Ising Model: Motivation

Why should we spend so much time talking about the Ising model?

•It's surprisingly **useful for helping us think** about all sorts of behaviors relating to *phase transitions*. For instance:

- It exhibits symmetry breaking in low-temperature phase .
- *'Critical point'* at a well-defined temperature

•It's one of few **exactly solvable models** where we can actually compute thermodynamic quantities and interpret them. In general, calculating thermodynamic quantities is hard because

- You have to sum up many terms. Remember that you can think about an equilibrium system as an *ensemble* of many states s , each weighted with their own probability P_s .

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- In this framework, the thermodynamic quantities that you observe correspond to averages over the ensemble. In particular, if you want to find the ensemble average of some observable $A(s)$, you need to find the sum $\langle A \rangle = \sum_s A(s)P(s)$ where the sum runs over *all the possible states*.

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- The problem with this, as you remember, is that the number of states of a thermodynamic system scales *exponentially* with the number of particles! Even for a moderate-sized system, there are just too many states for a computer to explicitly compute the average – let alone a thermodynamic system where N is on the order of 10^{23} .

•So we need to "be clever" to compute the partition function, and we ought to be thankful for exactly solvable systems!

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Definition: Ising Model

- The Ising model is a theoretical model in statistical physics that was originally developed to describe ferromagnetism.
- A system of magnetic particles can be modeled as a linear chain in one dimension or a lattice in two dimension, with one molecule or atom at each lattice site i.

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•An alloy; say, brass. Each of the sites is an atom in the lattice; -1 represents an copper atom at that site; +1 represents zinc.
•A "lattice gas". Each of the sites is the possible location of a particle; -1 means that site is empty and +1 means that site is occupied by a particle.

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- A system of magnetic particles can be modeled as a linear chain in one dimension or a lattice in two dimension, with one molecule or atom at each lattice site i.
- To each molecule or atom a magnetic moment is assigned that is represented in the model by a discrete variable σ_i. Each 'spin' σ_i can only have a value of $\sigma_i = \pm 1$. The two possible values indicate whether two spins σ_i and σ_j are align and thus parallel ($\sigma_i\ \sigma_j = +1$) or anti-parallel ($\sigma_i\ \sigma_j = -1$).

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Ising Model

- A system of two spins is considered to be in a lower energetic state if the two magnetic moments are aligned. If the magnetic moments points in opposite directions they are consider to be in a *higher energetic state*. Due to this interaction the system tends to align *all magnetic moments in one direction in order to minimize energy*.

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- If nearly all magnetic moments point in the same direction the arrangement of molecules behaves like a macroscopic magnet.

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Ising Model

- A phase transition in the context of the Ising model is a transition from an ordered state to a disordered state.
- A ferromagnet above the critical temperature T_c is in a disordered state. In the Ising model this corresponds to a random distribution of the spin values.

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- Below the critical temperature T_c (nearly) all spins are aligned, even in the absence of an external applied magnetic field H.

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- Below the critical temperature T_c (nearly) all spins are aligned, even in the absence of an external applied magnetic field H.

- *If we heat up a cooled ferromagnet, the magnetization vanishes at T_c and the ferromagnet switches from an ordered to a disordered state. This is a phase transition of second order.*

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Example Consider a system of three fixed particles, each having spin $\frac{1}{2}$ so that each spin can point either up or down (i.e., along or opposite some direction chosen as the z axis). Each particle has a magnetic moment along the z axis of μ when it points up, and $-\mu$ when it points down. The system is placed in an external magnetic field H pointing along this z axis.

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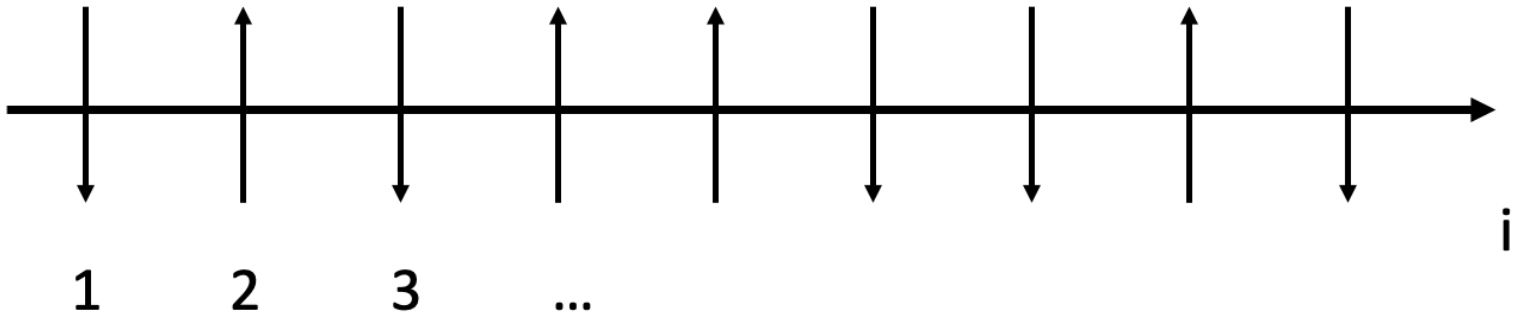
The state of the particle i can be specified by its magnetic quantum number m_i which can assume the two values $m_i = \pm\frac{1}{2}$. The state of the whole system is specified by giving the values of the three quantum numbers m_1, m_2, m_3. A particle has energy $-\mu H$ when its spin points up, and energy μH when its spin points down.

