1}{kT^2}\frac{\partial^2}{\partial\beta^2}\ln Z = \frac{1}{kT^2}\frac{\partial}{\partial\beta}\left(\frac{\partial}{\partial\beta}\ln Z\right),$$

where we recognize the partial derivative in the parenthesis as the negative mean energy.

$$\begin{aligned} C_V = \frac{1}{kT^2}\Bigg(&\frac{64J^2\cosh\left(8J\beta\right)\left(3 + \cosh\left(8J\beta\right)\right)}{\left(3 + \cosh\left(8J\beta\right)\right)^2} \\ &- \frac{64J^2\sinh^2\left(8J\beta\right)}{\left(3 + \cosh\left(8J\beta\right)\right)^2}\Bigg), \end{aligned}$$

by inserting for the mean energy and using the product rule. Further simplifications gives the mean heat capacity

$$C_V = \frac{64J^2}{k_B T^2}\left(\frac{\cosh(8\beta J)(3+\cosh(8\beta J)) - \sinh^2(8\beta J)}{(3+\cosh(8\beta J))^2}\right)$$

The susceptibility is given as

$$\chi = \frac{1}{kT}\left(\langle M^2\rangle - \langle M\rangle^2\right).$$

To find the susceptibility of the system we consider the mean magnetic moment

$$\langle M\rangle = \frac{1}{Z}\sum_i |M_i| e^{-\beta E_i},$$

where we find the magnetic moment for a given energy in Table 1. So the mean magnetic moment is

$$\langle M\rangle = \frac{1}{Z}\left(4e^{8J\beta} + 4\left(2e^0\right) + 4\left(-2e^0\right) + -4e^{8J\beta}\right) = 0.$$

Further we calculate the mean of the magnetic moment squared

$$\langle M^2\rangle = \frac{1}{Z}\sum_i M_i^2 e^{-\beta E_i},$$

and again referring to Table 1 we get

$$\begin{aligned}\langle M^2\rangle &= \frac{1}{Z}\left(16\left(2e^{8J\beta}\right) + 16\left(2e^0\right)\right)\\ &= \frac{8\left(e^{8J\beta}+1\right)}{3+\cosh\left(8J\beta\right)}.\end{aligned}$$

So the susceptibility of the system is given as

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

Further we find the mean of the absolute value of the magnetic moment by

$$\begin{aligned}\langle |M|\rangle &= \frac{1}{Z}\sum_i |M_i| e^{-\beta E_i}\\ &= \frac{1}{Z}\left(4e^{8J\beta} + 4\left(2e^0\right) + 4\left(|-2|e^0\right) + |-4|e^{8J\beta}\right)\\ &= \frac{2e^{8J\beta}+4}{3+\cosh\left(8J\beta\right)},\end{aligned}$$

after pulling out a factor 4 from the partition function. To summarize we have the following analytical expression for the system

$$\begin{aligned}\langle E\rangle &= -\frac{4}{Z}\left(8J\sinh\left(8J\beta\right)\right),\\ \langle |M|\rangle &= \frac{2e^{8J\beta}+4}{3+\cosh\left(8J\beta\right)},\\ C_V &= \frac{64J^2}{kT^2}\left(\frac{\cosh(8\beta J)(3+\cosh(8\beta J)) - \sinh^2(8\beta J)}{(3+\cosh(8\beta J))^2}\right),\\ \chi &= \frac{1}{kT^2}\frac{8\left(e^{8J\beta}+1\right)}{3+\cosh\left(8J\beta\right)}.\end{aligned}$$

2.2. *Ising model*

When the energy of the Ising model we consider the equation given in the introduction, Eq. (**??**), where the subscript of the sum means we are taking the sum over the neighbouring spins, N is the total amount of spins and s_k, $s_l = \pm 1$, represents the spin of the particles. Consider a random spin at the lattice, in the two-dimensional case it has a total of four neighbours that it interacts with. An example for a spin surrounded by four spin up.

$$\begin{matrix} & \uparrow & \\ \uparrow & \uparrow & \uparrow, \\ & \uparrow & \end{matrix}$$

with energy $E = -4J$. Changing one of the spins in the example above results in a new configuration with a new energy and magnetic moment. Following are five examples that show the different energies $E = 0, \pm 2J, \pm 4J$, and the resulting energy when flipping the spin we are located at:

$$E = -4J \quad \begin{array}{ccc} & \uparrow & \\ \uparrow & \uparrow & \uparrow \\ & \uparrow & \end{array} \quad \Longrightarrow \quad E = 4J \quad \begin{array}{ccc} & \uparrow & \\ \uparrow & \downarrow & \uparrow \\ & \uparrow & \end{array}$$

where the change of energy $\Delta E = E_{after} - E_{before} = 8J$.

$$E = -2J \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \uparrow & \uparrow \\ & \uparrow & \end{array} \quad \Longrightarrow \quad E = 2J \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \downarrow & \uparrow \\ & \uparrow & \end{array}$$

with $\Delta E = 4J$.

$$E = 0 \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \uparrow & \uparrow \\ & \downarrow & \end{array} \quad \Longrightarrow \quad E = 0 \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \downarrow & \uparrow \\ & \downarrow & \end{array}$$

with $\Delta E = 0$.

$$E = -2J \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \uparrow & \downarrow \\ & \downarrow & \end{array} \quad \Longrightarrow \quad E = 2J \quad \begin{array}{ccc} & \uparrow & \\ \downarrow & \downarrow & \downarrow \\ & \downarrow & \end{array}$$

with $\Delta E = -4J$.

$$E = 4J \quad \begin{array}{ccc} & \downarrow & \\ \downarrow & \uparrow & \downarrow \\ & \downarrow & \end{array} \quad \Longrightarrow \quad E = -4J \quad \begin{array}{ccc} & \downarrow & \\ \downarrow & \downarrow & \downarrow \\ & \downarrow & \end{array}$$

with $\Delta E = -8J$. We now see that for a random spin of the lattice we have known values for the change of energy ΔE.

2.3. *Implementation*

For a MC cycle we initialize the lattice by setting all the spins in either a random or an ordered state, and then calculating the energy and the magnetic moment. We then iterate over the lattice at random positions (i.e. we check L^2 random spins), for each of these positions we calculate the change in energy ΔE. Consider the ratio of the probability of the new energy $P(E_{new})$ and the previous energy $P(E_{prev})$:

$$\frac{P(E_{new})}{P(E_{prev})} = \frac{e^{-\beta E_{new}}/Z}{e^{-\beta E_{prev}}/Z} = e^{-\beta(E_{new} - E_{prev})} = e^{-\beta \Delta E},$$

where Z is the the partition function. We now perform the Metropolis test for a given ΔE;

$$r \leq e^{-\beta \Delta E}, \qquad r \in [0, 1]$$

i.e. if the ratio is larger than or equal to a random number $r \in [0, 1]$ we accept a new configuration, and flip the spin. We are looking at the change in energy if we were to flip a random spin; if the change of energy is large, the likelihood of this spin being flipped is small, so we reject this solution, on the other hand, if the probability is large, we accept the configuration. Since we expect the system to move to more likely state, we are looking for states that does not increase the systems energy. A large change in energy means we are looking at a spin that has half or more of its surrounding spins in the same configuration, and the system seems to locally move towards a steady state, therefore the local system is not changed. For each such Metropolis test that succeeds we add the flip of spin as a contribution to the systems energy and magnetic moment. When the calculations over the lattice is complete we conclude a single MC cycle and store the final value for the energy and magnetic moment.

2.4. *Critical temperature*

As the temperature of the system moves towards the critical temperature, the susceptibility χ and the heat capacity C_V moves towards an infinite value. We can see this by

$$C_V \sim |T_C - T|^{-\alpha}$$
$$\chi \sim |T_C - T|^{-\nu},$$

where α and ν are positive constants. For the results in this study we have clearer peaks for the susceptibility, so we will extract the critical temperature from these. We know that the critical tempeature scales as

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

where we set $\nu = 1$, and a is a positive constant. Solving the above equation for the critical temperature as the lattice size is infinite we get

$$T_C(L = \infty) \approx T_C(L) - \frac{1}{L}.$$

3. RESULTS

Following are the results produced in this study. The results are found in plots and tables, and the content is presented in the following subsections.

