Magnetism: Monte Carlo methods and the Ising model

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1 Monte Carlo methods

Monte Carlo methods are an important class of computational algorithms that make repeated use of random numbers to compute numerical results. These numerical techniques are prominent in statistical physics where they are used to compute thermal averages of classical many-body systems. Here, we will discuss their general use as a way to compute high-dimensional integrals and employ them to study the Ising model of a magnetic material. Monte Carlo methods can also be used to simulate the solution of differential equations such as the diffusion equation or the Schrödinger equation.

1.1 Monte Carlo integration

While there are Monte Carlo simulations where one is interested in reproducing on the computer a truly stochastic process (e.g. the behavior of a title in the stock market), one is often dealing with a problem which is not probabilistic in nature but tries to find a solution using probabilistic methods. This type of Monte Carlo simulations can ultimately be recast as the computation of an integral with statistical methods.

Monte Carlo integration is based on the fact that an integral can be expressed as an average. For instance, the one-dimensional integral of the function f can be written as

$$I = \int_a^b f(x)dx \; = (b-a)\langle f\rangle_{[a,b]}\,, \tag{1}$$

where $\langle f\rangle_{[a,b]}$ is the average of the function in the range $[a,b]$. A statistical estimate of the average can be obtained by randomly generating M points $(x_1, \ldots\, x_M)$ uniformly distributed in the domain $[a,b]$ and estimating the average as

$$\langle f\rangle_{[a,b]} \approx \frac{1}{M}\sum_{i=1}^{M} f(x_i)\,, \tag{2}$$

where x_i is sampled with probability $dx/(b-a)$. The estimate of the integral (Eq. 1) approaches I as $M \to \infty$ and one can therefore compute the integral by drawing a large number of points. Sampling from a uniform distribution will however be highly inefficient if $f(x)$ is sharply peaked in a small region: most points will be falling out of the important region and the fluctuations of the average will be very large (see Fig. 1).

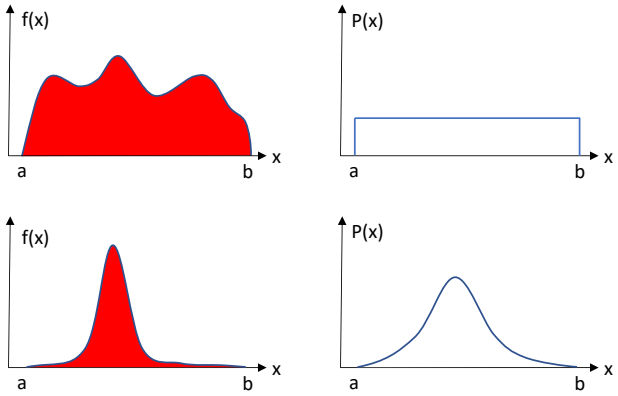

Figure 1: Uniform Monte Carlo sampling to compute the integral of $f(x)$ is appropriate for the (top) function $f(x)$ but less efficient for the peaked (bottom) function, where a probability distribution resembling the shape of $f(x)$ would lead to more efficient sampling.

Let us now rewrite the integral so that $f(x) = g(x)P(x)$:

$$\boxed{I = \int_a^b g(x)P(x)dx}\,, \tag{3}$$

and choose

$$\boxed{P(x) \geq 0} \quad \text{for every } x \in [a,b] \quad \text{and} \quad \boxed{\int_a^b P(x) = 1}\,. \tag{4}$$

Since it is positive and integrates to one, we can treat $P(x)$ as a probability density on the interval $[a,b]$. Moreover, if we choose the factorization so that $g(x)$ is more smooth that the original $f(x)$, it will be clearly advantageous to sample random configuration $(x_1, \ldots, x_M)$ distributed like $P(x)$ and estimate the integral as

$$\boxed{I = \langle g \rangle_{\rm P} \;\approx\; \bar{g} = \frac{1}{M}\sum_{i=1}^{M} g(x_i)}\,, \tag{5}$$

where x_i is sampled with probability $P(x_i)dx$. For large M, the sum over the $g(x_i)$ values satisfies the central limit theorem so that the root-mean-square deviation of the sample mean, $\bar{g}$, from the true expectation value, $\langle g \rangle_P$, can be interpreted as a statistical error

$$\Delta_g = \frac{\sigma_g}{\sqrt{M}}\,, \tag{6}$$

where the variance of the sampled values is

$$\sigma_g^2 = \langle g^2 \rangle_P - \langle g \rangle_P^2 = \int_a^b \left[g(x)^2 - \langle g \rangle_P^2 \right] P(x)dx\,. \tag{7}$$