State index r	*Quantum numbers* m_1, m_2, m_3	*Total magnetic moment*	*Total energy*
1	$+ + +$	3μ	$-3\mu H$
2	$+ + -$	μ	$-\mu H$
3	$+ - +$	μ	$-\mu H$
4	$- + +$	μ	$-\mu H$
5	$+ - -$	$-\mu$	μH
6	$- + -$	$-\mu$	μH
7	$- - +$	$-\mu$	μH
8	$- - -$	-3μ	$3\mu H$

One dimensional Ising Model



- Each spin can interact with its neighbors.
- No external magnetic field is considered.

- The interaction strength between two spins σ_i and σ_{i+1} is characterised by the coupling strength J. The Hamiltonian $\mathcal{H}$ of such a system is then given by

$$\mathcal{H} = \sum_{\langle ij \rangle} \sigma_i \sigma_j \,,$$

with a nearest neighbouring sum.

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- ❑ Our end goal is to find various **thermodynamic properties** of the 1D Ising model.
- ❑ Remember that thermodynamics means that the system is in *thermal equilibrium*; where the probability of each configuration/microstate is $\frac{e^{-\beta E}}{Z}$ (This also called the "canonical ensemble").
- ❑ Our system is defined by a **Hamiltonian** $\mathcal{H}$ a function that tells us its energy. From the Hamiltonian, we figure out the **energy eigenstates**, a.k.a. **configurations**, (or sometimes even "states") of the system. These are the basic states, and we will be *summing over* these states.
- ❑ We take limit $N \to \infty$

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One dimensional Ising Model

In the canonical ensemble, the probability of finding a particular spin configuration $\{s_i\}$ is,

$$p(\{s_i\}) = \frac{1}{Z}\exp(-\beta H(\{s_i\})), \quad \beta \equiv \frac{1}{k_B T} \tag{2}$$

where $Z = \sum_{\{s_i\}} \exp(-\beta H(\{s_i\}))$ is the partition function. Due to the Boltzmann factor, $e^{-\beta H}$, spin configurations with lower energies will be favored.

a.k.a. microstates (or sometimes even "states") of the system. These are the basic states, and we will be *summing over* these states.

- ❑ We take limit $N \to \infty$
- ❑ And our main target is to calculate partition functions $Z = \sum e^{-\beta E(s)}$, β is the related to inverse temp, and $E(s)$ is the energy of the system when it is in state s.
- ❑ Once we have found Z, we can calculate the free energy $F = -T \log Z$

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$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

- For a system with N_{tot} lattice sites, and two possible $\sigma_i -$ values, a total number of $2^{N_{\text{tot}}}$ possible configurations of the arrangements of particles exist. Summing over all configurations, *our main target* is obtain the partition sum Z as

$$Z = \sum_{\{i\}} e^{-\beta \mathcal{H}} = \sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} \ldots \ldots \sum_{\sigma_N = \pm 1} e^{\beta J (\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \cdots)}$$

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We introduce a new variable $\mu_i := \sigma_i . \sigma_{i+1}$

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We introduce a new variable $\mu_i := \sigma_i . \sigma_{i+1}$

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

Thus, for $N \gg 1$, $\quad Z = 2. \sum_{\{\mu\}} e^{\beta J \sum_{i=1}^{N-1} \mu_i}$

The factor of 2 in the partition function arises from the two possible configurations for the first spin in the chain.

One dimensional Ising Model

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \qquad Z = \sum_{\{i\}} e^{-\beta \mathcal{H}} = \sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} \dots \dots \sum_{\sigma_N = \pm 1} e^{\beta J (\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \cdots)}$$

$$Z = 2. \sum_{\{\mu\}} e^{\beta J \sum_{i=1}^{N-1} \mu_i} = 2 \sum_{\mu_1 = \pm 1} \sum_{\mu_2 = \pm 1} \dots \dots \sum_{\mu_{N-1} = \pm 1} e^{\beta J (\mu_1 + \mu_2 + \mu_3 + \cdots + \mu_{N-1})}$$

Open Boundary condition

$$= 2 \sum_{\mu_1 = \pm 1} \sum_{\mu_2 = \pm 1} \dots \dots \sum_{\mu_{N-2} = \pm 1} e^{\beta J (\mu_1 + \mu_2 + \mu_3 + \cdots + \mu_{N-2})} \underbrace{\sum_{\mu_{N-1} = \pm 1} e^{\beta J \mu_{N-1}}}_{e^{\beta J} + e^{-\beta J}}$$

$$= 2[2 \cosh(\beta J)]^{N-1} \approx [2 \cosh(\beta J)]^N$$

$$\cosh x = \frac{e^x + e^{-x}}{2}$$
$$\sinh x = \frac{e^x - e^{-x}}{2}$$
$$\frac{d}{dx} \cosh x = \sinh x$$
$$\frac{d}{dx} \sinh x = \cosh x$$
$$\tanh x = \frac{\sinh x}{\cosh x}$$
$$\frac{d}{dx} \tanh x = 1 - (\tanh x)^2$$