3.1. *Comparison of analytical and numerical values*

Table 2 shows a comparison of analytical and numerical values for a 2x2 lattice.

3.2. *Mean energy and magnetisation 20x20 lattice*

Figures 1a and 1b shows the energy and magnetisation of the ground state for temperature 1 kT/J, while figures 2a and 2b shows the same for temperature 2.4 kT/J. We see that the system stabilizes quickly. For the non-ground state plots see figures 4a and 4b for temperature 1 kT/J and figures 5a and 5b for temperature 2.4 kT/J.

3.3. *Accepted states in the Metropolis algorithm*

The accepted states as a function of temperature and MC cycles are found in figures 6 and 7 respectively, both are logarithmic plots.

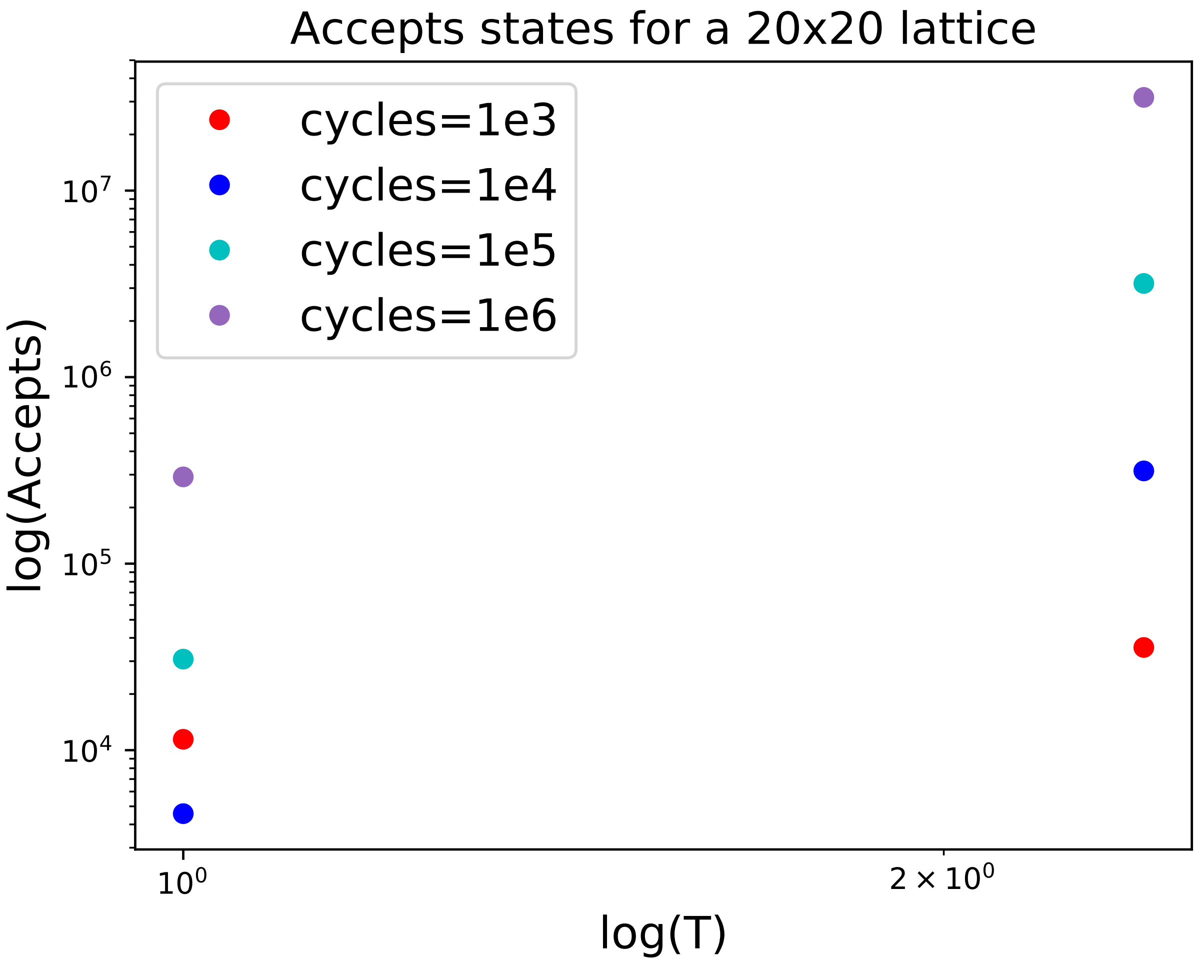
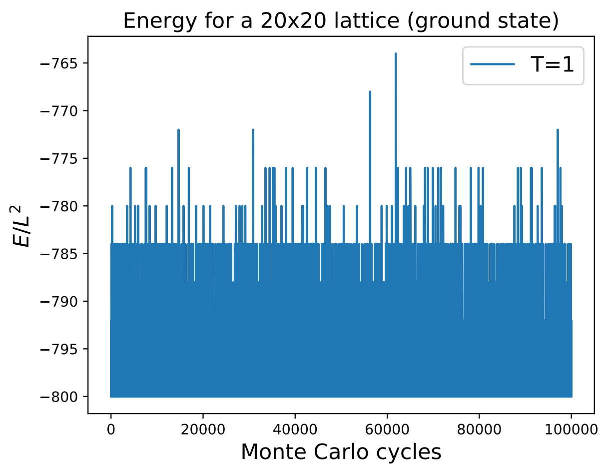


FIG. 6.— Logarithm of the accepted states as a function of the temperature for different number of Monte Carlo cycles. The left four dots corresponds to $T = 1$ kT/J, and the right four dots corresponds to $T = 2.4$ kT/J. The initial spins are randomly organized.

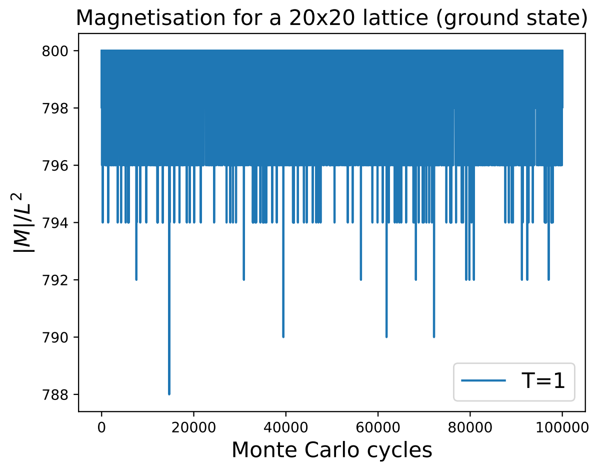
TABLE 2

MC cycles	$\langle E \rangle$	$\langle \lvert M \rvert \rangle$	C_V	χ
1e3	-7.984	3.996	0.127	0.019
5e3	-7.985	3.994	0.114	15.916
1e4	-7.981	3.994	0.146	15.769
1e5	-7.984	3.994	0.129	15.847
1e6	-7.984	3.994	0.127	15.973
Analytical	-7.983	3.994	0.128	15.973

NOTE. — Comparison of analytical and numerical results for various MC cycles. Lattice size is 2x2, temperature 1 kT/J and initial spin randomly set.

