

Maks Koncilja

Applying Monte Carlo methods to the Ising model

Eutopija project

Mentors: Prof. Dr. Laura Hernandez and Prof. Dr. Mihael Perman

Introduction

Ising model is mathematical model of ferromagnetism. The model consists of spins that can be in one of two states up or down (1 or -1). The spins are arranged in a lattice, where each spin interacts with its neighbours. In ferromagnets aligned neighbouring spins have lower energy than those who are misaligned, the system of spins tends to the lowest energy but the heat bath interrupts this tendency, allowing different micro-states.

Monte Carlo methods are algorithms that depend on repeated random sampling to obtain numerical results. It is a way to solve deterministic problems with randomness. In physics Monte Carlo methods (from now on written as MC methods) are used for simulating systems with coupled degrees of freedom, such as distorted materials, strongly coupled solids and fluids.

History

Wilhelm Lentz invented the The Ising model problem. His student Ernest Ising found a one-dimensional solution. The analytical two dimensional square lattice solution was proposed years later by Lars Onsager [3]. Greater dimensions don't have analytical solutions and are therefore studied numerically.

One of the first variants of MC methods was used to solve Buffon's needle problem, in which value of π can be estimated by dropping needles on the floor marked by equidistant strips. Enrico Fermi experimented with MC methods for studying neutron diffusion. Later Stanislaw Ulam invented modern version of the Markov Chain Monte Carlo while working at the Los Alamos National Laboratory.

In this project a simple Metropolis algorithm is used. It was developed by Nicholas Metropolis and his colleagues and published in 1953 article Equation of State Calculations by Fast Computing Machines [2].

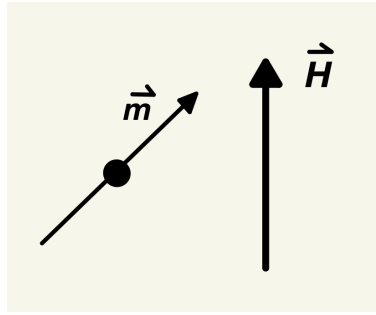
Purpose of this few pages is to help students learn and understand basics of Metropolis algorithm through practical example of Ising model. This seminar is mainly composed of lectures given by Professor Laura Hernandez during my short stay at Cergy.

Ising model

First we have to understand behaviour of a magnetic moment \vec{m} in a magnetic field \vec{H} .

Energy of magnetic moment in magnetic field is

$$E = -\vec{m} \cdot \vec{H} \begin{cases} \text{min value,} & \text{aligned } \vec{m} \uparrow \uparrow \vec{H} \\ \text{max value,} & \text{opposed } \vec{m} \downarrow \uparrow \vec{H} \\ 0, & \text{if } \vec{m} \perp \vec{H} \end{cases}$$



magnetic moment in a magnetic field

Magnetic moment is related to spin. In quantum mechanics components of angular momentum for spin s particle measured along any direction can take on the values:

$$S_i = \hbar s_i, \quad s_i \in \{-s, -(s-1), \dots, s-1, s\}$$

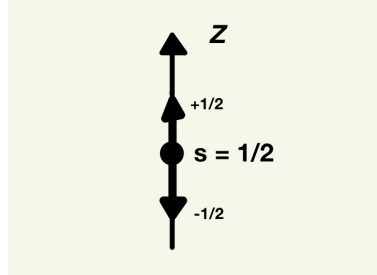
where S_i is the spin component along the i -th axis (x,y or z), where s_i is the spin projection quantum number along the i -th axis, and s is the principal spin quantum number. Conventionally the direction chosen is the z axis:

$$S_z = \hbar s_z, \quad s_z \in \{-s, -(s-1), \dots, s-1, s\}$$

where the S_z is the spin component along the z axis. There are $2s + 1$ possible values of s_z , the number " $2s + 1$ " is the multiplicity of the spin system.

Electron is a fermion and has spin value $s = 1/2$, there are only two possible values $s_z = +\frac{1}{2}$ and $s_z = -\frac{1}{2}$. These correspond to quantum states in which

the spin component is pointing in the $+z$ or z directions respectively, and are often referred to as “spin up” and “spin down” [4].



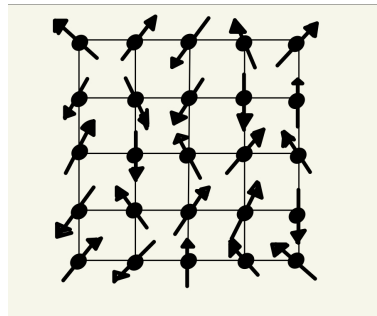
spin up and spin down

Model of a solid

2D solid can be presented as a lattice of atoms, each with its own spin (and therefore its own magnetisation).

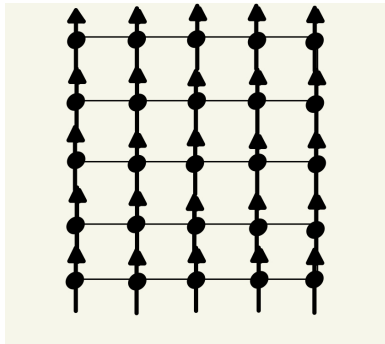
Paramagnet

In Paramagnet there are no interactions among spins of neighbouring atoms. In zero external magnetic field magnetic moments point in random directions. Magnetisation of a crystal (sum of individual magnetic moments) is therefore $\vec{M} = \sum_i \vec{s}_i = 0$.