This is the partition function of the one-dimensional Ising model *without* an external field.

$$F = -kT \ln Z_N$$

$$\overline{E} = -\frac{\partial \ln Z_N}{\partial \beta} = \frac{\partial(\beta F)}{\partial \beta}$$

$$C = \left(\frac{\partial \overline{E}}{\partial T}\right)_B = -k\beta^2 \frac{\partial \overline{E}}{\partial \beta}.$$

$$Z \approx [2\cosh(\beta J)]^N$$

$$E = -NJ \tanh \beta J.$$

$$C = Nk(\beta J)^2 (\operatorname{sech} \beta J)^2.$$

One dimensional Ising Model

Reason for learning Ising model in 1-D.
Strategy: for a given Hamiltonian construct the partition function.
Weakness: Ising;s 1-d solution was unable to find the phase transition.

Q: **What will happen if we add external magnetic field? How can we calculate that?**

One dimensional Ising Model: Transfer matrix approach

The next question we are going to answer is what happens to our system if we apply an external magnetic field H that can interact with the magnetic moment m of each spin. The Hamiltonian of such a system becomes:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \; - mH \sum_i \sigma_i$$

In that case, we will consider the periodic boundary condition. We define a transfer matrix in a following way,

$$e^{-\beta\mathcal{H}} = \underbrace{e^{\beta E(\sigma_1,\sigma_2)}}_{T_{1,2}} \underbrace{e^{\beta E(\sigma_2,\sigma_3)}}_{T_{2,3}} \ldots\ldots\ldots \underbrace{e^{\beta E(\sigma_{N-1},\sigma_N)}}_{T_{N-1,N}} \underbrace{e^{\beta E(\sigma_N,\sigma_1)}}_{T_{N-1,1}}$$

One dimensional Ising Model:Transfer matrix

$$e^{-\beta\mathcal{H}} = \underbrace{e^{\beta E(\sigma_1,\sigma_2)}}_{T_{1,2}}\underbrace{e^{\beta E(\sigma_2,\sigma_3)}}_{T_{2,3}} \ldots\ldots \underbrace{e^{\beta E(\sigma_{N-1},\sigma_N)}}_{T_{N-1,N}} e^{\beta E(\sigma_N,\sigma_1)}$$

$T_{N-1,1}$

So each transfer matrix is given by $T_{i,i+1} = \exp(\beta(J\,\sigma_i\sigma_{i+1} + \frac{1}{2}H(\sigma_i + \sigma_{i+1})))$

Every spin can have two possible values , so our transfer matrix becomes 2×2 matrix

$$T_{i,i+1} = \begin{pmatrix} T_{+1,+1} & T_{+1,-1} \\ T_{-1,+1} & T_{-1,-1} \end{pmatrix} = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}$$

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Now we can write down the partition function in terms of the transfer matrices

$$Z = \sum_{\{i\}} e^{-\beta\mathcal{H}} = \sum_{\sigma_1=\pm1} \sum_{\sigma_2=\pm1} \ldots\ldots \sum_{\sigma_N=\pm1} T_{1,2} \ldots\ldots T_{N,1}$$

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If we zoom in on the multiplication between the 1-2 transfer matrix and the 2-3 transfer matrix, we see that the transfer matrices are being multiplied by each other when we sum over their shared index σ_2

$$\sum_{\sigma_2} T_{1,2}\,T_{2,3} = (T \cdot T)_{\sigma_1\sigma_3}$$

One dimensional Ising Model:Transfer matrix

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So when we sum over σ_2, those two transfer matrices "collapse" together and we are left with a squared Transfer matrix between spin σ_1 and σ_3. If we repeat this process of "collapsing" all the transfer matrices together, we end up with

$$Z = \sum_{\sigma_1} (\underbrace{T\cdot T\cdot T\cdot \dots \cdot T}_{N\,\text{times}})_{\sigma_1\sigma_1},$$

$$Z = tr[T^N] = \lambda_1^N + \lambda_2^N$$

One dimensional Ising Model:Transfer matrix

$$T_{i,i+1} = \exp\left(\beta\left(J\,\sigma_i\sigma_{i+1} + \frac{1}{2}H(\sigma_i + \sigma_{i+1})\right)\right)$$

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1. Every symmetric (real) matrix can be diagonalized,

$$P = U \cdot D \cdot U^T \tag{27}$$

where U is a unitary matrix ($U \cdot U^T = I$), and D is a diagonal matrix. For 2×2 matrices, define $\lambda_+ \equiv D_{11}$, $\lambda_- \equiv D_{22}$ ($D_{12} = D_{21} = 0$). $\lambda_\pm$ are the eigenvalues of matrix P.

2. Trace is unchanged after diagonalization

$$\mathrm{Tr(P)} = \mathrm{Tr(D)} = \lambda_+ + \lambda_- \tag{28}$$

Hence the trace equals the sum of the eigenvalues.