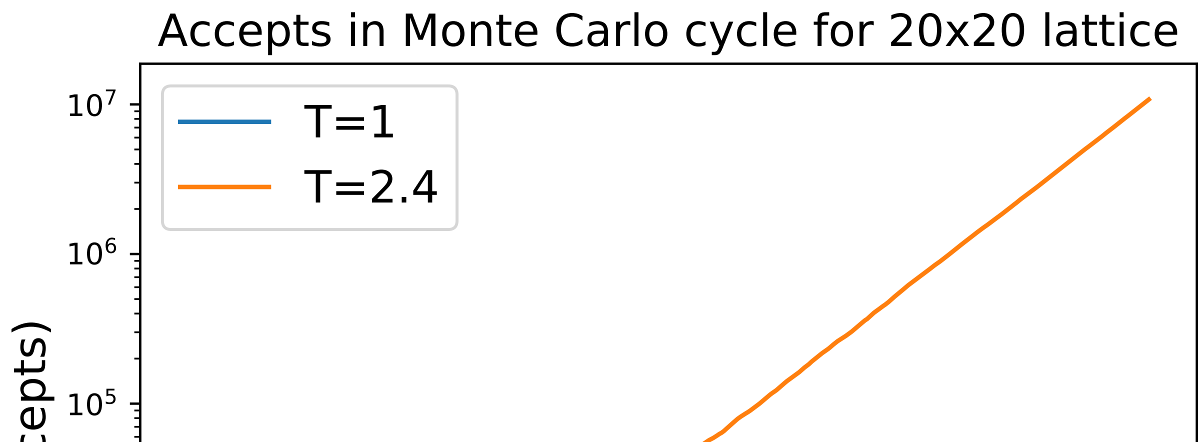


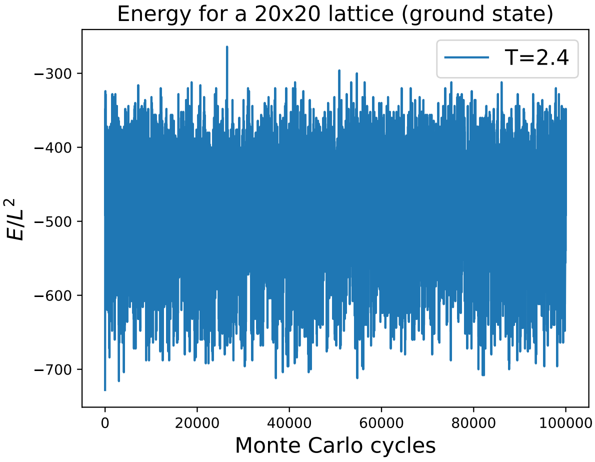
(a) Energy pr. spin.



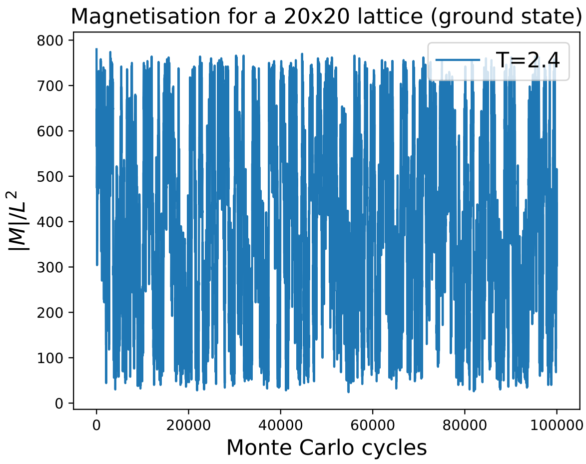
(b) Absolute value of the magnetic moment pr. spin.

FIG. 1.— Time evolution (MC cycles) of energy and magnetic moment of an ordered initial state with temperature 1 kT/J. 10^5 Monte Carlo cycles.





(a) Energy pr. spin.

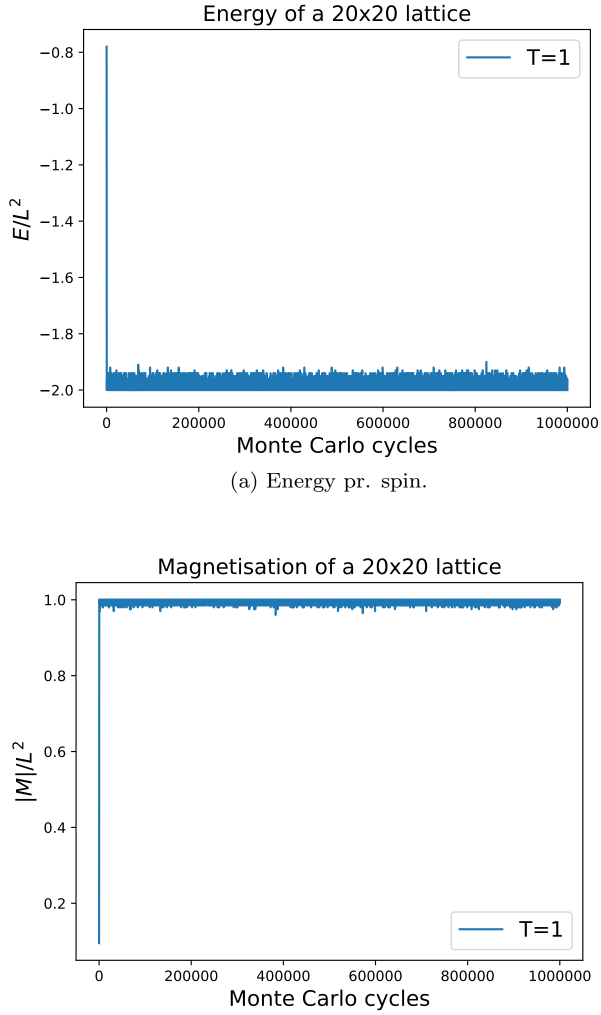


(b) Absolute value of the magnetic moment pr. spin.

FIG. 2.— Time evolution of energy and magnetic moment of an ordered initial state with temperature 2.4 kT/J. 10^5 Monte Carlo cycles.

3.4. *Varying temperature*

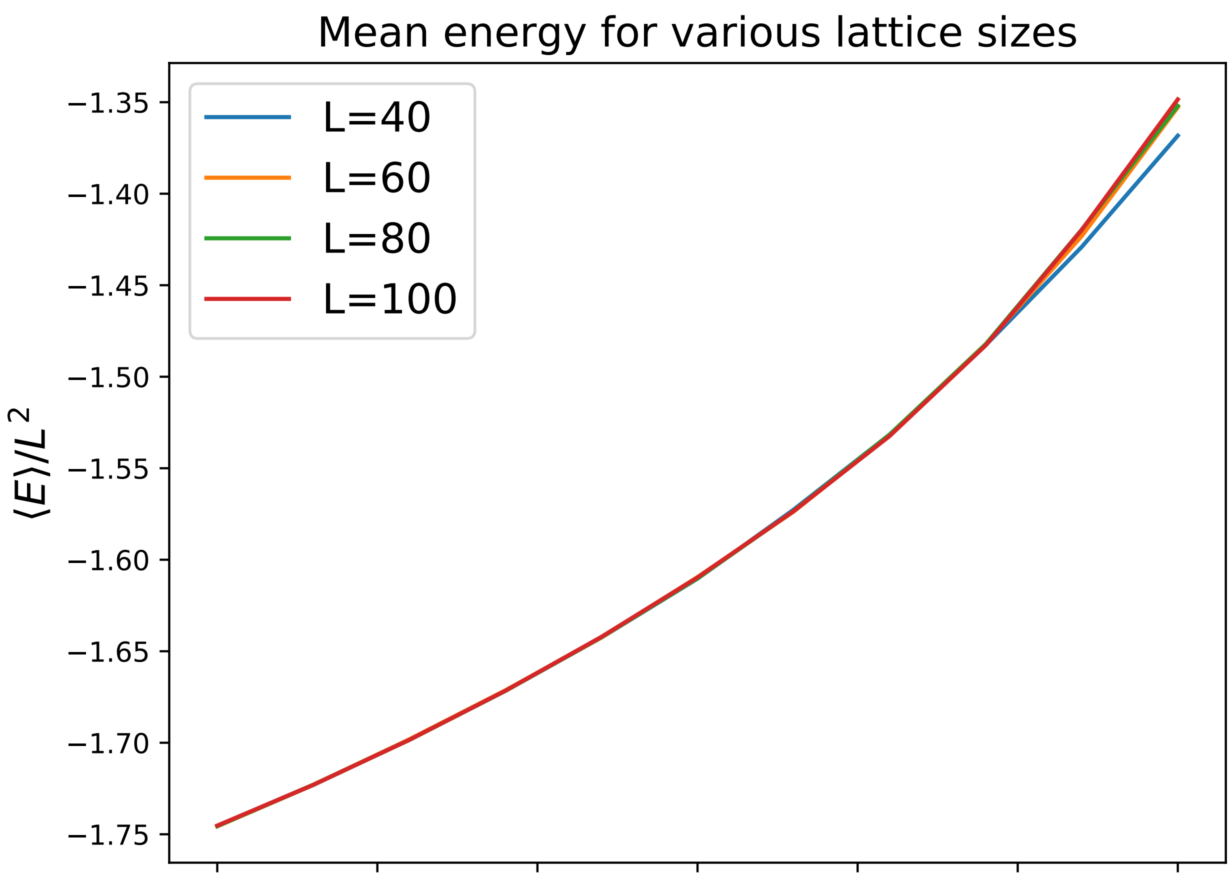
In figures 8-11 we can see plots of mean energy, mean magnetisation, heat capacity and susceptibility as a function of temperature. The temperature varies from 2-2.3 kT/J. The number of MC cycles are 10^6, with a random initial state for the spins. In figures 12-15 the temperature interval and temperature step are changed to $2.2 - 2.4$ kT/J and 0.01 respectively, this is done to focus on the temperature where we expect to find the critical temperature.