If $g(x)$ is smoother that $f(x)$, its fluctuations will be smaller and one can then estimate the integral with the desired accuracy with fewer Monte Carlo configurations $\{x_i\}$. Because of

the central limit theorem, you will have

$$\begin{aligned} \langle g \rangle_P &\in [\bar{g} - \Delta_g, \bar{g} + \Delta_g] \quad 68\% \text{ of the time} \\ &\in [\bar{g} - 2\Delta_g, \bar{g} + 2\Delta_g] \quad 95\% \text{ of the time} \\ &\in [\bar{g} - 3\Delta_g, \bar{g} + 3\Delta_g] \quad 99.7\% \text{ of the time}\,. \end{aligned} \tag{8}$$

In practice, in a Monte Carlo simulation, one estimates

$$\boxed{\langle g \rangle_{\rm P} \approx \bar{g} = \frac{1}{M} \sum_{i=1}^{M} g(x_i)} \quad \text{and} \quad \boxed{\langle g^2 \rangle_{\rm P} \approx \bar{g^2} = \frac{1}{M} \sum_{i=1}^{M} g(x_i)^2}\,, \tag{9}$$

and the actual error[1] as

$$\boxed{\Delta_g \approx \sqrt{\frac{\bar{g^2} - \bar{g}^2}{M-1}}}\,. \tag{10}$$

It is important to notice that

1) The $1/\sqrt{M}$ decay rate of the error on the estimate with the number of Monte Carlo configurations does **not** depend on the dimension of the integral!

2) All the problem has now been moved to how we can generate configurations $\{x_i\}$ with probability $P(x_i)dx$.

1.2 Monte Carlo simulations in statistical physics

The basic idea of Monte Carlo simulations is to generate non-uniform Monte Carlo sampling to compute an integral. While we work for simplicity in one dimension with x the configuration of your system (spin direction, particle position, etc.), recall that all formulas below are directly generalizable to many dimensions.

A thermal average in statistical physics is given in terms of the Boltzmann factor by:

$$\langle A \rangle = \frac{1}{Z} \int_a^b A(x) e^{-\beta E(x)} dx \tag{11}$$

where $E(x)$ is the energy of configuration x, $\beta = 1/(k_B T)$, and the partition function is

$$Z = \int_a^b e^{-\beta E(x)} dx\,. \tag{12}$$

The expectation value can be rewritten as

$$\boxed{\langle A \rangle = \int_a^b P(x) A(x) dx}\,, \tag{13}$$

where we defined

$$\boxed{P(x) = \frac{e^{-\beta E(x)}}{Z}}\,, \tag{14}$$

[1] We are here assuming that all sampled values are independent. This will not hold in your simulations of the Ising model with the Metropolis algorithm.

which we can treat as a probability distribution function since $P(x) \geq 0$ and $\int_a^b P(x) = 1$.

In statistical physics, $P(x)$ is a sharp exponential function and A is often a smooth low-order polynomial of the degrees of freedom of the system. Therefore, we are in a situation where sampling a uniform distribution to compute the average as in Eq. 1 is not the smartest choice. It is clearly advantageous to sample random configuration $(x_1, \ldots, x_M)$ distributed like $P(x)$ and estimate the average as

$$\langle A \rangle \equiv \langle A \rangle_P \approx \boxed{\bar{A} = \frac{1}{M} \sum_{i=1}^{M} A(x_i)}. \tag{15}$$

with a statistical error

$$\boxed{\Delta_A \approx \sqrt{\frac{\bar{A^2} - \bar{A}^2}{M-1}}}. \tag{16}$$

When is Monte Carlo integration convenient with respect to numerical integration? "Standard" numerical integration methods would use n points for every dimension d (e.g. $d = 3N$ for a configuration with N particles), so you would have a total of $M = n^d$ points and a scaling on the error as

- error $\propto 1/n$ (midpoint rule)
- error $\propto 1/n^2$ (trapezoidal rule)
- error $\propto 1/n^4$ (Simpson rule)

Therefore, in one dimension, the $1/\sqrt{M}$ rate of convergence of Monte Carlo is very slow. However, let us take Simpson rule in d dimensions and equate its scaling to the scaling of Monte Carlo integration (independent of d!),

$$\frac{1}{M^{4/d}} = \frac{1}{\sqrt{M}} \Longrightarrow d = 8! \tag{17}$$

Therefore, **Monte Carlo integration wins for d > 8**.