3. The same matrix U that diagonalizes P also diagonalizes P^N, because

$$P^N = (U \cdot D \cdot U^T) \cdot (U \cdot D \cdot U^T) \cdots (U \cdot D \cdot U^T) = U \cdot D^N \cdot U^T \tag{29}$$

4. Notice that

$$D^N = \begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} \tag{30}$$

We have

$$\mathrm{Tr}(P^N) = \mathrm{Tr}(D^N) = \lambda_+^N + \lambda_-^N \tag{31}$$

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$$\begin{aligned} \lambda_\pm &= e^{\beta J}\left[\cosh\beta h \pm \sqrt{\sinh^2\beta h + e^{-4\beta J}}\right] \\ U &= \begin{bmatrix} -e^{\beta J}\left(e^{\beta(J-h)-\lambda_+}\right) & 1 \\ 1 & -e^{\beta J}\left(e^{\beta(J+h)-\lambda_-}\right) \end{bmatrix} \\ \mathrm{Tr}(P) &= \lambda_+ + \lambda_- = 2\,e^{\beta J}\cosh\beta h \end{aligned}$$

h and H are same

$$\begin{aligned} Z &= \mathrm{Tr}(P^N) = \lambda_+^N + \lambda_-^N \\ &= e^{N\beta J}\left\{\left[\cosh\beta h + \sqrt{\sinh^2\beta h + e^{-4\beta J}}\right]^N \right. \\ &\qquad \left. + \left[\cosh\beta h - \sqrt{\sinh^2\beta h + e^{-4\beta J}}\right]^N\right\} \end{aligned}$$

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$$\frac{1}{N}\ln Z_N(T,H) = \ln\lambda_+ + \ln\left[1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right] \underset{N\to\infty}{\rightarrow} \ln\lambda_+,$$

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Statistical Physics Seminar by Prof. Wolschin
Anton Kabelac

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and the free energy per spin is given by

$$\frac{1}{N}F(T,H) = -kT\ln\left[e^{\beta J}\cosh\beta H + \left(e^{2\beta J}\sinh^2\beta H + e^{-2\beta J}\right)^{1/2}\right].$$

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$$M = \frac{\partial F}{\partial H} = N\frac{\sinh\beta H}{(\sinh^2\beta H + e^{-4\beta J})^{1/2}}.$$

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Anton Kabelac

One dimensional Isina Model:Transfer matrix

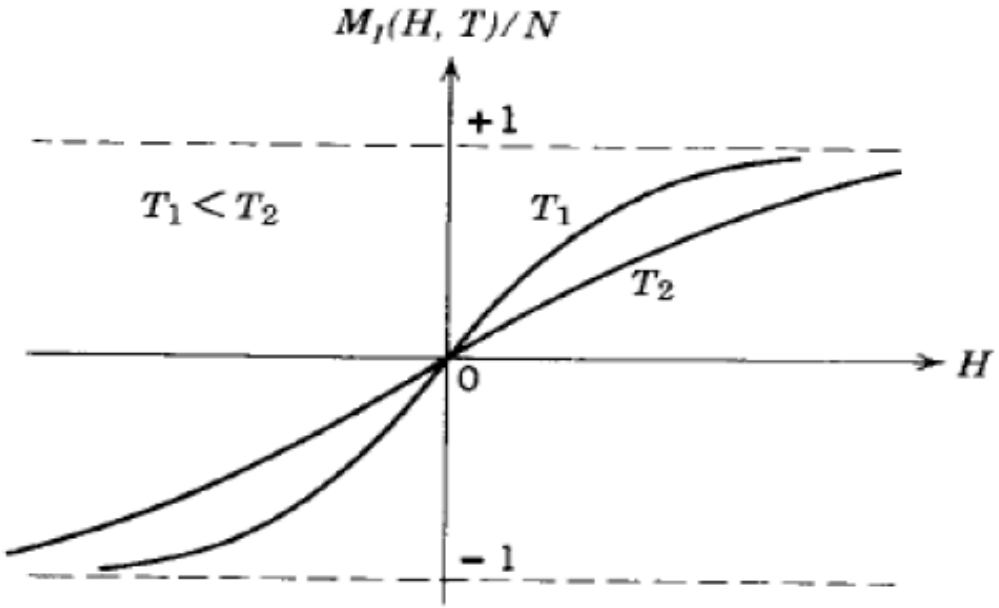


Fig. 14.16 Magnetization of the one-dimensional Ising model. There is no spontaneous magnetization.

$$M = \frac{\partial F}{\partial H} = N \frac{\sinh \beta H}{(\sinh^2 \beta H + e^{-4\beta J})^{1/2}}.$$

A system is paramagnetic if $M \neq 0$ only for $H \neq 0$, and is ferromagnetic if $M \neq 0$ for $H = 0$. For the one-dimensional Ising model, we see from (5.72) that $M = 0$ for $H = 0$, and there is no spontaneous magnetization at nonzero temperature. (Recall that $\sinh x \approx x$ for small x.) That is, the one-dimensional Ising model undergoes a phase transition from the paramagnetic to the ferromagnetic state only at $T = 0$. In the limit of low temperature ($\beta J \gg 1$ and $\beta H \gg 1$), $\sinh \beta H \approx \frac{1}{2} e^{\beta H} \gg e^{-2\beta J}$ and $m = M/N \approx 1$ for $H \neq 0$. Hence, at low temperatures only a small field is needed to produce saturation, corresponding to $m = 1$.