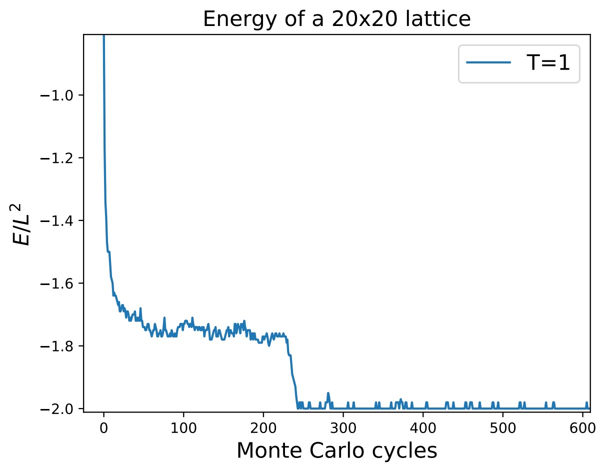


(a) Energy pr. spin.

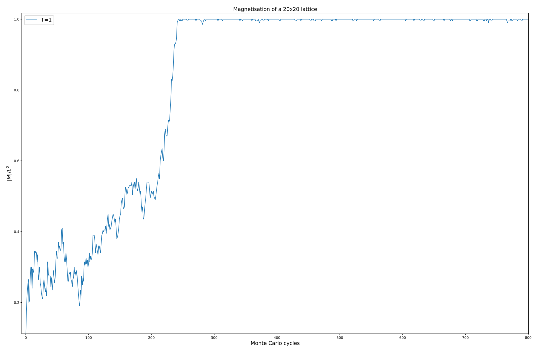
(b) Absolute value of the magnetic moment pr. spin.

FIG. 3.— Time evolution of energy and magnetic moment of an random initial state with temperature 1 kT/J. 10^6 Monte Carlo cycles.



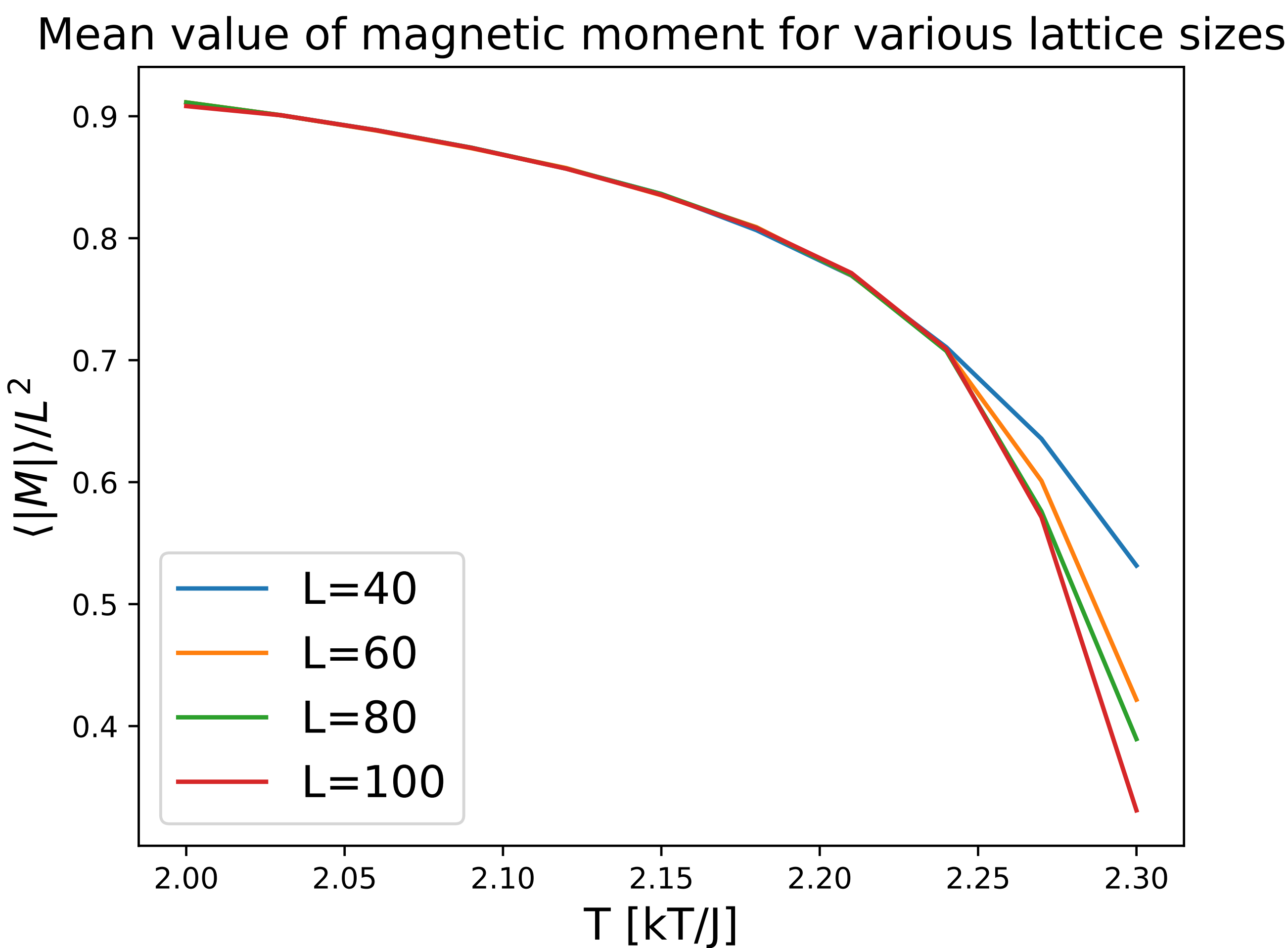


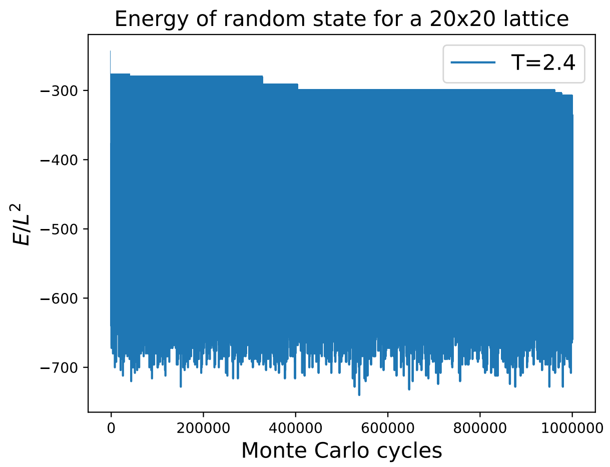
(a) Zoom of figure 4a.



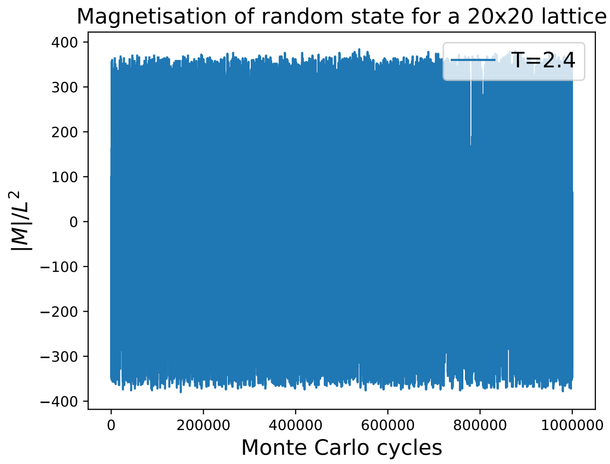
(b) Zoom of figure 4b.