If you are not convinced, let us do a reality check to appreciate Monte Carlo integration. Consider N particle in a box with a pair-interaction $v(\mathrm{r}_i - \mathrm{r}_j)$ so that

$$E(\mathrm{r}_1, \ldots, \mathrm{r}_N) = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i=1}^{N} \sum_{j=1, j<i}^{N} v(\mathrm{r}_i - \mathrm{r}_j)\,. \tag{18}$$

In statistical physics, the probability density is

$$P(\mathrm{r}_1, \ldots, \mathrm{r}_N) = \frac{e^{-\beta \sum_{i<j} v(\mathrm{r}_i - \mathrm{r}_j)}}{\int d\mathrm{r}_1 \ldots \int d\mathrm{r}_N \, e^{-\beta \sum_{i<j} v(\mathrm{r}_i - \mathrm{r}_j)}}\,, \tag{19}$$

and a typical average one cares about could be

$$\langle V \rangle = \int d\mathrm{r}_1 \ldots \int d\mathrm{r}_N \left[\sum_{i<j=1}^{N} v(\mathrm{r}_i - \mathrm{r}_j) \right] P(\mathrm{r}_1, \ldots, \mathrm{r}_N)\,. \tag{20}$$

Let us take $N = 100$ so that there are $3N = 300$ coordinates.

- With a **"standard" integration method** one would choose at least 10 points per variable (still very few) to compute $\langle V \rangle$. This means that we need to evaluate $\sum_{i<j=1}^{N} v(\mathrm{r}_i - \mathrm{r}_j)$ as many as 10^{300} times! This is simply **impossible**.

- With Monte Carlo integration, one needs to be able to write the average as $\int f(x)P(x)dx$ with $P(x)$ an effective probability density. Monte Carlo sampling is not always trivial but often doable with some thinking. Furthermore, the normalization of $P(x)$ is often unknown but this problem can be overcome as we will show later.

1.3 Metropolis algorithm

The Metropolis method is a very simple and powerful algorithm to obtain a sequence of configurations sampled from an arbitrary probability density irrespective of the analytical complexity and dimensionality. The Metropolis method represents the basic method behind almost all modern Monte Carlo simulations and is named after the first author of the paper: N. Metropolis, A. W. Rosenbluth, M. Rosenbluth, A. H. Teller, and E. Teller, *Equation of State Calculations by Fast Computing Machines*, Journal of Chemical Physics **21**, 1087 (1953). We will now see how it works.

We begin to generate a sequence of configurations, $\{x_1, \ldots, x_M\}$ (a so-called Markov chain), where, at each Monte Carlo step, a configuration x is modified (updated) to configuration x' according to a **transition probability** $\mathbf{W}(\mathbf{x} \to \mathbf{x}')$ satisfying

$$\boxed{W(x \to x') \geq 0} \quad \text{for } x, x' \in [a, b] \quad \text{and} \quad \boxed{\int_a^b W(x \to x')dx' = 1}. \tag{21}$$

This last condition means that if we start from x we have probability 1 to end up somewhere in $[a, b]$. We have therefore generated a sequence

$$\boxed{x_1 \xrightarrow{W} x_2 \xrightarrow{W} \ldots \xrightarrow{W} x_M}. \tag{22}$$

but we need to now impose some conditions on W so that the configurations are asymptotically distributed as $P(x)$.

It is reasonable to require that a "good" W obeys the following criteria:

1) W must preserve the distribution $P(x)$

$$P(x') = \int_a^b P(x)W(x \to x')dx\,. \tag{23}$$

In other words, if the configurations are distributed according to $P(x)$, they must remain distributed like $P(x)$. This is called **stationarity condition**.

2) The process must be **ergodic**. Starting from any configuration, repeated application of W must allow us to reach any other configuration in a finite number of steps.

It is possible to show that these two rather intuitive conditions are **sufficient** to guarantee that any initial distribution will approach the distribution $P(x)$ after an initial "thermalization" period.

The question now becomes on how to find a transition probability $W(x \to x')$ which satisfies Eq. 23. To this aim, we impose a more stringent (sufficient but not necessary) condition, namely, the so-called **detailed balanced condition**:

$$\boxed{P(x)W(x \to x') = P(x')W(x' \to x)} \tag{24}$$

which means that the flux from $x \to x'$ is equal to the flux from $x' \to x$. We can also see that the updates are microscopically reversible. It is easy to show that imposing detailed balance ensures that the condition in Eq. 23 is satisfied:

$$\int_a^b P(x)W(x \to x')dx = \int_a^b P(x')W(x' \to x)dx = P(x') \underbrace{\int_a^b W(x' \to x)dx}_{1} = P(x')\,, \tag{25}$$

where we used the property (Eq. 21) of W. Therefore, if we construct a transition W which satisfies detailed balance and the process is ergodic, starting form an arbitrary initial distribution we will end up in $P(x)$.