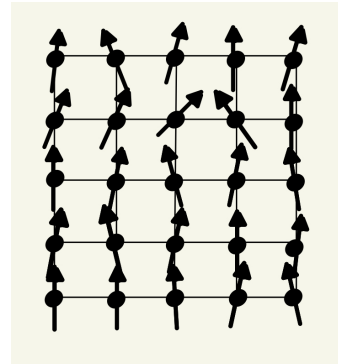


spin up and spin down

At low temperatures ($T \approx 0K$) in external magnetic field each spin follows individually an applied magnetic field. If temperatures are not really low, temperature bath and external magnetic field compete for direction of a spin (free energy $F = U - TS$, where $U \propto -\vec{m}_i \vec{H}$ and $TS \propto e^{-\frac{E}{kT}}$).



$$\vec{H} \neq 0, T \approx 0K$$



$$\vec{H} \neq 0, T \neq 0K$$

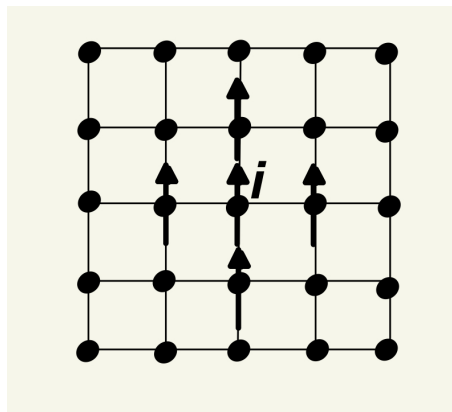
Paramagnet in external magnetic field at zero and non zero low temerature

Ferromagnets

Interactions among particles of ferromagnetic materials tend to align them. Interaction between two closest neighbours is written as:

$$E_{ij} = -J \vec{s}_i \cdot \vec{s}_j$$

where J is interaction constant, which by its positivne or negative sign categorises the material.



Ising hamiltonian

$$H = -J' \sum_{\langle ij \rangle} \tilde{s}_i \tilde{s}_j$$

where $\tilde{s}_i = \pm 1/2$, $\frac{J'}{4} = J$. We will rewrite the hamiltonian in the form:

$$H = -J \sum_{\langle ij \rangle} s_i s_j$$

where $s_i = \pm 1$ and J includes all the contents such that it has the dimension of an energy.

if $J > 0$, ferromagnetic phase

the ground state (minimum energy) of 2D square lattice of N particles

$$E = -4J \frac{N}{2} = -2JN$$

with degeneracy $g = 2$ (meaning two states with same energy)

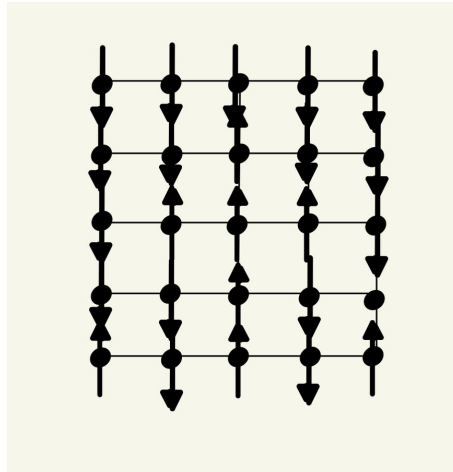
if $J < 0$, antiferromagnetic state

has a hamiltonian:

$$H = -J \sum_{\langle ij \rangle} s_i s_j = +|J| \sum_{\langle ij \rangle} s_i s_j$$

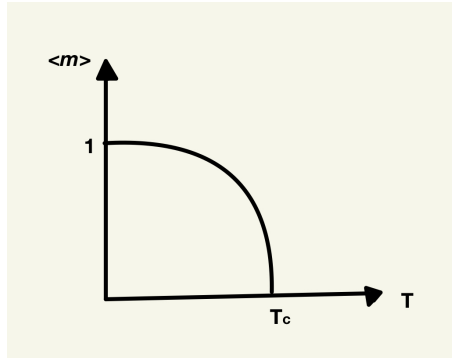
the ground state energy $E = -2JN$

Ising ferromagnet if $T \neq 0$ looks like figure bellow.



Ising ferromagnet at nonzero temperature

At critical temperature ferromagnet goes from ordered phase to disordered phase, which can be represented by a graph of average magnetisation per spin $\langle m \rangle = \frac{M}{N}$ as a function of temperature.



Graph of average magnetisation per as a function of temperature

The canonical ensemble

- micro-state of a system $l = (s_1, s_2, s_3, \dots, s_N)$.
- macro-state of a system is associated to the energy. (n spins up (\uparrow) and $N - n$ spins (\downarrow))

It is important to recognise that one macro-state may have many micro-states associated to it.

For purpose of this seminar we will use the notation p_i for probability of micro-state i in the canonical ensemble

$$p_i = \frac{e^{-\beta E_i}}{Z}$$

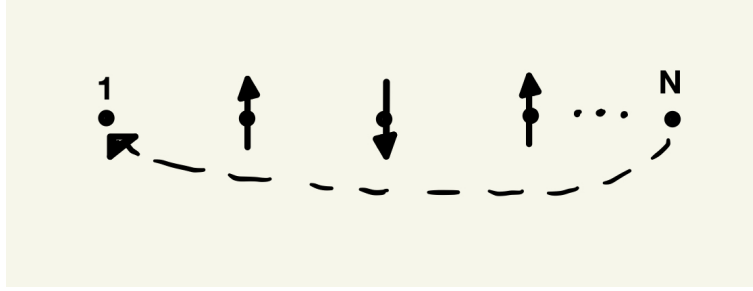
where canonical ensemble is written as sum over all micro-states:

$$Z = \sum_i e^{-\beta E_i}$$

writing energy of a lattice as a function of variables $E_l(s_1^l, s_2^l, s_3^l, \dots, s_N^l)$ where s_k^l is a spin of a particle k in the micro-state l .

Analytical solution of Ising model in 1 dimension

In this subsection we will find analytical solution of Ising model in 1 dimension. 3D and higher dimensional Ising models don't have analytical solutions.



Ising model in 1 dimension

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j = \mathcal{H} = -J \sum_i s_i s_{i+1}$$

we have to take in to account periodic boundary contions $s_{N+1} = s_1$

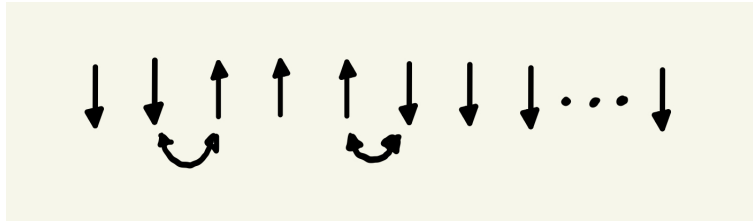
the ground state with two possible macro-states all up or all down gives us $H = -JN = E_0$ degeneracy is 2

$$Z = \sum_l e^{-\beta \mathcal{H}} = 2e^{-\beta E_0} + \dots$$

1st excited state has energy $E_1 = -(N-2)J + 2J$

there are $\binom{N}{2}$ possible ways to choose 2 broken links among N possible.

first excited states brings $\binom{N}{2} e^{-\beta E_1}$ to canonical ensemble.



