Investigation of the Ising model using the Metropolis algorithm

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The application of the Markov Chain Monte Carlo Metropolis algorithm to the Ising model is investigated. The theoretical prediction of the critical temperature $T_c \approx 2.269\frac{J}{k_B}$ for the two-dimensional Ising model is adopted as benchmark. By studying the absolute magnetisation $|m|$, the susceptibility χ, the specific heat capacity C_V and the fourth-order Binder cumulant U_4, an estimate of the critical temperature $T_c \in [2.193\frac{J}{k_B}, 2.425\frac{J}{k_B}]$ was obtained. The precision of such measurement is affected by the limited computing power adopted and the finite scaling inherent to finite-size lattices. Additionally, the dependence of the phase transition on the topology of the lattice is investigated, yielding results consistent with the literature.

1. INTRODUCTION AND THEORY

1.1. The Ising model

In 1925 Ernst Ising[5] published the analytic solution to the Ising Model in one dimension. The model describes the spin interaction between particles and their nearest neighbours with possible collinear spin projections $S_i = \pm 1$. The two-dimensional model was solved analytically by Lars Onsager[8] in the absence of an external magnetic field on a square lattice. The two-dimensional Ising model represents an interesting example of Monte Carlo simulations in statistical physics, as it is both exactly solvable and nontrivial.

The Ising model is defined by the Hamiltonian

$$H = -\sum_{\langle ij \rangle} J_{ij} S_i S_j - h \sum_i S_i \tag{1}$$

where the $S_i = \pm 1$ is a spin degree of freedom on the lattice cite i, J_{ij} is a coupling constant (on a isotropic lattice the coupling constant has the same value J in all directions, as assumed in this paper), $\langle ij \rangle$ denotes the nearest neighbour summation and h is an external applied magnetic field, assumed throughout this paper to have the units of $\frac{J}{\mu}$ or T.

The theoretical predictions by Onsager state that for the two-dimensional Ising model there exists a critical temperature T_c for which the system transitions from an ordered state to a disordered state as a function of the temperature gradient. The ordering refers to the spin alignment in the lattice. Specifically, for the coupling constant $J > 0$, the ordered system is ferromagnetic for $T < T_c$, with the energy minimised by the spin alignment condition $S_i S_j = +1$ around $0\frac{J}{k_B}$. On the contrary, a disordered state denotes a random distribution of spin alignments, referred to as paramagnetic phase at $T > T_c$.

Onsager's analytical solution on an isotropic square lattice predicts that the critical temperature for the two-dimensional Ising model will occur at

$$T_c = \frac{2J}{\ln 1 + \sqrt{2}} \approx 2.269\frac{J}{k_B} \tag{2}$$

where k_B is Boltzmann's constant. This result will be adopted throughout this paper as a benchmark to test the accuracy of the simulations.

1.2. Physical observables

Macroscopic physical observables are studied in this simulation[1]. The average change in energy per spin site is given by the difference between the Hamiltonian given by eq.(1) with a spin flip and the original Hamiltonian in the considered state, so that

$$\Delta E_i = 2(J \sum_{\langle ij \rangle} S_i S_j + h \sum_i S_i) \tag{3}$$

where J is taken to be the isotropic coupling constant.

The magnetisation of the system is given my

$$M = \langle \sum_i S_i \rangle \tag{4}$$

where the sum is over the total number of spins N on the lattice.

In the absence of and external magnetic field h, for temperature values $T > T_c$, the magnetisation fluctuates around zero as the system is in a paramagnetic phase.

For $T \simeq T_c$ clusters of parallel spins appear, resulting in a non-zero magnetisation.

For temperature values $T < T_c$ domains of positive and negative magnetisation are formed, domain walls diffuse and interact, finally resulting in a single domain for temperatures close to $0\frac{J}{kB}$. Under such conditions, the system is in a fully ferromagnetic phase (with $J > 0$), with a total magnetisation evaluating to unity.

The variance of the energy and the magnetisation yield two observables of interest[4]: the magnetic susceptibility

[1] The complete repository of python and shell scripts used to produce the results presented can be found at `https://github.com/delanebl/Ising`. The codes were run on locally on an Apple MacBook Pro, processor 2.6 GHz Intel Core i5, RAM 8 GB 1600 MHz DDR3.

χ and the heat capacity at constant volume given by C_V given by

$$\chi = \frac{1}{k_B T}(\langle M^2 \rangle - \langle M \rangle^2) \tag{5}$$

$$C_V = \frac{1}{k_B T^2}(\langle E^2 \rangle - \langle E \rangle^2) \tag{6}$$

2. METHODS

In order to avoid carrying out the computationally expensive task of computing the expectation value of an observable over all microstates, a finite set of states are sampled from, according to the Metropolis algorithm[6].