Phase Transition in 2-d Ising model

Phase Transition in 2-d Ising model of a Ferromagnet

The two-dimensional Ising model was solved exactly in zero magnetic eld for a rectangular lattice by Lars Onsager in 1944. Onsager's calculation was the first exact solution that exhibited a phase transition in a model with short-range interactions. Before his calculation, some people believed that statistical mechanics was not capable of yielding a phase transition.

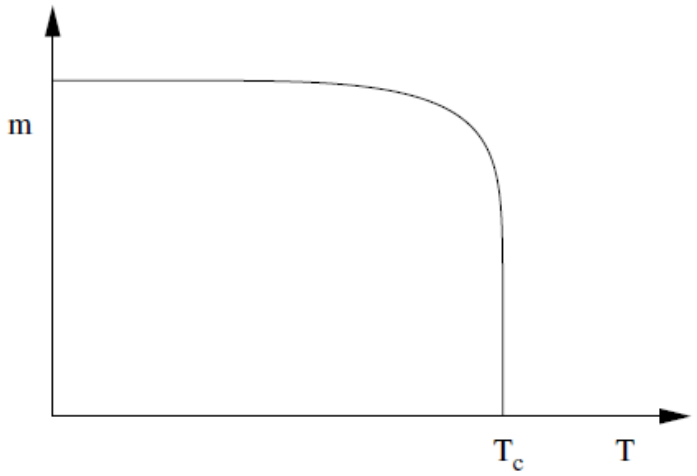


Figure 5.8: The temperature-dependence of the spontaneous magnetization of the two-dimensional Ising model.

The most important results of the exact solution of the two-dimensional Ising model are that the energy (and the free energy and the entropy) are continuous functions for all T, m vanishes continuously at $T = T_c$, the heat capacity diverges logarithmically at $T = T_c$, and the zero-field susceptibility diverges as a power law. When we discuss phase transitions in more detail in Chapter 9, we will understand that the paramagnetic $\leftrightarrow$ ferromagnetic transition in the two-dimensional Ising model is *continuous*. That is, the order parameter m vanishes continuously rather than discontinuously. Because the transition occurs only at $T = T_c$ and $H = 0$, the transition occurs at a *critical point*.

Phase Transition in 2-d Ising model of a Ferromagnet

In most ordinary materials the associated magnetic dipoles of the atoms have a random orientation. In effect this non-specific distribution results in no overall macroscopic magnetic moment. However in certain cases, such as iron, a magnetic moment is produced as a result of a preferred alignment of the atomic spins.

This phenomenon is based on two fundamental principles, namely energy minimization and entropy maximization.

These are competing principles and are important in moderating the overall effect. Temperature is the mediator between these opposing elements and ultimately determines which will be more dominant

Jacques Kotze
arXiv:0803.0217v1

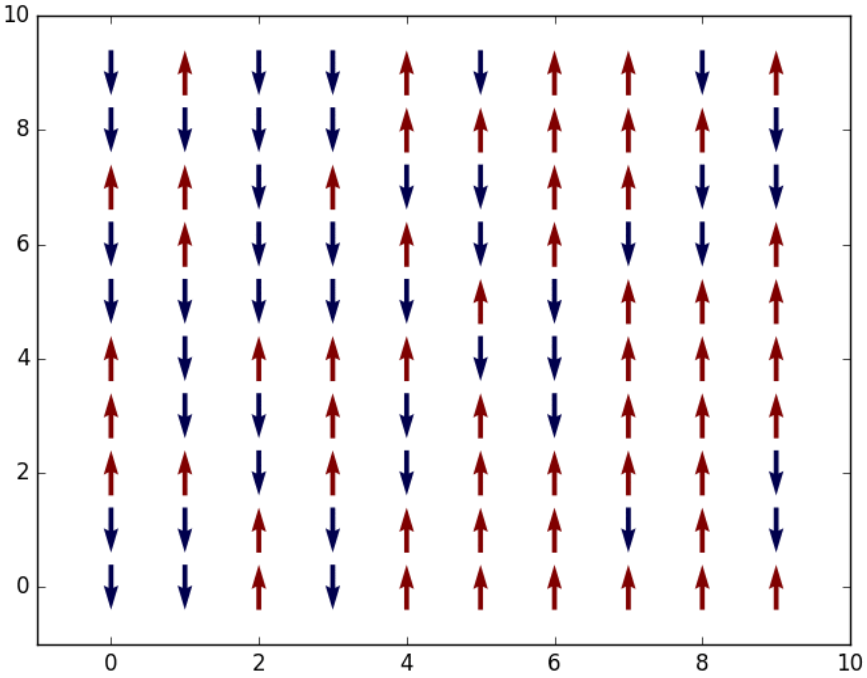
Phase Transition in 2-d Ising model of a Ferromagnet

Aim: Critical Temperature for phase transition

Let $s_{i,j}$ denote a spin state at lattice coordinates i and j having either spin up or spin down, $s_{i,j} = \pm 1$. The Hamiltonian or total energy of the system in a particular state $\{s_{i,j}\}$ is

$$H(\{s_{i,j}\}) = -J \sum_{i,j} s_{i,j}(s_{i+1,j} + s_{i-1,j} + s_{i,j+1} + s_{i,j-1})$$

Here, in 2D Ising model, the spins are lying in xy-plane and oriented only along either $+y$ or $-y$ directions.



https://ruihaoqiu.github.io/MC-Magnetic-Phase-Transition/

Phase Transition in 2-d Ising model of a Ferromagnet

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Periodic boundary condition (2 d lattice folded in torus) and only a nearest neighbour coupling is allowed.