1st excited state of Ising model in 1 dimension

from here we can guess that energy of n-th excited state is

$$E_n = -\frac{J}{2}[(N-2n) - 2n] = -\frac{JN}{2} + 2Jn$$

for calculation of canonical ensemble we will take in to account degeneracy for each energy

$$Z = \sum_n g_n e^{-\beta E_n} = \sum_{n=0}^{N/2} \binom{N}{2n} e^{-\beta(-\frac{JN}{2} + 2Jn)} = (e^{\beta J})^{N/2} \sum_{n=0}^{N/2} \binom{N}{2n} (e^{\beta J})^{-2n}$$

mathematical binom intermezzo

$$(1+u)^N = \sum_{p=0}^N \binom{N}{p} 1^p u^{N-p} = \sum_{p=0}^N \binom{N}{p} u^{N-p}$$

$$(1-u)^N = \sum_{p=0}^N \binom{N}{p} 1^p (-u)^{N-p} = \sum_{p=0}^N \binom{N}{p} u^{N-p} (-1)^{N-p}$$

$$(1-u)^N + (1+u)^N = \sum_{p=0}^N \binom{N}{p} u^{N-p} [1 + (-1)^{N-p}]$$

which for even value of $N-p$ gives

$$(1-u)^N + (1+u)^N = 2u^N \sum_{n=0}^{N/2} \binom{N}{p} u^{-2n}$$

from the similarity we can write:

$$Z = \frac{(1+u)^N + (1-u)^N}{2u^{\frac{N}{2}}}$$

final form is

$$Z = 2^N [ch(\frac{\beta J}{2})^N + sh(\frac{\beta J}{2})^N]$$

Average energy is defined (formulas from statistical thermodynamics)

$$\langle E \rangle = -(\frac{\partial \ln(Z)}{\partial \beta})_{V,N}$$

calculating average energy for our case

$$\langle E \rangle = -\frac{JN}{2} \frac{ch^{N-1}(\frac{J\beta}{2}) sh(\frac{J\beta}{2}) + sh^{N-1}(\frac{J\beta}{2}) ch(\frac{J\beta}{2})}{ch^N(\frac{\beta J}{2}) + sh^N(\frac{\beta J}{2})}$$

Let's calculate the average number of broken links $\langle x \rangle$. For this case energy is not fixed therefore n is not fixed. We can write

$$E_n = -\frac{JN}{2} + 2Jn \Rightarrow \langle E \rangle = -\frac{JN}{2} + 2J \langle n \rangle$$

$\langle x \rangle$ is normalized by size of a lattice $\langle x \rangle = \frac{2\langle n \rangle}{N}$

$$\frac{\langle E \rangle}{N} = -\frac{J}{2} + J \langle x \rangle$$

final formula for $\langle x \rangle$

$$\langle x \rangle = \frac{\langle E \rangle}{JN} + \frac{1}{2} = \frac{e^{-\frac{\beta J}{2}}}{2ch(\frac{\beta J}{2})} \frac{1 - th^{N-1}(\frac{\beta J}{2})}{1 + th^{N-1}(\frac{\beta J}{2})}$$

high temperature limit $T \gg 0K$

$$\langle x \rangle = \frac{1}{2}$$

low temperature limit $T \approx 0K$

$$\langle x \rangle = \frac{1}{1 + e^{\beta J}} \approx e^{-\beta J} \rightarrow 0$$

Notions of Monte Carlo method

We work in canonical ensemble, using notation \vec{x}_l for l -th micro-state of the system. For Ising system of N particles $\vec{x}_l = (s_1^l, s_2^l, \dots, s_N^l)$

Probability of lattice being in micro-state l

$$P(\vec{x}_l) = \frac{e^{-\beta E(\vec{x}_l)}}{Z}$$

where canonical ensemble is a sum over all the micro-states.

$$Z = \sum_l e^{\beta E(\vec{x}_l)}$$

Problem is that if particles are not independent canonical ensemble becomes extremely hard to compute analytically. This is the reason we will later introduce Metropolis Monte Carlo method.

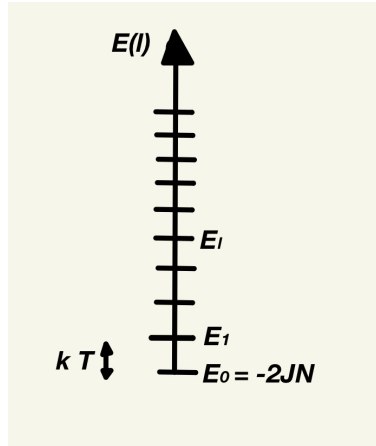
First principle of thermodynamics:

$$\Delta U = Q + W$$

where U is internal energy, Q , W are heat and work received by the system. For elementary quantities of heat and work exchanged we can rewrite into form

$$dU = \delta Q + \delta W$$

Internal energy U is average energy of the system $\langle E \rangle$. In statistical mechanics commonly used $\beta = \frac{1}{kT}$ represents energy difference between two energy levels.



Energy levels differ for a coefficient β

$g(E)$ is density of states with energy E and $g(E)dE$ is a number of micro-states between $(E, E + dE)$. Total number of possible micro-states for a system of N particles in Ising system is $\Omega_T = 2^N$ (since each spin can either be up or down).

For example a lattice of hundred particles $N = 100$, which means that there are $\Omega_T = 2^{100} \approx 10^{30}$ possible states.

Average energy of a system is

$$\langle E \rangle = \sum_l E(\vec{x}_l) P(\vec{x}_l)$$

where $E(\vec{x}_l)$ is an energy of micro-state \vec{x}_l . Calculating average energy of the system and canonical ensemble is undoable. This is the reason we need MC methods.