The simulation used allows for the main properties of the lattice to be set (shape, dimensions). l sweeps are performed throughout the lattice iterating the Metropolis algorithm to bring the system to equilibrium. A second set of iterations $l' = \frac{l}{2}$ of the Metropolis algorithm is performed to collect the statistics of the observables, normalising by the quantity l' to yield the correct mean. The above is reiterated for a set of temperatures to yield the evolution of the system as a function of the temperature gradient. The reader is invited to consult the appendices D and E to view the flow chart describing this routine.

3. RESULTS AND ANALYSIS

3.1. Physical observables

The following results were produced using the IPython script `Ising2D.ipynb` for a 50×50 isotropic square lattice, for temperatures between $0.1\ \frac{J}{k_B}$ and $4.0\ \frac{J}{k_B}$, with the isotropic coupling constant $J = 1.0$ and the external magnetic field $h = 0$.

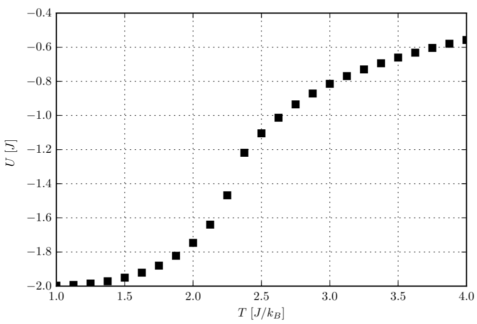

FIG. 1: Average energy U per spin site versus temperature (black).

Figure 1 illustrates the average spin energy as a function of temperature. This increases in a nonlinear fashion with temperature, exhibiting the highest variation around the temperature value $T = 2.269 \frac{J}{k_B}$ at which a phase transition between ferromagnetic and paramagnetic phase is expected, according to the theory.

The order parameter describing the phase dependence on temperature for the Ising model is the magnetisation per site $m = \frac{\langle M \rangle}{N}$ with N the total number of spin sites.

Figure 2 illustrates the average absolute magnetisation per spin site $| \langle m \rangle |$ as a function of the temperature. Onsager's solution for the two-dimensional square lattice[8] is plotted in red for the spontaneous magnetisation given by

$$|m(T)| = \begin{cases} (1 - \sinh^{-4}(\frac{2J}{T}))^{\frac{1}{8}} & \text{if } T < T_c \\ 0 & \text{if } T > T_c \end{cases} \tag{7}$$

Additionally, the theoretical value of the critical temperature for the isotropic two-dimensional square lattice $T_c \simeq 2.269 \frac{J}{k_B}$ is shown in cyan.

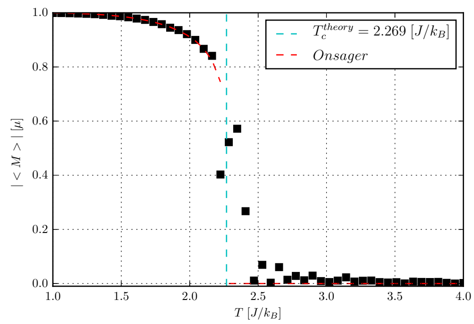

FIG. 2: Average magnetisation per spin site versus temperature (black), Onsager's analytical prediction for the spontaneous magnetisation (red), Onsager's prediction for the critical temperature in an isotropic square lattice with $h = 0$ (cyan).

As it can be seen, a phase transition from a ferromagnetic phase to a paramagnetic phase is evident with a critical temperature fully consistent with the analytical predictions. The magnetisation decreases from its unity value at low temperatures to its saturation zero value at high temperatures.

In order to identify the critical temperature at which the phase transition occurs with higher precision, it is useful to analyse the fluctuations of the magnetisation, given by eq.(5) for the susceptibility χ.

From figure 3 it is possible to observe a marked peak for a temperature value $T \in [2.263 \frac{J}{k_B}, 2.241 \frac{J}{k_B}]$, where fluctuations of the magnetisation are strongest and the susceptibility χ diverges. This is in good agreement with the behaviour of the magnetisation discussed above.

The behaviour exhibited by the macroscopic observables shown above and the estimation of the critical temperature T_c is confirmed by looking at the specific heat capacity at constant volume C_V (eq.(6)), which characterises the fluctuations of the internal energy per site.