FIG. 4.— Zoom of previous plot to show where the energy and magnitisation stabilized.



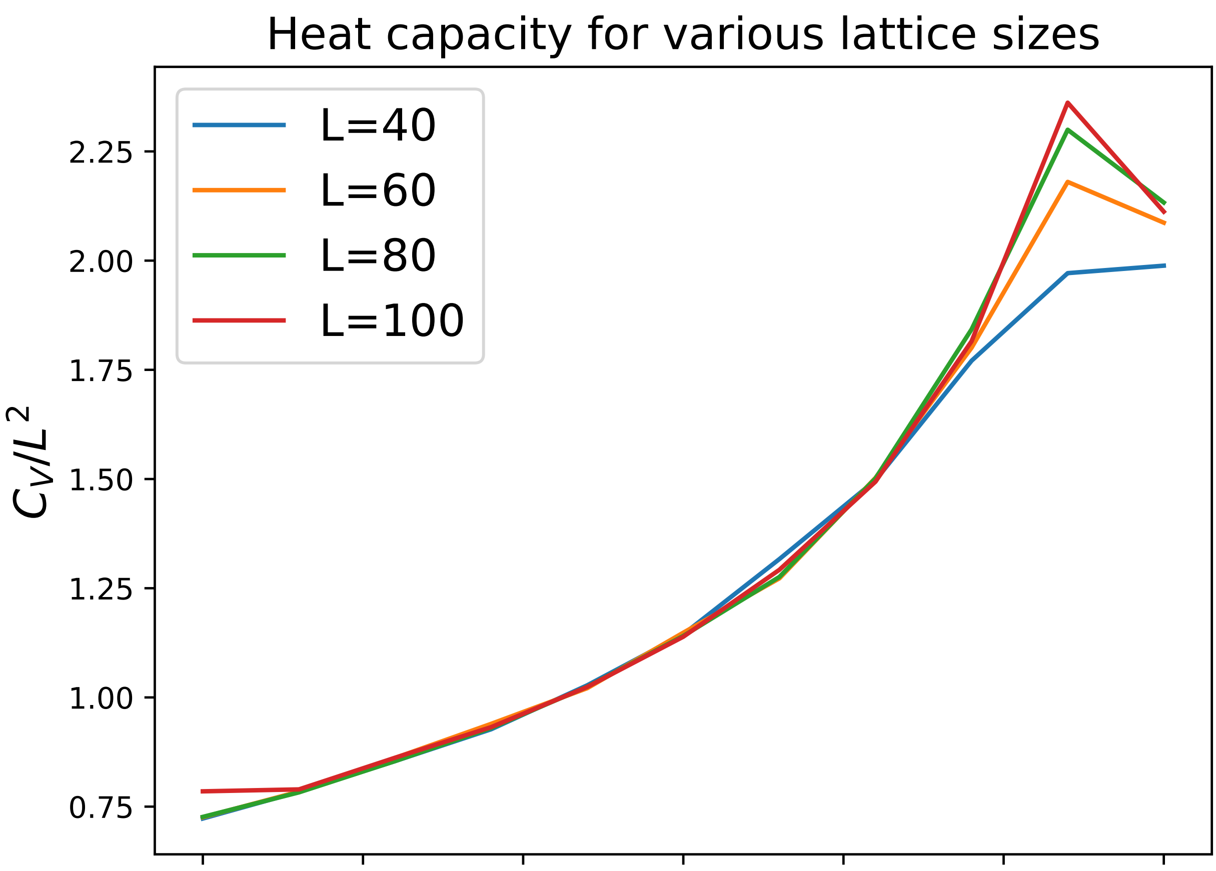


(a) Energy pr. spin.



(b) Absolute value of the magnetic moment pr. spin.

FIG. 5.— Time evolution (MC cycles) of energy and magnetic moment of an random initial state with temperature 2.4 kT/J. 10^6 Monte Carlo cycles.



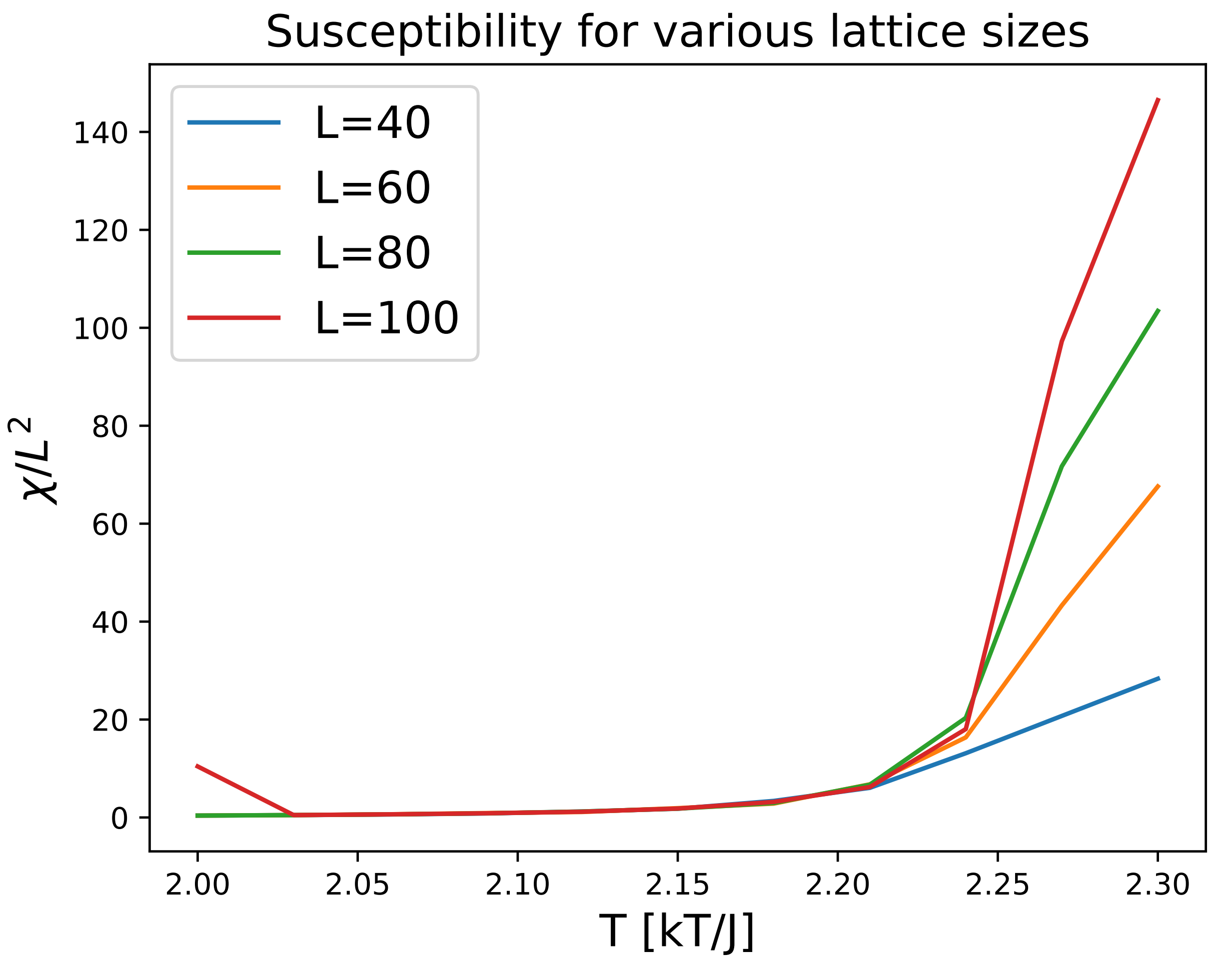


Fig. 11.— Susceptibility pr. spin for various lattice sizes. 10^6 MC cycles.. Initial spin state is random. Temperature varies with a step size of 0.03, making it ten steps.