Naive solution is simple sampling of M micro-states. Where $M \gg 1$ to cover big enough sample but still much smaller than the number of all possible micro-states $M \ll 2^N$. Picking the micro-states at random implies over-representing high E micro-states which have $p(\vec{x}_l) \rightarrow 0$ at finite T .

Importance Sampling is the way to go. The idea is to pick \vec{x}_l that are the most probable at temperature T .

Lets start form the basic form for calculating average value of certain function of energy at temperature T .

$$\langle A \rangle = \sum_l A(\vec{x}_l) P(\vec{x}_l)$$

sum l goes over all micro-states l . Lets write $P(\vec{x}_l) = \pi(\vec{x}_l) = e^{-\beta E(\vec{x}_l)}/Z$

$$\langle A \rangle = \frac{\sum_l A(\vec{x}_l) \frac{\pi(\vec{x}_l)}{\pi(\vec{x}_l)} e^{-\beta E(\vec{x}_l)}}{\sum_l e^{-\beta E(\vec{x}_l)} \frac{\pi(\vec{x}_l)}{\pi(\vec{x}_l)}}$$

Now lets write $A(\vec{x}_l) \pi(\vec{x}_l) = A(\vec{x}_k)$ and lets cut the sum to the M most probable micro-states.

$$\langle A \rangle \approx \frac{\sum_{k=1}^M A(\vec{x}_k) \frac{e^{-\beta E(\vec{x}_k)}}{\pi(\vec{x}_k)}}{\sum_{k=1}^M \frac{e^{-\beta E(\vec{x}_k)}}{\pi(\vec{x}_k)}}$$

by taking into account $\pi(\vec{x}_l) = e^{-\beta E(\vec{x}_l)}/Z$ we get

$$\langle A \rangle = \frac{\sum_{k=1}^M A(\vec{x}_k) Z}{Z M}$$

$$\langle A \rangle_T = \frac{1}{M} \sum_{k=1}^M A(\vec{x}_k)$$

The important question is how do we select the most probable micro-states among the $\Omega_T = 2^N$. We build a chain of states such that the probability of being on a given state at time t only depends on the state at the previous time step. Let $P(\vec{x}_l, t)$ be the probability that the system is at state \vec{x}_l at time t .

We can write Master equation

$$\frac{\Delta P(\vec{x}_l, t)}{\Delta t} = - \sum_{x_{l'}} W(\vec{x}_l \rightarrow \vec{x}_{l'}) P(\vec{x}_l, t-1) + \sum_{x_{l'}} P(\vec{x}_{l'}, t-1) W(\vec{x}_{l'} \rightarrow \vec{x}_l)$$

where $W(\vec{x}_l \rightarrow \vec{x}_{l'})$ is transition probability per unit time to pass from $\vec{x}_l \rightarrow \vec{x}_{l'}$ by a local change and $P(\vec{x}_l, t-1)$ is probability of system being in micro-state \vec{x}_l in previous time step.

In equilibrium state

$$\frac{\Delta P(\vec{x}_l, t)}{\Delta t} = 0$$

$$\sum_{x_{l'}} -W(\vec{x}_l \rightarrow \vec{x}_{l'}) P(\vec{x}_l, t-1) + \sum_{x_{l'}} P(\vec{x}_{l'}, t-1) W(\vec{x}_{l'} \rightarrow \vec{x}_l) = 0$$

Sufficient condition is that each term of the sum is zero. Form of detailed balance condition is

$$W(\vec{x}_l \rightarrow \vec{x}_{l'}) P(\vec{x}_l, t) = P(\vec{x}_{l'}, t) W(\vec{x}_{l'} \rightarrow \vec{x}_l)$$

$$\frac{W(\vec{x}_l \rightarrow \vec{x}_{l'})}{W(\vec{x}_{l'} \rightarrow \vec{x}_l)} = \frac{P(\vec{x}_{l'}, t)}{P(\vec{x}_l, t)}$$

where the $P(\vec{x}_{l'}, t) = P_{eq}(\vec{x}_{l'})$ should not depend on t at equilibrium. But probability for equilibrium state is $P_{eq}(\vec{x}_l) = \frac{e^{-\beta E(\vec{x}_l)}}{Z}$

$$\frac{W(\vec{x}_l \rightarrow \vec{x}_{l'})}{W(\vec{x}_{l'} \rightarrow \vec{x}_l)} = \frac{e^{-\beta E(\vec{x}_{l'})}}{Z} \frac{Z}{e^{-\beta E(\vec{x}_l)}}$$

$$\frac{W(\vec{x}_l \rightarrow \vec{x}_{l'})}{W(\vec{x}_{l'} \rightarrow \vec{x}_l)} = e^{-\beta(E(\vec{x}_{l'}) - E(\vec{x}_l))}$$

Metropolis choice for $W(\vec{x}_l \rightarrow \vec{x}_{l'})$ is

$$W(\vec{x}_l \rightarrow \vec{x}_{l'}) = \begin{cases} \frac{1}{\tau_1} e^{-\beta[E(\vec{x}_{l'}) - E(\vec{x}_l)]}, & \text{if } \Delta E > 0 \\ \frac{1}{\tau_1}, & \text{otherwise.} \end{cases}$$

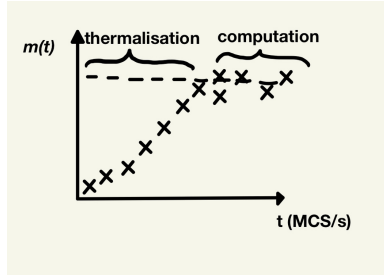
where τ_1 is a temporal scale for the transition note. $\tau_1 = 1$

Practically Metropolis algorithm is done by:

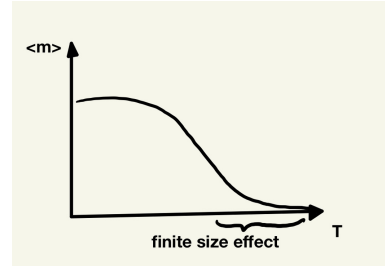
1. Initializing the system at random configuration.
2. Do many MCS/s (MC steps per spin, meaning N trials of local modifications) as thermalization process.
3. Measure variables and check for stability

Ex: $m = \frac{1}{N} \sum_{i=1}^N s_i$, $E = -J \sum_{\langle ij \rangle} s_i s_j$

lets assume that we start with random configuration at low temperature $T(\neq 0)$ **Metropolis importance sampling MC pseudocode**



thermalisation of a system



Average magnetisation $\langle m \rangle$ as a function of temperature T .