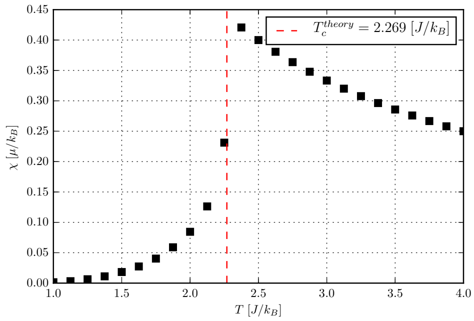

FIG. 3: Susceptibility χ versus temperature (black), Onsager's prediction for the critical temperature in an isotropic square lattice with $h = 0$ (red).

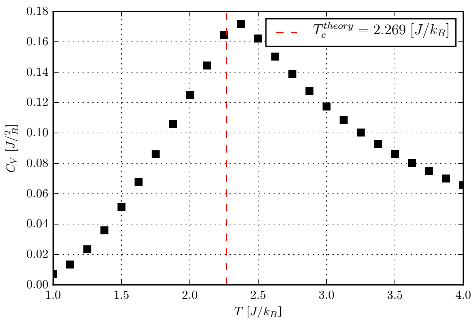

FIG. 4: Heat capacity C_V versus temperature (black), Onsager's prediction for the critical temperature in an isotropic square lattice with $h = 0$ (red).

The behaviour of the heat capacity is consistent with the divergence shown for the magnetic susceptibility, with a peak at a temperature value $T \in [2.267\frac{J}{k_B}, 2.425\frac{J}{k_B}]$. This is slightly higher than the estimation allowed by figure 3, with a less pronounced divergence as C_V diverges logarithmically and not as a power-law[1].

3.2. Phase transition and estimation of the critical temperature

One of the most common physical problems studied in simulations are phase transitions in various forms, such as the transition from ferromagnetism to paramagnetism. Most phase transitions can be described by an order parameter[9]. Mathematically, this is zero in one phase (usually called the disordered phase), non-zero in the other phase (ordered phase). Thus, it cannot be an analytic function at the transition point. In this paper, the magnetisation $|m|$ is adopted as the preferred order parameter for the Ising model.

Normally, transitions are either first or second order. The name comes from the number of derivatives of the free energy $F = -T \log Z$ that must be computed before a clear discontinuity appears. It can be shown that the magnetisation and the susceptibility are given by the first and second derivative of F with respect to h, yielding a second order phase transition for the two dimensional Ising model.

The dependence of the critical temperature on lattice size is evident in the work of Dolfi *et al.*[3]: for larger lattice sizes, the critical temperature, at which the susceptibility χ diverges, approaches the theoretical value $T_c \approx 2.269\frac{J}{k_B}$. In order to further investigate the value of T_c, the fourth-order Binder cumulant[2, 3] U_4 was used.

$$U_4 = 1 - \frac{\langle m^4 \rangle}{3\,\langle m^2 \rangle^2} \tag{8}$$

At low temperatures, the ratio $\frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}$ tends to unity, whereas Gaussian fluctuations of the order parameter give a value 3 in the high temperature phase. The non-trivial feature of the Binder cumulant resides in its value at the critical point, which can be shown to be universal and independent of the system size. Therefore, a plot of the Binder cumulant versus temperature allows a determination of T_c at the crossing points of the curves with different system sizes. To this end, the work of Selke and Shchur[10] was reproduced for an isotropic square lattice. Figure 5 provides an estimate of the critical temperature $T_c \approx 2.193\frac{J}{k_B}$ with a critical Binder cumulant $U^* \approx 0.631$. These results are in partial agreement with Selke and Shchur's, and are most likely affected by the fact that this result was produced using 20 temperature values and could have been bettered by using more computationally expensive simulations.

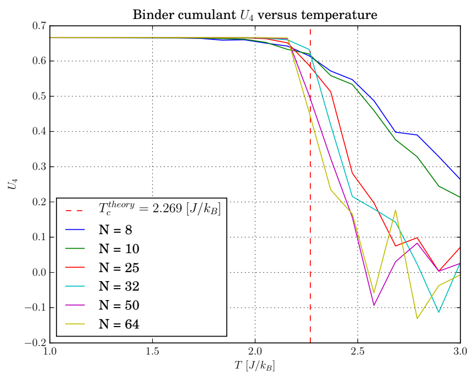

FIG. 5: Binder cumulant U_4 versus temperature for different lattice sizes, $T_c^{theory} = 2.269\frac{J}{k_B}$ (red, dashed).

The difference in the critical temperatures inferred from C_V, χ and U_4 can be explained by the *finite scaling.* Such small differences are expected on small finite systems. The effective critical temperature $T_c(N)$ can be defined at the position of the peaks, and is expected to drift with system size according to $T_c(N) = T_c + AL^{-\frac{1}{\nu}}$. The constant A can be different with different ways of defining T_c, and, according to the literature, $\nu = 1$ [1]. The quality of the estimates for the critical temperature increases considerably when using larger system sizes. For further information regarding the divergence of the physical observables caused by finite scaling and encoded by the *critical exponents*, the reader is invited to consult the work by Nightingale and Privman[7].