In a typical simulation, one starts from x_1 and does not consider all possible configurations x' but a small subset by making "small" changes in x_1. For instance, for a system of spins on a lattice, one can flip one spin at random. For a system of particles, one can move a randomly chosen particle (or loop through the particles) by a displacement Δx chosen randomly in a box surrounding the current position (Fig. 2).

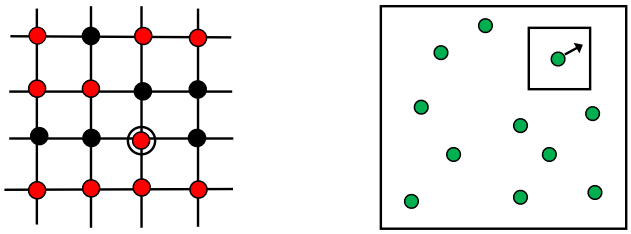

Figure 2: Possible Monte Carlo moves: flip a spin at random (left); move a particle by a random displacement in a box centered at the current position of the particle (right).

To proceed, one writes the transition probability W as the product of the probability T for attempting the move (e.g. flipping the spin or moving the particle) and the probability A of accepting the move:

$$\boxed{W(x \to x') = T(x \to x') \times A(x \to x')}\,, \tag{26}$$

where we choose $T(x \to x') \geq 0$ in $[a, b]$ and $\displaystyle\int_a^b T(x \to x')dx' = 1$.

Then, we can rewrite the detailed balance condition as

$$\begin{aligned} \frac{W(x \to x')}{W(x' \to x)} &= \frac{P(x')}{P(x)} \\ \frac{A(x \to x')}{A(x' \to x)} &= \frac{T(x' \to x)P(x')}{T(x \to x')P(x)}\,. \end{aligned} \tag{27}$$

For a given T, this condition can be fulfilled by an infinite choice of acceptance functions, A, but the choice which maximizes acceptance is the original choice of Metropolis *et al.*

$$A(x \to x') = \min\left\{1, \frac{T(x' \to x)P(x')}{T(x \to x')P(x)}\right\}. \tag{28}$$

Sometimes, one chooses **T symmetric**, namely, $T(x \to x') = T(x' \to x)$ as in the cases of Fig. 2. If T is symmetric, it cancels out from the above ratio and one obtains the simpler acceptance as in the original Metropolis algorithm:

$$\boxed{A(x \to x') = \min\left\{1, \frac{P(x')}{P(x)}\right\}}. \tag{29}$$

This expression is quite intuitive: If the probability density at the new configuration is higher, the move is accepted. Otherwise, it is accepted with a probability equal to the ratio the new and old weights. To determine whether to accept or reject the case when $A(x \to x') < 1$, compare A against a random number $r \in [0, 1]$. There are two possibilities:

1) If $r < A(x \to x')$, the move is accepted and you take x' as new configuration.

2) If $r > A(x \to x')$, the move is rejected and you take $x' = x$ as new configuration.

1.4 How do we sample configurations with $P(x) = \frac{1}{Z}e^{-\beta E(x)}$?

In statistical physics, we want a sequence of configurations distributed as $P(x) = \frac{1}{Z}e^{-\beta E(x)}$.

Starting from some initial configuration of the system, we propose a move to a new configuration with a chosen T (symmetric) and simply accept the move with

$$A(x \to x') = \min\left\{1, e^{-\beta[E(x')-E(x)]}\right\}. \tag{30}$$

Therefore, if $E(x') < E(x)$, the move is always accepted. Otherwise, it will accepted/rejected by comparing the exponential to a random number as discussed above.

Important bonus of the Metropolis algorithm is that Z (which we did not know how to compute) drops out of the equation! The method suffers however from two disadvantages:

1) The sampling process is only correct asymptotically.

2) Subsequent configurations are strongly correlated.

We will get back to these two issues in the exercises of the Monte Carlo simulations of the Ising model.

2 The Ising model

The Ising model is historically very important since it was the first statistical model exactly solvable, which exhibits a phase transition. From the exact results, it was possible to start developing concepts such as scaling, critical exponents, and universality which are widely used to analyze critical phenomena. The model was proposed by Wilhelm Lenz in 1920 and solved exactly in one dimension by his student Ernst Ising in 1925. The one-dimensional model does however not exhibit a phase transition. In 1944, Lars Onsager solved the Ising model exactly in two dimensions in the absence of an external magnetic field and showed that there is a phase transition in two dimensions.