- (1) Choose an initial state
- (2) Choose a site i
- (3) Calculate the energy change ΔE which results if the spin at site i
- (4) Generate a random number r such that $0 < r < 1$
- (5) If $r < \exp(-\Delta E/k_b T)$, flip the spin
- (6) Go to the next site and go to (3)

Ising model Practically

Ising model (for the purpose of this seminar $\vec{H} = 0$)

$$E = -J \sum_{\langle i,j \rangle} s_i s_j = E_i + E'$$

where E_i is energy of spin i and E' is energy of the rest of the lattice. Flipping the spin i results in $\Delta E = \Delta E_i + 0$

$$E_i = -J s_i \sum_{j \in nn} s_j = -J s_i \eta$$

nn means nearest neighbours. Energy E'_i after flipping spin i is

$$E'_i = E = -J(-s_i)\eta$$

$$\Delta E_i = E'_i - E_i = 2J s_i \eta$$

η is sum of the values that depend on a spin position of neighbours relative to spin i .

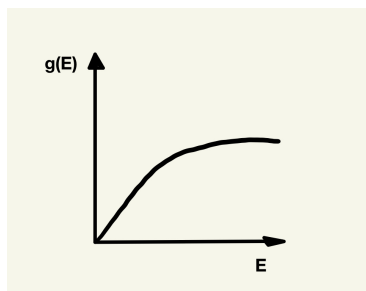
For Ising model this means $\eta \in (-4, -2, 0, 2, 4)$

Forgetting the initial state

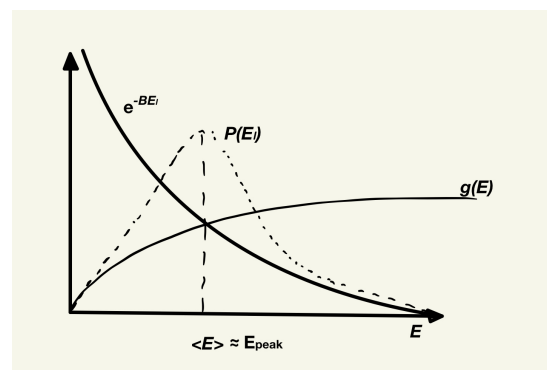
$$P(\vec{x}_l) = \frac{e^{-\beta E(\vec{x}_l)}}{Z}$$

$$P(E_l) = g_l \frac{e^{-\beta E_l}}{Z}$$

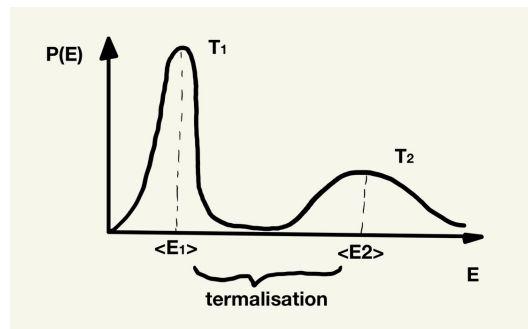
At the start we have random configuration, but there are many other \vec{x}_l with the same energy E_l . g_l represents the degeneracy of l -th energy level.



degeneracy of energy level as a function of energy $g(E)$



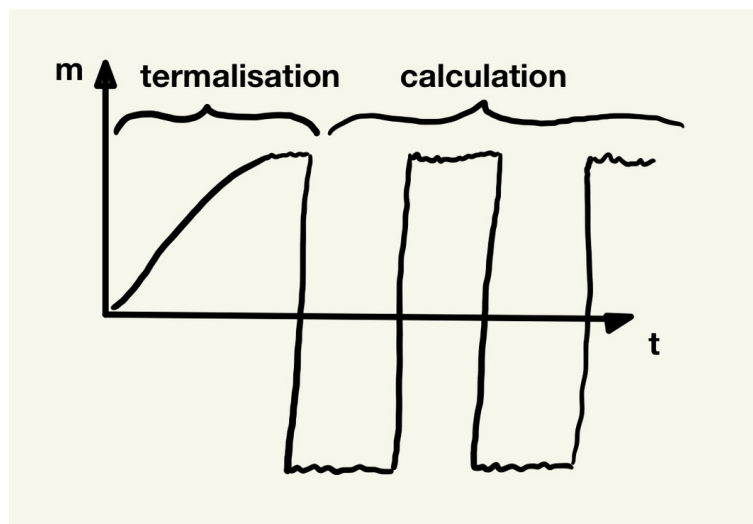
graph sketch of probability of energy state l , finding average energy



Termalisation a process of trail and error to get into most probable energy state at given energy.

Let's imagine a MC at low temperature T and you choose an initial random state, which is not one of the most probable at low T . Termalisation is a process of trail and error to get into most probable energy state at given low T .

Warning: due to the symmetry of Ising model in zero field exactly opposite states of the system are equiprobable (ex.: $\uparrow\uparrow\uparrow$ and $\downarrow\downarrow\downarrow$ are equiprobable). So you can observe:



equiprobable opposite states showcased on example of magnetisation

Calculated values

We can compute:

1. $\langle m \rangle$ magnetisation per spin $m = \frac{1}{N} \sum_{i=1}^N s_i = \frac{S_{TOT}}{N}$