3.3. Phase transitions and the topology of the lattice

The concluding analysis of this paper explores the dependence of the order parameter, the absolute magnetisation $|m|$, thus the phase transition, on the topology of the lattice. The reader is invited to view the relevant graphs placed in the appendix.

The three-dimensional Ising model remains unsolved analytically. A phase transition is expected, with the critical temperature approximately known from Monte Carlo simulations: $T_c \simeq 4.51142 \frac{J}{kB}$. It must be noted that T_c and the values of the critical exponents depend on the dimensionality of the system, and are thus not equal for the two- and three-dimensional Ising models. Additionally, higher values of the isotropic coupling constant yield a higher critical temperatures.

In the case of nearest neighbour interactions, E. Ising provided an exact solution of the one dimensional model[5]. At any positive temperature the free energy is analytic and the truncated two-point spin correlation decays exponentially fast. At zero temperature, there is a second order phase transition: the free energy is infinite and the truncated two point spin correlation remains constant. Therefore, for the one-dimensional Ising model, the critical temperature is $T = 0 \frac{J}{k_B}$.

Finally, in the presence of a nonzero external magnetic field h no phase transition for the two-dimensional Ising model is evident, as the external field disrupts the spontaneous magnetisation of the system as the spin sites will tend to take a value ± 1 depending on the sign of h.

4. CONCLUSIONS

The application to the Markov Chain Monte Carlo Metropolis algorithm to the Ising model was investigated. The two-dimensional Ising model represents an interesting example of Monte Carlo simulations in statistical physics, as it is both exactly solvable and nontrivial, and was thus taken as the main focus of this analysis. The dependence of the second order phase transition on the temperature gradient and the topology of the lattice were explored by studying the absolute magnetisation $|m|$, used as order parameter. For an accurate estimate of the critical temperature, the susceptibility χ, the specific heat capacity C_V and the Binder cumulant U_4 were obtained, yielding the estimate $T_c \in [2.193 \frac{J}{k_B}, 2.425 \frac{J}{k_B}]$, consistent with Onsager's predictions, although limited by the computing power available and finite scaling inherent to the simulations. As a corollary to this investigation, Ising's prediction was verified for the one-dimensional model as the divergence of $|m|$ was observed for temperatures close to $0 \frac{J}{k_B}$ (Appendix A). The three-dimensional model remains unsolved analytically. However, the findings shown in appendix A suggest the presence of a phase transition consistent with the literature. Finally, the two-dimensional model does not exhibit any phase transition in the presence of a non-zero external magnetic field h, as expected, with the dependence of the observable statistics on the lattice size and higher values of J made evident by the graphs shown in appendix A.

In conclusion, the investigation of the Metropolis algorithm proved successful in showcasing some of the main points of interest of the Ising model, subject to systematic biases given by the limited computing power and finite scaling.

[1] *ALPS 2 Tutorials:MC-07 Phase Transition* [n.d.], `http://alps.comp-phys.org/mediawiki/index.php/ALPS_2_Tutorials:MC-07_Phase_Transition`.

[2] Binder, K. [1981], 'Finite size scaling analysis of ising model block distribution functions', *Zeitschrift für Physik B Condensed Matter* **43**(2), 119–140.

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[4] Hutzler, S. [2014], 'PY3C01 Computer Simulations I Numerical and Statistical Methods', `http://www.tcd.ie/Physics/Foams/LectureNotes/`.

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[6] Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H. and Teller, E. [1953], 'Equation of state calculations by fast computing machines', *The journal of chemical physics* **21**(6), 1087–1092.

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[8] Onsager, L. [1944], 'Crystal statistics. i. a two-dimensional model with an order-disorder transition', *Physical Review* **65**(3-4), 117.

[9] Rummukainen, K. [n.d.], 'Monte Carlo Simulation methods, Phase transitions and finite size scaling', `http://www.helsinki.fi/~rummukai/simu/fss.pdf`.

[10] W.selke, L. N. S. [n.d.], 'Critical Binder cumulant revisited', `https://www.physik.uni-leipzig.`

de/~janke/CompPhys07/Folien/selke-poster2.pdf.

Appendix A

1. 1D Ising Model

Figure 6 illustrates the phase order parameter $|m|$ as a function of temperature, with $J = 1$, $h = 0$, and a spin chain with 100 spin sites. The plot suggests the singularity predicted by Ising for the one-dimensional model, with a phase transition at $0\ \frac{J}{k_B}$, for the nearest neighbour interactions.