The Ising model is a lattice model to describe magnetism in solids and consists of a collection of magnetic moments, which we can think as being atoms with spin $\frac{1}{2}$ moments. For simplicity, we will place the spin on a regular lattice and assume that each spin s_i can point in the $+z$ or $-z$ direction. For convenience, we set $\mathbf{s_i = \pm 1}$ at each site and further simplify the model by having **spins interact only with the nearest neighbors**. The energy of a particular state (configuration) of the Ising model is given by

$$\boxed{E = -J \sum_{\langle ij \rangle} s_i s_j - B \sum_i s_i}\,, \tag{31}$$

where the notation $\langle ij \rangle$ means that we sum over all nearest neighbor pairs in the lattice. B is a possible external magnetic field.[2]

The interaction energy of nearest neighbors is called the exchange interaction J. If $\mathbf{J > 0}$, neighboring spins prefer to be aligned ($\uparrow\uparrow$ or $\downarrow\downarrow$) and such a system is a **ferromagnet**. If $\mathbf{J < 0}$, the spins want to anti-align ($\uparrow\downarrow$) as in an **antiferromagnet**.

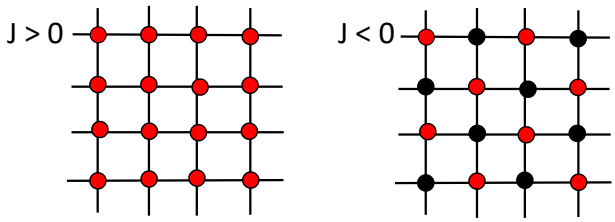

Figure 3: Parallel and antiparallel alignment of the spins in a ferromagnet ($J > 0$) and antiferromagnet ($J < 0$).

2.1 Important thermodynamic quantities

Let us quickly go through some important quantities we will use to study the magnetic behavior of the Ising model. You will derive some of these expressions as part of the exercises.

We denote a global spin configuration of the system as

$$S = (s_1, \ldots, s_N)\,, \tag{32}$$

[2]Comments on the notation: B should be properly denoted by H but we use B to avoid confusion with the Hamiltonian. We have omitted the factor μ for the magnetic moment, which has been absorbed in B. Finally, the magnetic moment of the electron is antiparallel to the spin, so the sign in the second term of the energy above should in fact be positive, but the negative term is used conventionally.

where N is the total number of sites. The total number of states is $K = 2^N$ and a thermal average over the possible states is given by

$$\boxed{\langle A \rangle = \frac{1}{Z} \sum_{i=1}^{K} A(S_i) e^{-\beta E(S_i)}}, \tag{33}$$

and the partition function is

$$Z = \sum_{i=1}^{K} e^{-\beta E(S_i)} . \tag{34}$$

The free energy of the system is given by

$$F = E - TS = -\frac{1}{\beta} \ln(Z) . \tag{35}$$

where S in $F = E - TS$ is the entropy (do not confuse it with the spin configuration).

The value of the **total magnetization** for a given spin configuration $S = (s_1, \ldots, s_N)$ is

$$\boxed{M(S) = \sum_{i=1}^{N} s_i}, \tag{36}$$

and its average value

$$\langle M \rangle = \frac{1}{Z} \sum_{i=1}^{K} M(S_i) e^{-\beta E(S_i)} . \tag{37}$$

The magnetization is also related to the first derivative of the free energy (at constant temperature) as

$$\langle M \rangle = -\frac{\partial F}{\partial B} . \tag{38}$$

In the following, we will often discuss about the mean magnetization per site defined as

$$m = \frac{1}{N} \langle M \rangle . \tag{39}$$

The **magnetic susceptibility** (at constant temperature) is the response of the magnetization to a change in the external magnetic field and is defined as

$$\boxed{\chi = \frac{\partial \langle M \rangle}{\partial B}}. \tag{40}$$

It is easy to show that the susceptibility can be expressed in terms of the thermal fluctuations of the magnetization around its average

$$\boxed{\chi = \beta \left[\langle M^2 \rangle - \langle M \rangle^2 \right]}. \tag{41}$$