The system of spins is considered to be in contact with a heat bath at temperature T. The set of spins can exchange energy with the heat bath, in such a way that the system can come into thermal equilibrium with the heat bath. In thermal equilibrium, the probability of finding the system in a particular microstate α is :

$$P_\alpha \propto e^{-\frac{E_\alpha}{kT}}$$

Phase Transition in 2-d Ising model of a Ferromagnet

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If the energy of each possible state of the system is specified, then the Boltzmann distribution function, gives the probability for the system to be in each possible state (at a given temperature) and therefore macroscopic quantities of interest can be calculated by doing probability summing. This can be illustrated by using magnetization and energy as examples. For any fixed state α, the magnetization is proportional to the 'excess' number of spins pointing up or down while the energy is given by the Hamiltonian H

$$M(\alpha) = N_{up}(\alpha) - N_{down}(\alpha)$$

Jacques Kotze

Phase Transition in 2-d Ising model of a Ferromagnet

Aim: Critical Temperature for phase transition

Let $s_{i,j}$ denote a spin state at lattice coordinates i and j having either spin up or spin down, $s_{i,j} = \pm 1$. The Hamiltonian or total energy of the system in a particular state $\{s_{i,j}\}$ is

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$$M(\alpha) = N_{up}(\alpha) - N_{down}(\alpha)$$

Thus, expected value $\langle M \rangle = \sum_\alpha M(\alpha) P_\alpha$. similarly, $\langle E \rangle = \sum_\alpha E(\alpha) P_\alpha$

These calculation pose a drastic problem from a practical perspective. Considering we have two spin orientations (up & down) and there are N spins which implies that there are 2^N different states. As N becomes large it is evident that computations become a daunting task if calculated in this manner.

Jacques Kotze

Quantum Mechanics of Magnetism Summarized

- Due to the motion of their electrons, some atoms can have intrinsic magnetic moments. Other atoms develop magnetic moments when placed in an external magnetic field.
- If atoms have zero magnetic moment, then an applied field H induces magnetic moments that are aligned anti-parallel to the applied field. The magnetization M is such that $M/H < 0$. This is **diamagnetism.**
- If atoms have non-zero magnetic moments that point in random directions then the sum over many atoms gives zero magnetization. An applied field tends to align the magnetic moments so that $M/H > 0$. This is **paramagnetism.**
- If atoms have non-zero magnetic moments that point in the same direction then the sum over many atoms gives finite magnetization. This is **ferromagnetism.**

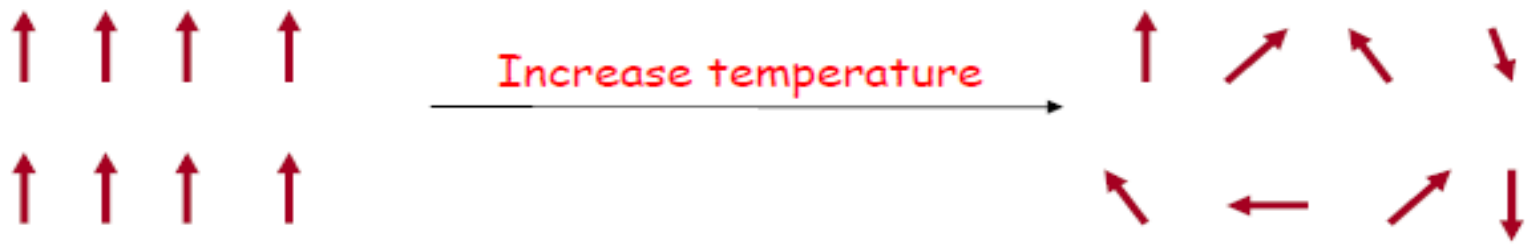
Bohr-van Leeuwen Theorem: At any finite temperature, and in all finite applied electric or magnetic fields, classical magnetization of a collection of electrons in thermal equilibrium vanishes identically.

Branislav K. Nikolić

Magnetization as Order Parameter of Alligned Quantum Spins

Ferromagnet:
Spins aligned

Paramagnet:
Spins disordered



- Spontaneous magnetization (in the absence of magnetic field): '**Order Parameter**'.
- Ordered phase spontaneously breaks spin rotation symmetry.
- **First Order Phase Transitions:** discontinuity in the order parameter or energy (i.e., first derivative of the free energy).
- **Second order Phase Transitions:** divergence in the susceptibility or specific heat (i.e., second derivative of the free energy).

How to Evade **Analytic** Computation of Ising Model Partition Function?

- Suppose we want to calculate the exact partition function **Z** numerically. Need to do this for all **T**, but let us start with just one temperature.

- Real system has $O(10^{23})$ spins, try first 32x32 lattice with $O(10^3)$ spins:

  → Number of configurations in the sum = $2^{32\times 32} \sim 10^{300}$

  → Gigantic parallel supercomputer with 10 million processors: Each processor could generate a configuration ***C***, calculate its energy **E(*C*)** and the Boltzmann factor **exp[-E(*C*)/kT]**, and add it to the sum over configurations in one **nanosecond**.