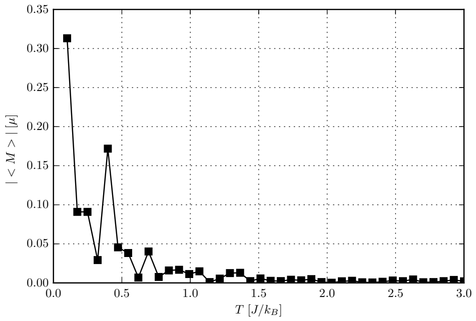


FIG. 6: Absolute magnetisation versus temperature, one-dimensional Ising model.

2. 3D Ising Model

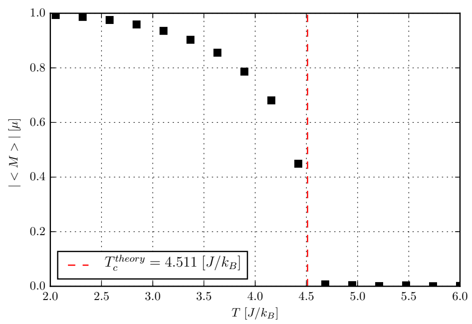


FIG. 7: Absolute magnetisation versus temperature, three-dimensional Ising model. $T_c^{theory} = 4.511 \frac{J}{k_B}$ in red, dashed.

Figure 7 illustrates the phase order parameter $|m|$ as a function of temperature, with $J = 1$, $h = 0$, for an isotropic cubic lattice with $50 \times 50 \times 50$ sites. A phase transition is evident and is fully consistent with the theory.

3. 2D Ising model

Figure 8 illustrates how higher values of isotropic coupling constant J yield higher critical temperatures.

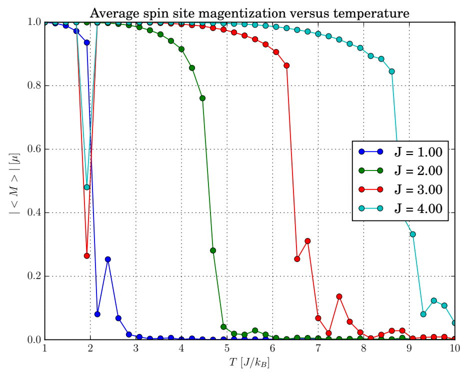


FIG. 8: Absolute magnetisation versus temperature, two-dimensional Ising model for J = 1.0 (blue), J = 2.0 (green), J = 3.0 (red), J = 4.0 (cyan), for N = 50, $h = 0$.

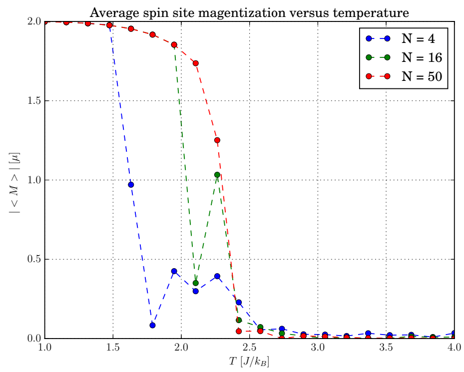


FIG. 9: Absolute magnetisation versus temperature, two-dimensional Ising model for lattice side size N = 4 (blue), N = 16 (green), N = 50 (red).

Figure 9 illustrates the dependence of the absolute magnetisation with $|m|$ with $J = 1$, $h = 0$, and the accuracy of the statistical analysis carried out, on the length of the lattice sides. In order to balance accuracy and run time, the results presented in the paper we obtained using a 50×50 lattice.

The action of an external field disrupts the spontaneous magnetisation of the system, as shown in figure 10.

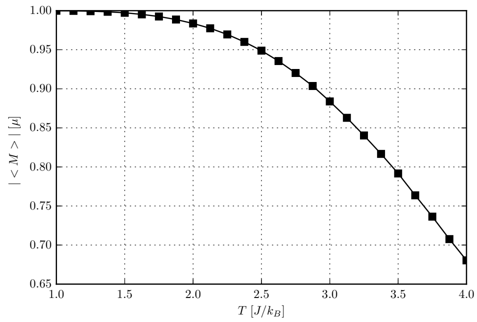


FIG. 10: Absolute magnetisation versus temperature with `J = h = 1.0` for a 2D isotropic 50×50 square lattice.