The total energy of the system is given by

$$\langle E \rangle = \frac{1}{Z} \sum_{i=1}^{K} E(S_i) e^{-\beta E(S_i)} , \tag{42}$$

and the **heat capacity** (at constant field) is the response of the energy of the system to a change in temperature

$$\boxed{C_B = \frac{\partial \langle E \rangle}{\partial T}}, \tag{43}$$

which, similarly to the magnetic susceptibility, can be express in terms of the thermal fluctuations of the energy around the mean value

$$\boxed{C_B = k_B \beta^2 \left[\langle E^2 \rangle - \langle E \rangle^2 \right]}. \tag{44}$$

2.2 Phase transitions and spontaneous symmetry breaking

A phase transition occurs when there is a singularity in the free energy or in one of its derivatives, and is visible as a sharp change in the macroscopic properties of the system as some external parameter (e.g. temperature) is varied. Unless otherwise stated, we will work with the Ising model of a **ferromagnet** ($J > 0$) in **two dimensions**. The results below are valid in the **thermodynamic limit**, namely, $N \to \infty$.

To analyze the characteristic of the phase transitions in the Ising model, we begin by describing the behavior of the **magnetization as a function of the temperature** (see also Fig. 4):

- $\mathbf{B \neq 0}$. The magnetization changes smoothly as the temperature is varied and is positive or negative according to the sign of the field. At very large temperature, the magnetization goes to zero since the entropy associated with the spin fluctuations is dominant over the energetically preferable state of aligned spins. As $T \to 0$, the magnetization smoothly goes to the values of $m = \pm 1$ which minimizes the energy, with all the spins pointing in the same direction (either up or down).

- $\mathbf{B = 0}$. The magnetization does not behave smoothly but turns off abruptly at the critical temperature $T_c > 0$. For $T > T_c$, the average magnetization is zero (paramagnetic phase) and, for $T < T_c$, a magnetization emerges even in the absence of a magnetic field (ferromagnetic phase) and the system can sit in one of two magnetized states. We say that the system displays a **paramagnetic $\leftrightarrow$ magnetic phase transition** as we vary the temperature across T_c.

  As T goes below the critical temperature at $B = 0$, the system is said to **spontaneously break the symmetry**. This means that, even though the Hamiltonian is

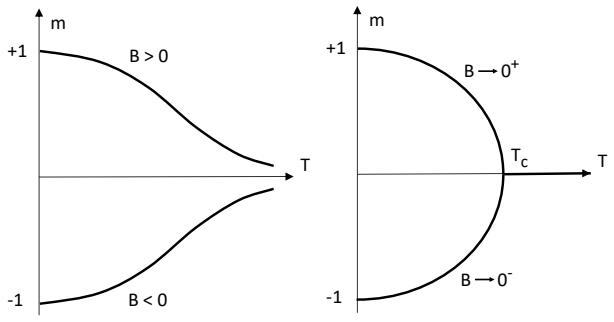

Figure 4: Magnetization as a function of temperature for $B \neq 0$ (left) and $B = 0$ (right).

symmetric with respect to flipping all spins, the system chooses the ferromagnetic state, which is not invariant under $S \to -S$.

The **phase diagram** in the B–T plane of the two-dimensional Ising model is shown in Fig. 5 and displays **a line of first-order phase transition which ends in a critical point** at the temperature T_c. All transitions happen at $B = 0$ because of the symmetry of a ferromagnet to reversal of the field. Let us elaborate on this some more:

- If we fix $T < T_c$, we do have a phase transition if we vary B from positive to negative:

$$\begin{cases} M > 0 & B = 0^+ \\ M < 0 & B = 0^- \end{cases} \tag{45}$$

  The magnetization jumps discontinuously from a positive to a negative value. Since the magnetization is a first derivative of the free energy, this is a **first-order phase transition**.

- For $T > T_c$, it is possible to move continuously from a state of positive magnetization to one of negative magnetization.

- The critical point $T = T_c$ separates these two behaviors. At the critical point, the magnetization is continuous (the transition is not first order) but the derivatives are discontinuous. This results in divergences of the response functions, namely, the specific heat and the susceptibility.