2. $\langle E \rangle$ average energy $E = -J \sum_{\langle ij \rangle} s_i s_j$

3. C_H specific heat we derive from first principle of thermodynamics

$$dU = \delta Q + \delta W$$

for magnetic systems variables are M, T, \vec{H} . Reversibly exchanged heat is $Q_{rev} = T dS$, work done by the system is $\delta W = H dM$. Rewritten first principle of thermodynamics:

$$dU = T dS + H dM$$

Legendre transformations, Enthalpie $E = U - MH$

$$dE = dU - M dH - H dM$$

$$= T dS + H dM - M dH - H dM$$

$$dE = T dS - M dH$$

$$C_H = \frac{dE_H}{dT_H} = \frac{dE}{d\beta} \Big|_H \frac{d\beta}{dT}, \text{ where } \beta = \frac{1}{kT} \text{ and } \frac{d\beta}{dT} = -\frac{1}{kT^2}$$

$$C_H = -\frac{1}{kT^2} \frac{dE}{d\beta} \Big|_H$$

$$E = \frac{1}{Z} \sum_{\{s_i\}} H e^{-\beta H}$$

$$C_H = -\left\{ \frac{1}{Z^2} \sum_{\{s_i\}} H e^{-\beta H} \frac{dZ}{d\beta} + \frac{1}{Z} \sum_{\{s_i\}} (-H^2 e^{-\beta H}) \right\} \left(-\frac{1}{kT^2} \right)$$

$$\frac{\partial Z}{\partial \beta} = \sum_{\{s_i\}} -H e^{-\beta H}$$

$$C_H = -\frac{1}{kT^2} \left\{ \frac{1}{Z^2} \left[\sum_{\{s_i\}} H e^{-\beta H} \right]^2 - \frac{1}{Z} \sum_{\{s_i\}} H^2 e^{-\beta H} \right\}$$

$$C_H = -\frac{1}{kT^2} \left(\langle H^2 \rangle - \langle H \rangle^2 \right)$$

4. Magnetic susceptibility

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - \bar{\mu} H \sum_{i=1}^N s_i = \mathcal{H}_0 - \bar{\mu} H \sum_{i=1}^N s_i$$

$$Z = \sum_{\{s_i\}} e^{-\beta \mathcal{H}}$$

$$M(T, H) = \frac{\sum_{\{s_i\}} \bar{\mu} S_{TOT} e^{-\beta \mathcal{H}}}{Z}$$

where $S_{TOT} = \sum_{i=1}^N s_i$.

Definition of magnetic susceptibility is $\chi_T = \lim_{H \rightarrow 0} \frac{\partial M(T, H)}{\partial H} \Big|_T$

$$\chi_T = -\frac{1}{Z^2} \sum_{\{s_i\}} \bar{\mu} S_{TOT} e^{-\beta \mathcal{H}} \frac{\partial Z}{\partial H} + \frac{1}{Z} \sum_{\{s_i\}} \bar{\mu} S_{TOT} \frac{\partial e^{-\beta \mathcal{H}}}{\partial H}$$

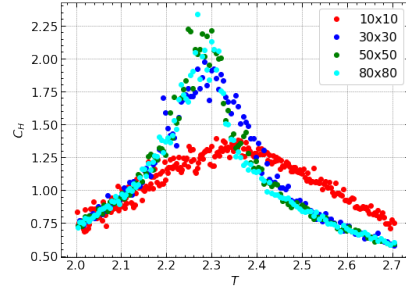
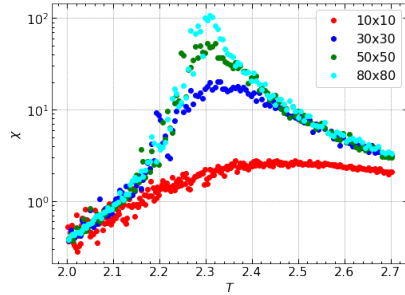
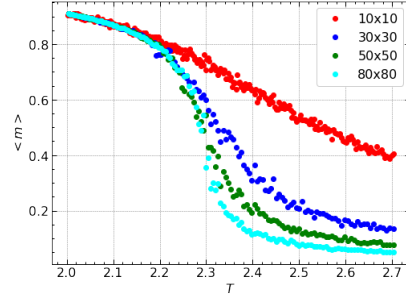
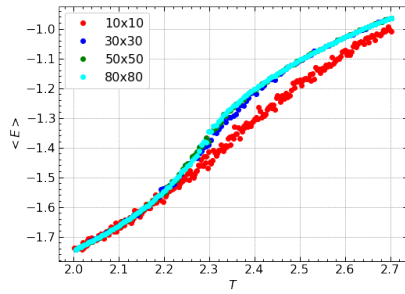
$$\frac{\partial(e^{-\beta \mathcal{H}})}{\partial H} = -\beta \frac{\partial \mathcal{H}}{\partial H} e^{-\beta \mathcal{H}} = \beta \bar{\mu} S_{TOT} e^{-\beta \mathcal{H}}$$

$$\frac{\partial Z}{\partial H} = \sum_{\{s_i\}} e^{-\beta \mathcal{H}} (\beta \bar{\mu} S_{TOT})$$

$$\chi_T = \frac{1}{Z} \sum_{\{s_i\}} \beta \bar{\mu}^2 S_{TOT}^2 e^{-\beta \mathcal{H}} + \frac{1}{Z^2} \bar{\mu}^2 \beta \sum_{\{s_i\}} S_{TOT} e^{-\beta \mathcal{H}} \sum_{\{s_i\}} S_{TOT} e^{-\beta \mathcal{H}}$$

$$\chi_T = \beta \bar{\mu}^2 \left(\langle S_{TOT}^2 \rangle - \langle S_{TOT} \rangle^2 \right)$$

Graphs of $\langle E \rangle$, $\langle m \rangle$, χ and C_H as a function of T



Criticality and finite size (finite size scaling)