Appendix B: Error analysis

The Ising Model produces correlated samples, with the number of independent samples is reduced

$$\Delta A = \sqrt{\frac{Var(A)}{M}(1 + 2\tau_A)} \tag{B1}$$

with the autocorrelation time defined as

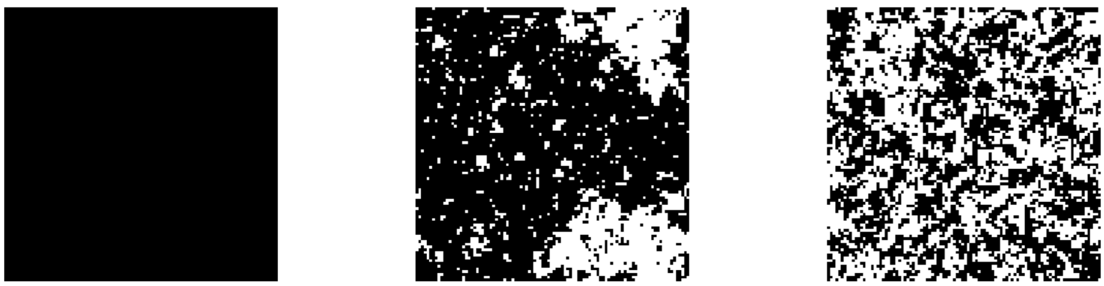
$$\tau_A = \frac{\sum_{t=1}^{\infty}(\langle A_{i+t}A_i\rangle - \langle A\rangle^2}{Var(A)} \tag{B2}$$

All the calculations performed were carried out subect to the machine round-off error of $\mathcal{O}(10^{-23})$. This is a systematic bias affecting all double-precision calculations. Such a bias could have been reduced using the python type `decimal`. However, for the purposes (precision and speed) of this analysis, it was deemed unnecessary to cast the variables into this python-specific type.

Finally, in order to achieve higher computing power, an application of parallel computing in python was attempted using the module `multiprocessing`. This proved unsuccessful due to the sequential order of the sampling loop in the main routine.

Appendix C: Visualising the phase transition

Figure 11 illustrates the transition from a ferromagnetic to a paramagnetic phase, for a 100×100 isotropic square lattice.



(A) $T = 0.3\frac{J}{k_B}$ (B) $T = 2.269\frac{J}{k_B}$ (C) $T = 3.0\frac{J}{k_B}$

FIG. 11: 2D Ising model, $J = 1.0$, $h = 0$ transitions from ferromagnetic to paramagnetic phase.

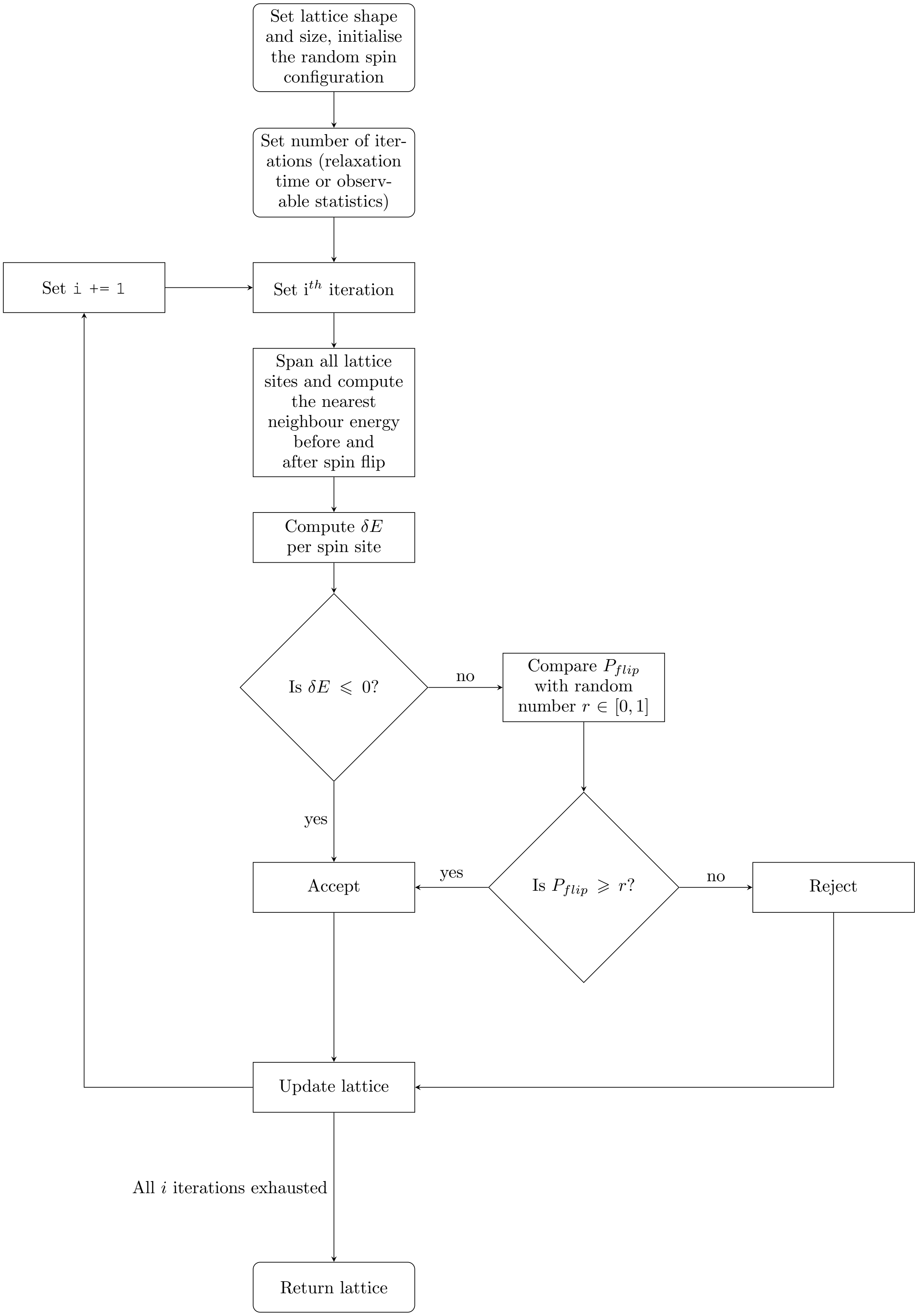
The ground state is achieved with a complete spin alignment. This is given by the number of edges connecting each spin site to its nearest neighbours, multiplied by $-JN$, divided by 2 as $S_i = \pm 1$. Thus, for an isotropic square lattice