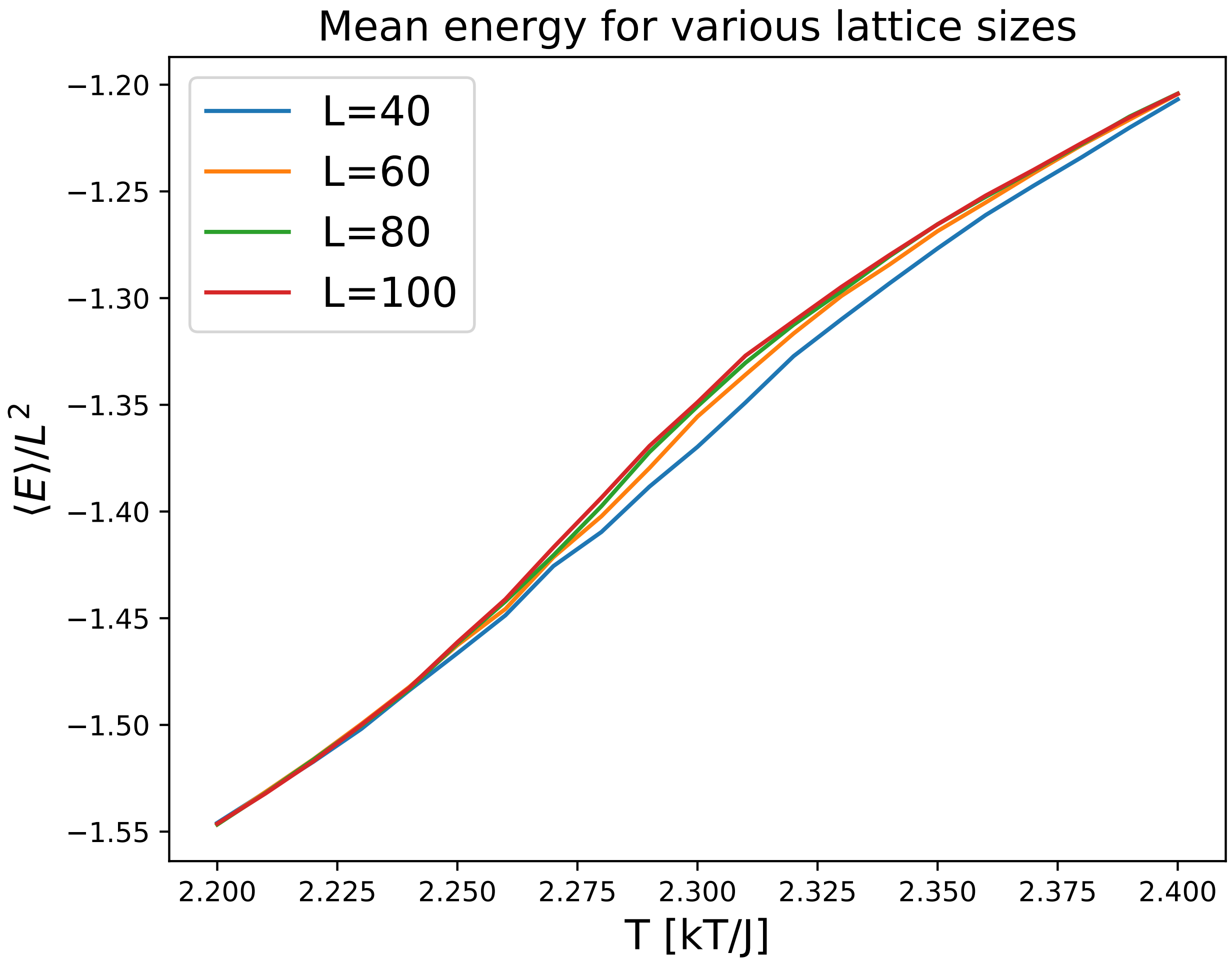


FIG. 12.— Mean energy pr. spin for various lattice sizes. 10^6 MC cycles. Initial spin state is random. Temperature varies with a step size of 0.01, making it twenty steps.

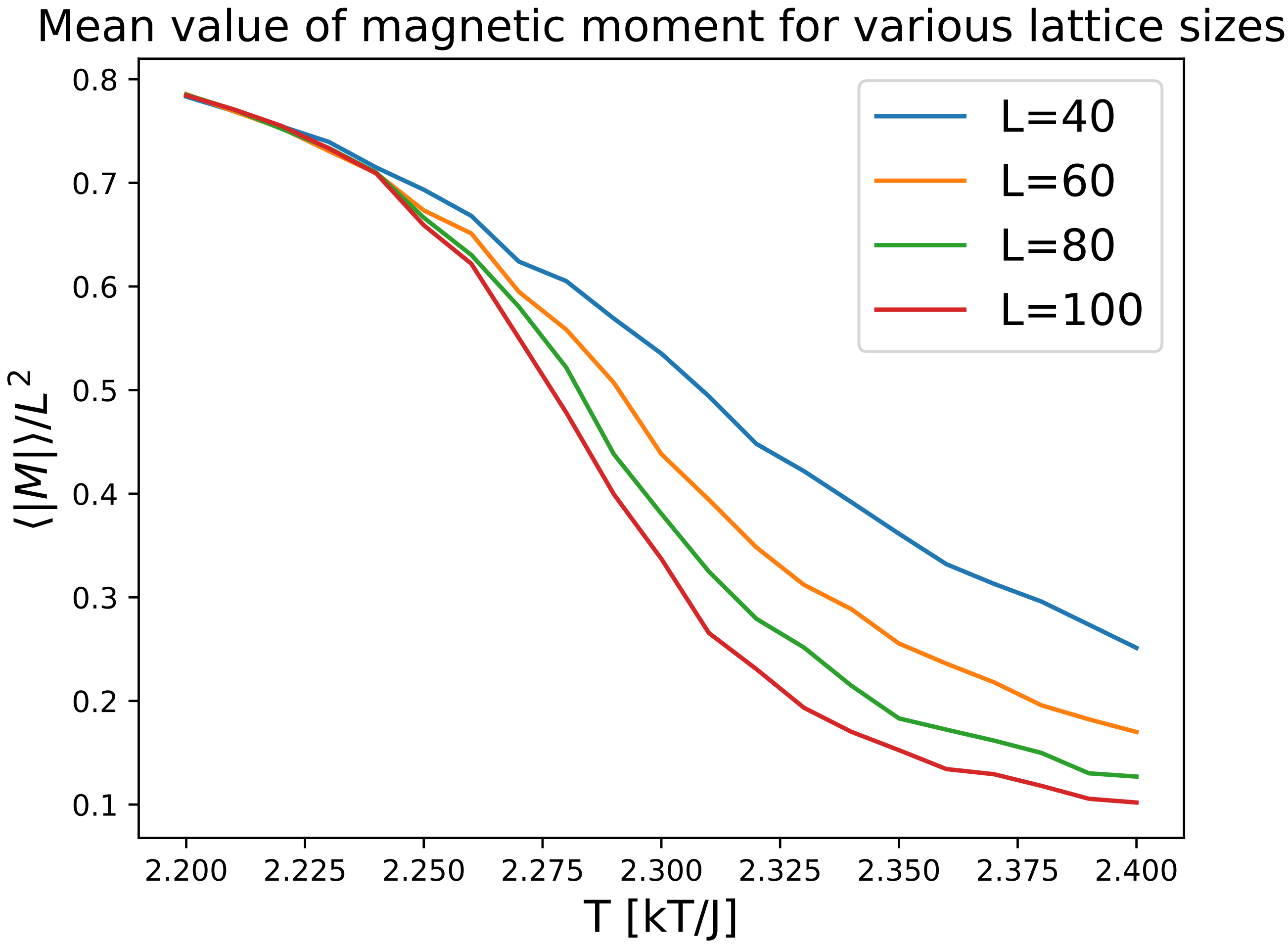


FIG. 13.— Mean abslute value of the magnetic moment pr. spin for various lattice sizes. 10^6 MC cycles.. Initial spin state is random. Temperature varies with a step size of 0.01, making it twenty steps.