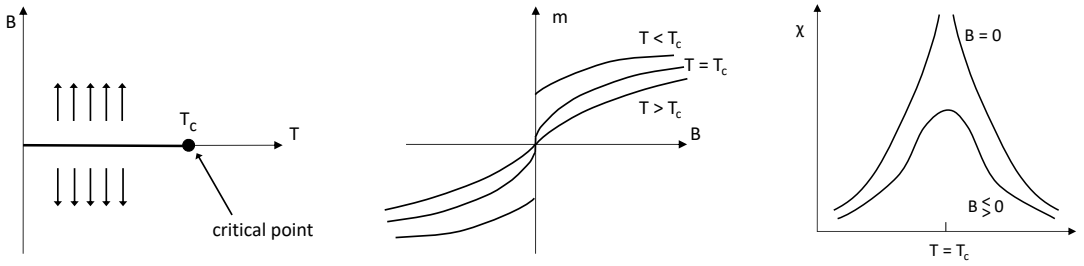

Figure 5: Phase diagram of the Ising model in the B-T plane (left). The co-existence curve is along the $B = 0$ axis and terminates in a critical point. Isotherms in the M-B plane (center). Note the emergence of flat piece for $T < T_c$. Dependence of the susceptibility on the temperature (left).

The magnetization is the so-called **order parameter** of the system, measuring the degree of order across the boundaries of the phase transition. For the Ising model, the word "order" refers to the behavior of the spins mostly aligned in the same direction below T_c, while pointing randomly in both directions above T_c. As we vary the temperature at $B = 0$, the **paramagnetic $\leftrightarrow$ ferromagnetic transition** at the critical temperature T_c is called a **continuous phase transition** because the order parameter m vanishes continuously rather than discontinuously.

Before discussing further the Ising model, it is important to point out the similarities of the phase transition of a Ising model with a very different system, namely, the liquid-gas phase transition depicted in Fig. 6. The order parameter of this transition is the density of the

fluid. The co-existence curve separates the gas and liquid phases characterized by different densities ρ_g and ρ_l. Along the co-existence curve, the fluid can can exist in the two different forms and in the co-existence region it will phase separate in a mixture of gas and liquid with densities ρ_g and ρ_l, and required total density ρ. The co-existence curve terminates in the critical point T_c, P_c, ρ_c. The difference between the densities of the coexisting liquid and gas phases vanishes on approaching T_c with $\rho_l \to \rho_g$ as $T \to T_c^-$. The isothermal compressibility (the response of the volume to a change in pressure) diverges at the critical point. Due to the termination of the coexistence line, it is possible to go from the gas phase to the liquid phase continuously (without a phase transition) by going around the critical point. Thus there are no fundamental differences between the liquid and gas phases (i.e. there is no change of fundamental symmetry).

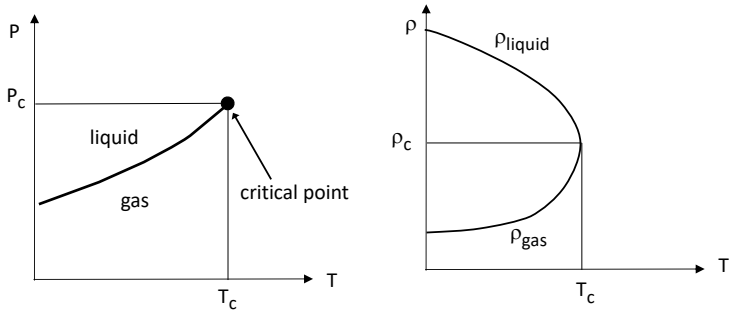

Figure 6: Phase diagram of a fluid. The first-order line of the gas/liquid phase transition ends at a critical point. The order parameter is here the density ρ of the fluid. The density of the gas and the liquid become the same at the critical point.

2.3 Critical exponents

The singular behavior in the vicinity of the critical point is characterized by a set of critical exponents. These exponents describe the non-analyticity of various thermodynamic functions. It turns out that, while the critical temperature T_c depends sensitively on the details of the interactions of the system, the critical exponents depend on few fundamental parameters (e.g. for systems with short range interactions, the dimensionality of space d and the symmetry of the order parameter). Remarkably, transitions as different as the liquid/gas and ferromagnetic transition in 3 dimensions can be described by the same set of critical exponents and are said to belong to the same **universality class**. Therefore, even though a phase transition in a system of spins on a lattice or a liquid/gas system may seem totally unrelated, the order parameters and higher derivatives of the free energies will behave similarly at the critical point as if all memory of the microscopic physics – the type of particles, the nature of the interactions – has been lost at the critical point.