$$E_{ground} = -JN(\frac{4}{2}) = -2JN \tag{C1}$$

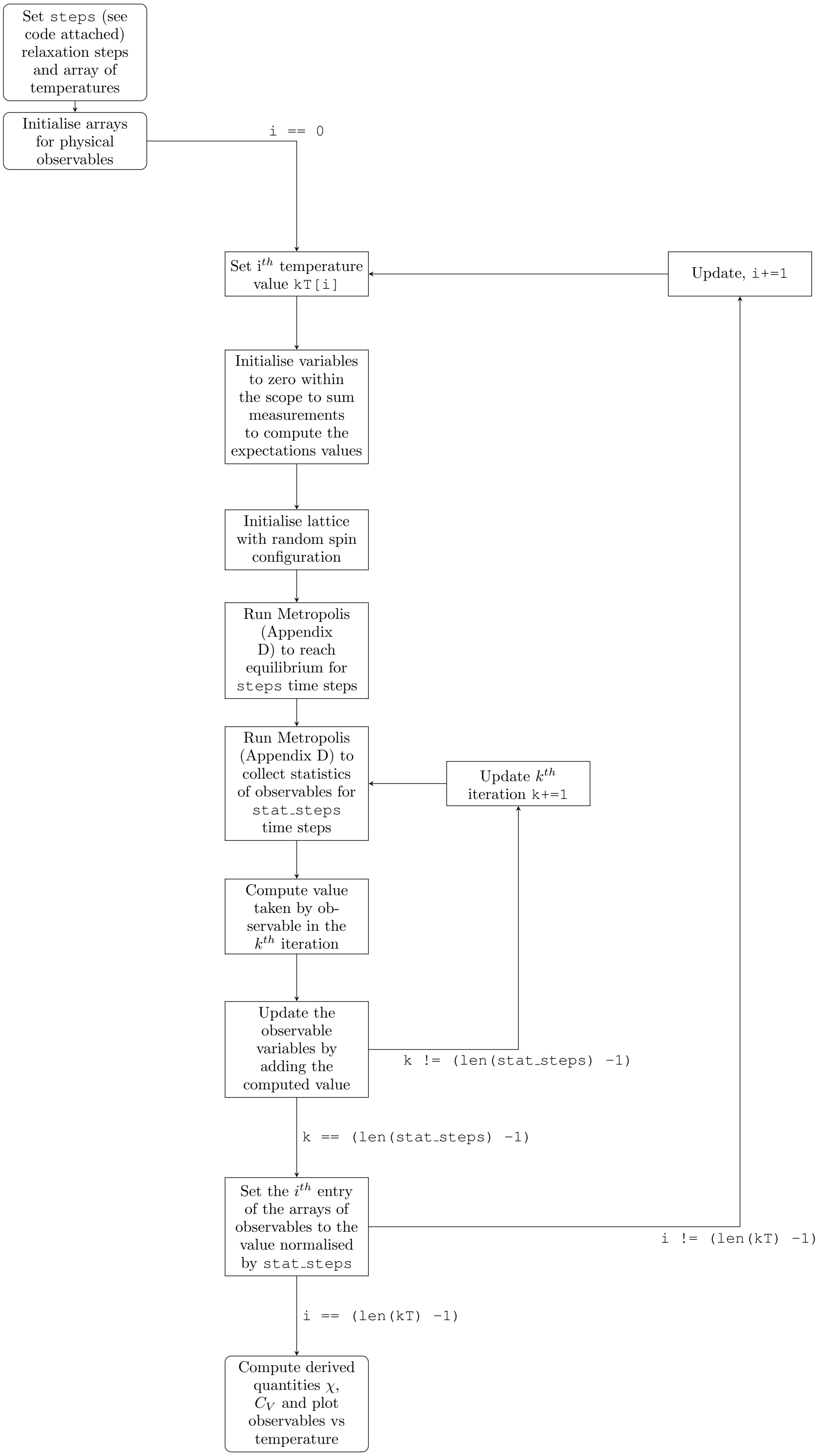
The transition from a ferromagnetic to a paramagnetic phase is characterised by the decrease of the size of clusters of aligned spins with increasing temperature. The mean size of such clusters is referred to as correlation length. For $T \approx 0\frac{J}{k_B}$ the correlation length is null. The correlation length increases with temperature as local clusters start to form and diverges at infinity at T_c as the system exhibits no global magnetisation. For $T > T_c$, the ordered clusters shrink and in the limit $T \to \infty$ the correlation goes to zero.