Characteristic feature of second order phase transition is correlation length at a critical temperature. This leads to singularities of the specific heat, magnetisation susceptibility parameterized by the critical exponents (analytically 2D Ising model $\nu = 1, \gamma = 7/4, \beta = 1/8$)

$$\xi \sim \left(\frac{T-T_C}{T_C} \right)^{-\nu}, \quad E = \frac{T-T_C}{T_C}$$

$\nu \rightarrow$ critical exp of the correlation length

In a finite system of $N = L \times L$ square lattice ξ can at most be $\xi \sim L$ (it cannot go to ∞). The "critical" temperature depends on the $T_C(L)$

$$\xi_L \sim L \sim \left(\frac{|T - T_C(L)|}{T_C(L)} \right)^{-\nu}$$

$$L^{-1/\nu} \sim \frac{|T - T_C(L)|}{T_C(L)} = E(L)$$

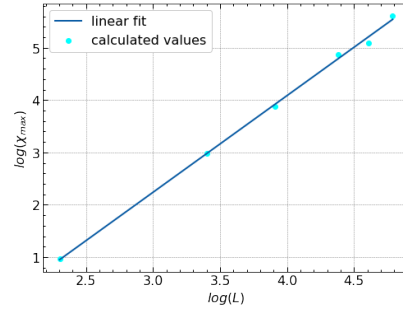
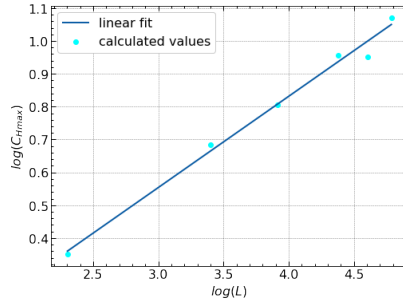
Critical exponents

$$m \sim (-E)^{-\beta/\nu}$$

$$C_H \sim (E)^{\alpha/\nu}$$

$$\chi_T \sim (E)^{\gamma/\nu}$$

numerically calculated critical exponents α and γ ,



Slope of a linear graph $\log(C_{Hmax})$ as a function $\log(L)$ is $\alpha = 0.28$

Slope of a linear graph $\log(\chi_{max})$ as a function $\log(L)$ is $\gamma = 1.85$

correlation function $\rightarrow \Gamma(r) = \sum_{|i-j|=r} (\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle)$

at $T \gg T_C$ it is $\langle s_i s_j \rangle = \langle s_i \rangle \langle s_j \rangle \implies \Gamma(r) \rightarrow 0$ for $\forall r$

at very low $T \ll T_C$ most of s_i are aligned $\Gamma(r) \rightarrow 0$

at finite temperature near T_C correlation function is $\Gamma(r) = \frac{e^{-r/\xi}}{r^{d-2+\eta}}$

where d is dimension and η is critical exponent

at $T \rightarrow T_C$ all the system is correlated $\xi \rightarrow \infty$

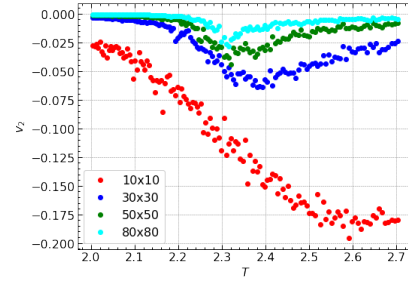
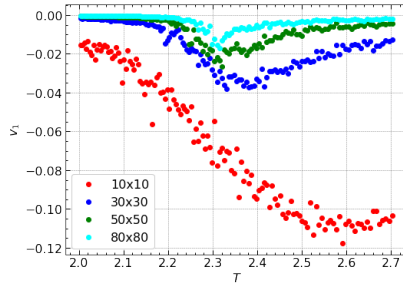
means $\frac{r}{\xi} \rightarrow 0$ $e^{-r/\xi} \rightarrow 1$ we get a power law $\Gamma(r) \sim \frac{1}{r^{d-2+\eta}}$

Comulants

$$v_1 = \frac{\partial \ln(m)}{\partial \beta} = \frac{\langle m E \rangle - \langle m \rangle \langle E \rangle}{\langle m \rangle}$$

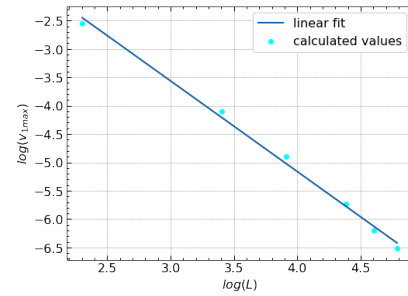
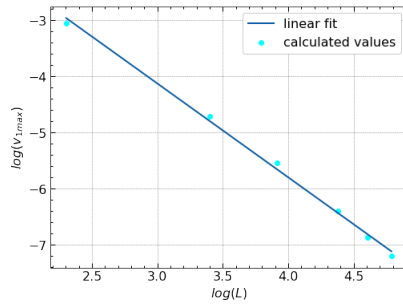
$$v_2 = \frac{\partial \ln(m^2)}{\partial \beta} = \frac{\langle m^2 E \rangle - \langle m^2 \rangle \langle E \rangle}{\langle m^2 \rangle}$$

graphs of first v_1 and second v_2 comulants as a function of temperature T



$v_1 \sim E^{-\nu}$ and $v_2 \sim E^{-\nu}$

linear graphs of $\log(v_{max1})$ and $\log(v_{max2})$ as a function of $\log(L)$ and their slopes $\nu_1 = 1.67$ and $\nu_2 = 1.60$



Hoshen Kopelman algorithm

Hoshen Kopelman algorithm [5] is used for labeling clusters on a grid, where each cell of a grid can either be occupied or unoccupied.

The algorithm was originally published in a paper "Percolation and cluster distribution. I. Cluster multiple labeling technique and critical concentration algorithm," by J. Hoshen and R. Kopelman [1]. HK- algorithm is really just a special application of the Union-Find algorithm, commonly used by computer scientists.

The general idea of HK-algorithm is to scan through the grid looking for occupied cells and assigning them a label corresponding to the cluster to which the cell belongs.

If the cell doesn't have occupied neighbours than we assign to it a cluster label we have not yet used, creating a new cluster.

If the cell has one occupied neighbour, than we assign it to the same cluster.

If the cell has more than one occupied neighbouring cell we choose the lowest-numbered cluster label of the occupied neighbours to use as the label for the current cell. If these neighbours are a part of a different clusters, we must make a note that these different labels correspond to the same cluster since we found a link between them.

The Union-Find algorithm

Calling the function $union(x, y)$, states that items x and y are members of the same equivalence class. Equivalence relation is transitive, items equivalent to x are all equivalent to all items equivalent to y . For any item x there is a set of items which are all equivalent to x ; this set is the equivalence class of which x is a member. Function $find(x)$ returns a representative member of the equivalence class to which x belongs.