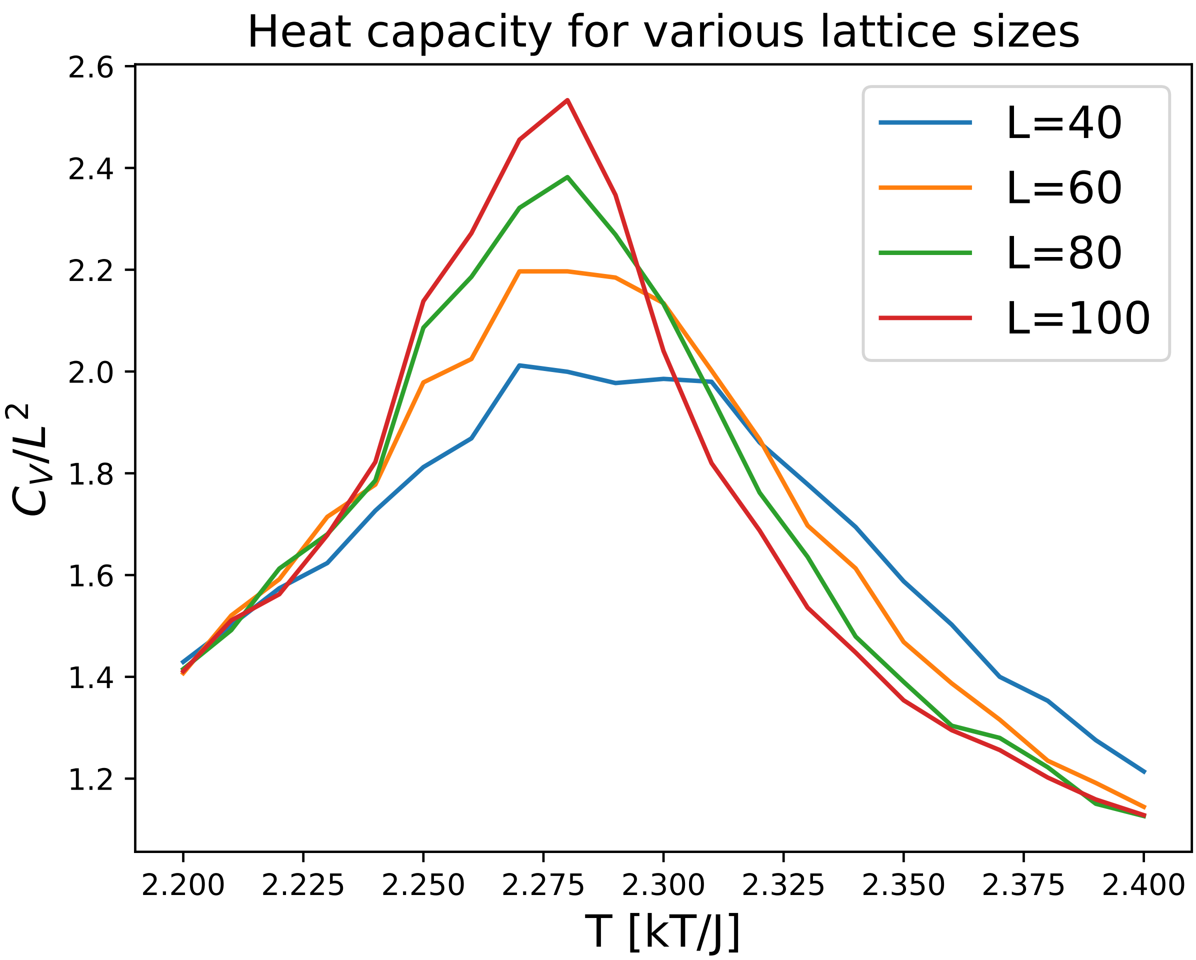


FIG. 14.— Heat capacity pr. spin for various lattice sizes. 10^6 MC cycles.. Initial spin state is random. Temperature varies with a step size of 0.01, making it twenty steps.

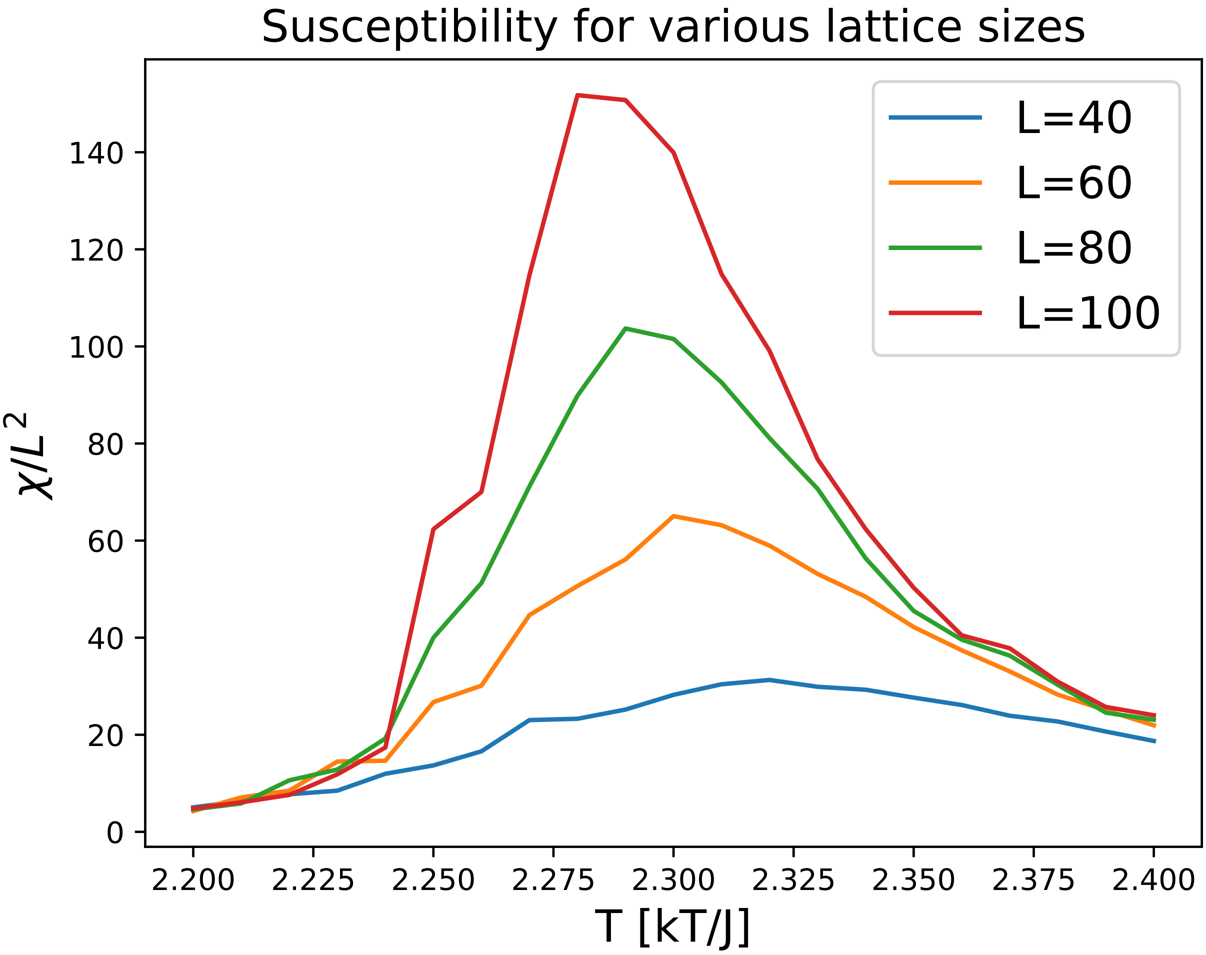


FIG. 15.— Susceptibility pr. spin for various lattice sizes. 10^6 MC cycles. Initial spin state is random. Temperature varies with a step size of 0.01, making it twenty steps.

3.5. *Critical temperature*

Figure 16 the critical temperature as a function of 1/L is plottet. Critical temperature was extracted from the susceptibility plotted in figure 15, that is; we have extracted the corresponding temperature of the highest value of the susceptibility. Linear regression gives the function $y(x) = 1.586x + 2.256$. When $L \to \infty$, this corresponds to $1/L \to 0$. We can see that $y(0) = 2.256$, which is the numerical value for the critical temperature when the lattice size $L \to \infty$.