  → The calculation runs during the whole age of the Universe:

$$10^7\,\text{CPU}\times 10^9\,\frac{\text{configurations}}{\text{CPU}\times\text{s}}\times 10^{14}\,\frac{\text{sec}}{\text{year}}\,10^{10}\ \text{years}$$

$$\sim 10^{40}$$ (just for a single temperature!)

Phase transition: computation(2 d lattice)

0. Start with some spin configuration $\{s_i\}$.
1. Randomly choose a spin s_i
2. Attempt to flip it, i.e. $s_i := -s_i$ (trial).
3. Compute the energy change ΔE due to this flip.
4. If $\Delta E < 0$, accept the trial.
5. If $\Delta E > 0$, accept the trial with probability $p^{\text{acc}} = e^{-\beta \Delta E}$.
6. If trial is rejected, put the spin back, i.e. $s_i := -s_i$.
7. Go to 1, unless maximum number of iterations is reached.

$$H(\{s_{i,j}\}) = -J \sum_{i,j} s_{i,j}(s_{i+1,j} + s_{i-1,j} + s_{i,j+1} + s_{i,j-1})$$

Phase transition: computation(2 d lattice)

```
adj = neighbors(1:N^2,N);
% grid = sign(randn(N,N));
p=.5; % average proportion of initial +1 spins
grid = sign(p-rand(N));
```

Phase transition: computation(2 d lattice)

```
adj = neighbors(1:N^2,N);
% grid = sign(randn(N,N));
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grid = sign(p-rand(N));
```

```
for T = 1.57:0.1:5;
kT = 1*T;
s=randi(N^2);
% location of ith spin
% s = spin(i);
% Calculate the change in energy of flipping s
dE = 2*J*grid(s)*sum(grid(adj(s,:)));
% Calculate the transition probability
p = exp(-dE/kT);
% Decide if a transition will occur
if dE<=0 || rand <= p,
grid(s) = -1*grid(s);
end
```

$$H(\{s_{i,j}\}) = -J \sum_{i,j} s_{i,j}(s_{i+1,j} + s_{i-1,j} + s_{i,j+1} + s_{i,j-1})$$

Metropolis- Hastings algorithm

The Monte Carlo approach (Hammersley and Handscomb, 1964; Rubinstein, 1981) emerged with computers, at the end of WWII, as it relies on the ability of producing a large number of realisations of a random variable distributed according to a given distribution, taking advantage of the stabilisation of the empirical average predicted by the Law of Large Numbers.

However, producing simulations from a specific distribution may prove near impossible or quite costly and therefore the (standard) Monte Carlo may also face intractable situations.

Metropolis- Hastings algorithm

An indirect approach to the simulation of complex distributions and in particular to the curse of dimensionality met by regular Monte Carlo methods is to use a Markov chain associated with this target distribution, using Markov chain theory to validate the convergence of the chain to the distribution of interest and the stabilisation of empirical averages (Meyn and Tweedie, 1994).

Markov chains construct a progressive picture of the target distribution, proceeding by local exploration of the state space X until all the regions of interest have been uncovered. An analogy for the method is the case of a visitor to a museum forced by a general blackout to watch a painting with a small torch. Due to the narrow beam of the torch, the person cannot get a global view of the painting but can proceed along this painting until all parts have been seen.