The HK-algorithm scans the grid, each time an occupied cell is encountered, algorithm checks whether this cell has any already scanned neighbours. If so, first a *union* operation is performed, to specify that neighboring cells are members of the same equivalence class. Then a *find* operation is performed in order to find a representative member of equivalence class with which the algorithm labels the current cell. If, the current cell has no occupied neighbors, it is assigned a new label. After the whole grid is scanned, the algorithm scans it a second time, performing only *find* operations at each cell, to re-label the cells with their final assignment of a representative element.

In our case where we work with lattices with 'up' and 'down' spins we run two KH-algorithms simultaneously. Firstly it is determined for each spin if it is in 'up' or 'down' orientation and then algorithm checks whether this

cell has any already scanned neighbours of the same orientation.
For Ising model with periodic boundary conditions we have to implement scanning for neighbours on the other side of the grid for boundary cells. In the figures below we have a lattice of 'up' and 'down' spins on which KH-algorithm was preformed to give as a lattice of labeled equivalence classes.

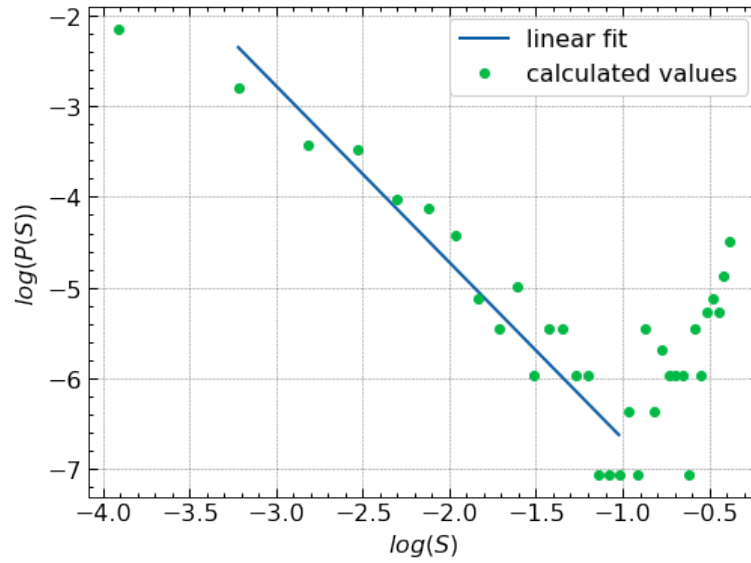
[[-1. 1. -1. -1. 1. 1. 1. -1. -1. -1.]	[[1. 2. 3. 3. 4. 4. 4. 1. 1. 1.]
[1. 1. -1. 1. 1. -1. 1. 1. -1. 1.]	[2. 2. 3. 4. 4. 8. 4. 4. 1. 2.]
[-1. -1. 1. -1. 1. 1. -1. -1. 1. 1.]	[1. 1. 10. 11. 4. 4. 12. 12. 2. 2.]
[-1. -1. -1. 1. 1. -1. -1. 1. 1. 1.]	[1. 1. 1. 4. 4. 12. 12. 2. 2. 2.]
[-1. 1. 1. 1. 1. -1. 1. -1. -1. 1.]	[1. 4. 4. 4. 4. 12. 18. 1. 1. 2.]
[-1. -1. 1. -1. -1. 1. -1. -1. -1. -1.]	[1. 1. 4. 20. 20. 21. 1. 1. 1. 1.]
[1. 1. -1. -1. 1. -1. -1. 1. -1. -1.]	[23. 23. 20. 20. 4. 1. 1. 27. 1. 1.]
[-1. -1. 1. -1. 1. 1. -1. -1. -1. -1.]	[1. 1. 4. 20. 4. 4. 1. 1. 1. 1.]
[-1. 1. 1. 1. 1. 1. 1. -1. -1. -1.]	[1. 4. 4. 4. 4. 4. 4. 1. 1. 1.]
[1. -1. 1. 1. -1. -1. 1. -1. -1. -1.]]	[31. 32. 4. 4. 33. 33. 4. 1. 1. 1.]]

On the left is a lattice of spins 'up' and 'down' on which KH-algorithm was preformed. On the right is the end result a lattice of labeled equivalence classes.

Studying formed clusters at critical temperature gives us an interesting correlation. Lets define S as a normalised cluster size $S = n/N$ where n is a number of cells in cluster and N size of a lattice. $P(S)$ is a probability of finding cluster size S . At critical temperature we get scale free power distribution

$$P(S) \sim S^{-\eta}$$

Ploting $\log(P(S)) \sim -\eta \log(S)$ for 300 thermalised lattices size $N = 100$ at critical temperature gives us value $\eta = 1.94$



References

- [1] J. Hoshen and R. Kopelman. “Percolation and cluster distribution. I. Cluster multiple labeling technique and critical concentration algorithm”. In: *Physical Review B* 14.8 (Oct. 1976), pp. 3438–3445. DOI: 10.1103/physrevb.14.3438. URL: <https://doi.org/10.1103/physrevb.14.3438>.
- [2] A. H. Teller, N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, and E. Teller. “Equation of State Calculations by Fast Computing Machines”. In: *The Journal of Chemical Physics* 21.6 (June 1953), pp. 1087–1092. DOI: 10.1063/1.1699114. URL: <https://doi.org/10.1063/1.1699114>.
- [3] Lars Onsager. “Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition”. In: *Physical Review* 65.3-4 (Feb. 1944), pp. 117–149. DOI: 10.1103/physrev.65.117. URL: <https://doi.org/10.1103/physrev.65.117>.
- [4] *Spin (physics)*. 2022. URL: [https://en.wikipedia.org/wiki/Spin_\(physics\)#Spin_projection_quantum_number_and_multiplicity](https://en.wikipedia.org/wiki/Spin_(physics)#Spin_projection_quantum_number_and_multiplicity).
- [5] Tobin Fricke. *The Hoshen-Kopelman Algorithm*. 2007. URL: <https://www.ocf.berkeley.edu/~fricke/projects/hoshenkopelman/hoshenkopelman.html>.