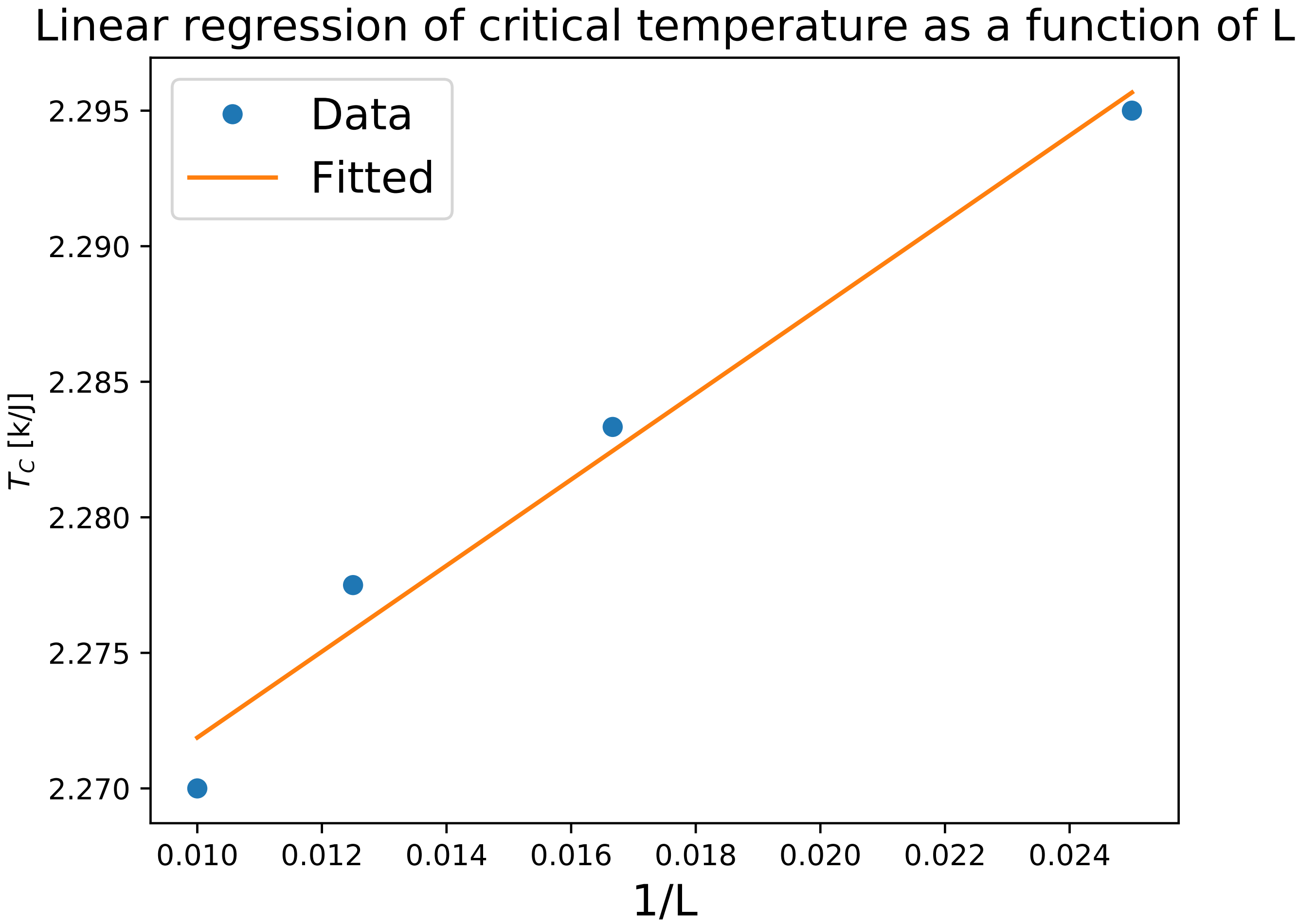


FIG. 16.— Linear regression used on the critical temperatures at points of 1/L for L = 40, 60, 80 and 100 gives the function $y(x) = 1.586x + 2.256$.

3.6. *Probability of energy*

In figures 17 and **??** we can see the probability distribution for a given energy for temperature 1 kT/J and 2.4 kT/J respectively. The variance of the energy $\sigma_E^2 = 9.398$ for temperature 1 kT/J and $\sigma_E^2 = 3264.7$ for temperature 2.4 kT/J.

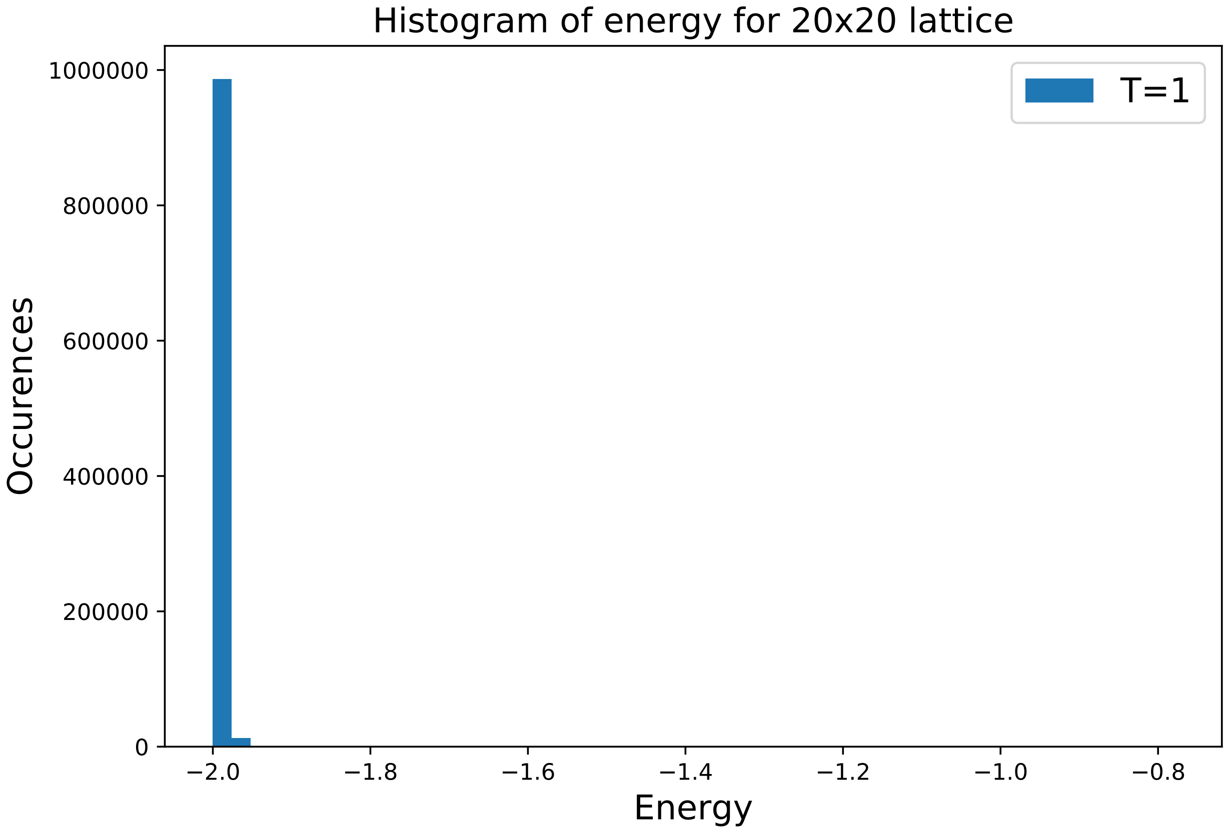


Fig. 17.— Histogram of the probability as a function of energy. Temperature is 1 kT/J. Initial spin states are random. 1e6 MC cycles.

REFERENCES

Górski, K. M., Hinshaw, G., Banday, A. J., Bennett, C. L., Wright, E. L., Kogut, A., Smoot, G. F., and Lubin, P. 1994, ApJL, 430, 89

TABLE 3

Run	1 core	4 core	Difference
1	13.910	4.448	9.461
2	14.348	4.530	9.817
3	14.407	4.636	9.770
Average	14.221	4.538	9.683

NOTE. — Run times for a 40x40 lattice for 10^5 Monte Carlo cycles. Temperature set to 1 kT/J and the initial state for the spins are random.

TABLE 4

Run	1 core	4 core	Difference
1	91.137	34.434	62.702
2	83.662	30.455	53.207
3	86.905	28.534	58.371
Average	87.235	31.141	58.093

NOTE. — Run times for a 100x100 lattice for 10^5 Monte Carlo cycles. Temperature set to 1 kT/J and the initial state for the spins are random.