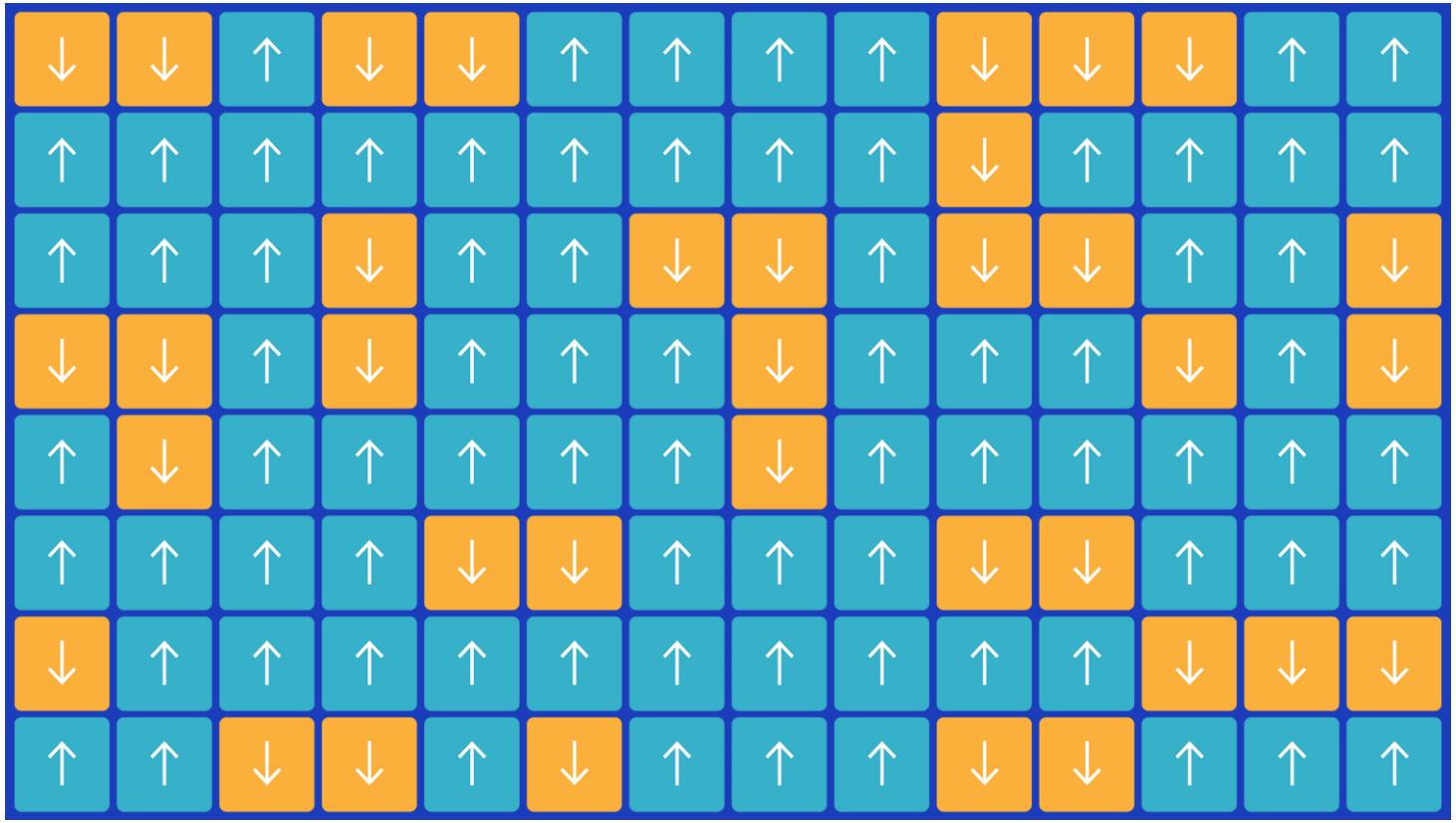
C.P Robert

Metropolis algorithm

Let $f(x)$ be a function that is proportional to the desired probability distribution $p(x)$ (a.k.a. a target distribution).

1. **Initialization:** Choose an arbitrary point x_t to be the first sample and choose an arbitrary probability density $g(x|y)$ (sometimes written $Q(x|y)$) that suggests a candidate for the next sample value x given the previous sample value y In this section, g is assumed to be symmetric; in other words, it must satisfy $g(x|y) = g(y|x)$. A usual choice is to let satisfy $g(x|y)$ be a Gaussian distribution centered at y so that points closer to y are more likely to be visited next, making the sequence of samples into a random walk The function g is referred to as the *proposal density* or *jumping distribution*.
2. **For each iteration t :** *Generate* a candidate x' for the next sample by picking from the distribution $g(x'|x_t)$. *Calculate* the *acceptance ratio* $\alpha = \frac{f(x')}{f(x_t)}$, which will be used to decide whether to accept or reject the candidate. Because f is proportional to the density of P, we have that $\frac{f(x')}{f(x_t)} = \frac{P(x')}{P(x_t)}$
3. ***Accept or reject*:**
    1. Generate a uniform random number $u \in [0,1]$.
    2. If $u \leq \alpha$ then *accept* the candidate by setting $x_{t+1} = x'$,
    3. If $u > \alpha$, then *reject* the candidate and set $x_{t+1} = x_t$ instead.

Ising Model: Motivation



https://www.bdhammel.com/ising-model/
https://www.quantamagazine.org/the-cartoon-picture-of-magnets-that-has-transformed-science-20200624/

https://stanford.edu/~jeffjar/statmech/lec3.html

Theory Behind Metropolis Monte Carlo: Markov Chains and Detailed Balance

- Let us set up a so-called Markov chain of configurations by the introduction of a fictitious dynamics → the "time" t is computer time (marking the number of iterations of the procedure), NOT real time since our statistical system is considered to be in equilibrium, and therefore time invariant.
  - →Probability to be in configuration A at time T is: $P(A,t)$
  - →The transition probability (per unit time) to go from A to B is: $W(A \to B)$

$$P(A,t+1) = P(A,t) + \sum_B [W(B \to A)P(B,t) - W(A \to B)P(A,t)]$$

$$= 0$$

- Equilibrium $\lim_{t\to\infty} P(A,t) = p(A)$ can be ensured by satisfying detailed balance
- For the special case of the Boltzmann probability distribution $p(A) = e^{-E(A)/kT}/Z$

$$\frac{W(A \to B)}{W(B \to A)} = \frac{p(B)}{p(A)} = \frac{e^{-E(B)/kT}}{e^{-E(A)/kT}} = e^{-\Delta E/kT}$$

$$\Delta E = E(B) - E(A)$$

Over Los Alamos dinner party in 1953

Metropolis, Teller, and Rosenbluth chose:

$$W(A \to B) = \begin{cases} e^{-\Delta E/kT}, & \Delta E > 0 \\ 1, & \Delta E \le 0 \end{cases}$$