The diverging correlation length at the transition causes the system interruption to spread quickly over all the small clusters, changing the spin configuration. The divergence of the observables discussed above are caused by the divergence of the correlation length at the phase transition.

Appendix D: Metropolis algorithm



Appendix E: Ising model main routine



Appendix F: Code

Adapted from Ising2D.ipynb. Please consult the module IsingClass.py and the scripts Ising.sh and Ising.py for further information.
Available on github at `https://github.com/delanebl/Ising`.

```

# coding: utf-8

# # The 2D Ising Model
#

# This is the IPython notebook compiled by me, Blaise Delaney (Junior Sophister Theoretical Physics, ID: 12313570), to tackle the tasks set by Dr. Thomas Archer for the course PY3C01, Trinity College, University of Dublin.

from __future__ import division #necessary to perform division of ints effectively cast into floats before division

import math
import numpy as np
import matplotlib.pyplot as plt
import numpy.random as rand

import IsingClass #module written to carry out the required calculations (metropolis, neighbours, energy, magnetization, etc.)

#ipython, plot in notebook
get_ipython().magic(u'matplotlib inline')


N = 50 #grid dimensions
J = 1.0 #coupling in the hamiltonian
h = 0.0 #external magnetic field



model = IsingClass.Ising(N,J,h) #constructor



steps = 3000 #steps for equilibrium
temp_steps = 25 #step size for increase in temperature [J/k]

kT = np.linspace(1.0,4.0,temp_steps) #temperature values

#arrays for future plotting
magnetization = np.zeros(temp_steps)
Energy = np.zeros(temp_steps)
susceptibility = np.zeros(temp_steps)
specific_heat = np.zeros(temp_steps)
mag_square = np.zeros(temp_steps)
e_square = np.zeros(temp_steps)
binder = np.zeros(temp_steps)
mag_four = np.zeros(temp_steps)

for l in range(len(kT)):
    temperature = kT[l]

    #initialise observables to zero
    M = 0
    E = 0
    M_sq = 0
    E_sq = 0

    M_fth = 0

    #reset to random initial configuration
    lattice = model.spin_config()
```

```
    #set out to reach equilibrium
    for t in range(steps):
        model.metropolis(lattice, temperature)

    #collect statistics allowing the system to evolve
    stat_steps = int(steps/2)
    for k in range(stat_steps):

        #model.metropolis(lattice, temperature,N,N,J,h)
        model.metropolis(lattice, temperature)

        mag = model.mag_per_spin(lattice)
        mag2 = model.mag2_per_spin(lattice)
        engy = model.energy(lattice)
        engy2 = model.energy2(lattice)


        M += mag
        E += engy
        M_sq += mag2
        E_sq += engy2



    #observables, after equilibrium is achieved, normalised by sweeps
    magnetization[l] = abs(M)/stat_steps
    Energy[l] = E/stat_steps
    mag_square[l] = M_sq/stat_steps
    e_square[l] = E_sq/stat_steps

#perform manipulation directly on array instead of loop
susceptibility = (mag_square - magnetization**2)/kT
specific_heat = (e_square - Energy**2)/(kT**2)
```

: Ising2D.py