Back to the Ising model in two dimensions. From the analytic solution at $B = 0$, we have that the critical temperature is given by

$$\boxed{\frac{kT_c}{J} = \frac{2}{\ln(1+\sqrt{2})}}. \tag{46}$$

and, in the following, we introduce the reduced temperature difference

$$t = \frac{T - T_c}{T_c} \,. \tag{47}$$

We have that the magnetization is zero for $T > T_c$ and vanishes for $T \to T_c^-$ as

$$m(T) \sim (-t)^\beta \,, \tag{48}$$

where β is the critical exponent, not to be confused with the temperature!
The zero-field susceptibility diverges for T near T_c as

$$\chi \sim |t|^{-\gamma} \,, \tag{49}$$

while the heat capacity diverges logarithmically at $T = T_c$ as

$$C_B \sim -\ln|t| \,. \tag{50}$$

Since the divergence of C_B is logarithmic and, therefore, slower than any power of t, one writes a power law as $\sim |t|^{-\alpha}$ with a critical exponent $\alpha = 0$.

Another important exponent is related to the behavior of the spin-spin correlation function:

$$G(r) = \langle s_k s_{k+r} \rangle - \langle s_k \rangle \langle s_{k+r} \rangle = \langle s_k s_{k+r} \rangle - m^2 \,, \tag{51}$$

where $\langle s_k \rangle = \langle s_{k+r} \rangle = \langle M \rangle / N = m$ is the magnetization per site. Since all lattice sites are equivalent, $G(r)$ is independent of the choice of k and, for a given B and T, depends only on the separation between the two spins in units of the lattice constant.

This function measures the degree of correlation between spins at different sites. If the spins are not correlated, $G(r) = 0$. At high temperatures, the interaction between spins is less important, and hence the spins are randomly oriented in the absence of an external field. Thus, in the limit of high temperatures, $G(r) \to 0$ for fixed r. For fixed T and B, we expect that if spin k is up, then the adjacent spins will have a greater probability of being up than down. For spins further away from spin k, the probability that spin $k + r$ is up (correlated with k) will decrease. Hence, $G(r) \to 0$ as $r \to \infty$. Close to the critical point, we have $G(r) \sim \exp(-r/\xi)$ with a correlation length ξ which diverges as

$$\xi \sim |t|^{-v} \,. \tag{52}$$

We will discuss the implication of this results on our ability of performing Monte Carlo simulations in proximity of the critical point.

The exponents are summarized in Table 1. In the exercises, you will numerically investigate the behavior of these properties close to the critical point and compare them to the mean-field model of the Ising system you have already seen in the Statistical Physics course.

2.4 Does symmetry breaking make sense?

Let us take $B = 0$ and $T < T_c$. The expression of the magnetization is given

$$\langle M \rangle = \frac{1}{Z} \sum_{i=1}^{K} M(S_i) e^{-\beta E(S_i)} \,. \tag{53}$$

You may ask yourself some questions:

Quantity	Singular behavior	Critical exponent
Order parameter (B=0)	$m \sim(-t)^{\beta}$	1/8
Susceptibility (B=0)	$\chi \sim\|t\|^{-\gamma}$	7/4
Specific heat (B=0)	$C_B\sim\|t\|^{-\alpha}$	0 (log)
Correlation length	$\xi \sim\|t\|^{-\nu}$	1

Table 1: Critical exponents of the two-dimensional Ising model.

- On the right-hand side of the equation, you have analytic functions. How can $\langle M\rangle$ display discontinuities at $B = 0$ or be non-analytic as a function of temperature?
- Under $S \to -S$, $E(S)$ is even and $M(S)$ is odd. Therefore the product $M(S)e^{-\beta E(S)}$ is odd. Summing over all values an odd function, you should get zero. How can we get $\langle M\rangle$ different than zero?

For spontaneous symmetry breaking to occur, you need two ingredients:

1) You need a small symmetry breaking field.

2) The system size must be infinite ($N \to \infty$).

The first requirement is automatically satisfied in a real system. For example, for the ferromagnetic transition, we always have a small but finite magnetic field in any experiment. Therefore, in reality, what you obtain in an experiment is

$$\langle M\rangle_+ = \lim_{B\to 0^+} \langle M(B)\rangle\,, \tag{54}$$

and

$$\langle M\rangle_- = \lim_{B\to 0^-} \langle M(B)\rangle\,, \tag{55}$$

with

$$\lim_{B\to 0^+} \langle M(B)\rangle \neq \lim_{B\to 0^-} \langle M(B)\rangle\,. \tag{56}$$

Therefore, you can think that you have obtained the upper and lower curve in Fig. 4 taking the limits $B \to 0^+$ or $B \to 0^-$, respectively. Alternatively, you can think that you have an infinitesimally small field always present which will break the symmetry.

To understand why we have a discontinuity in $\langle M\rangle$ with analytic functions, you need to think that you have a singularity in your system, namely, $N \to \infty$. If you have a function $f_i(x)$ with $i = 1, 2, 3, \ldots$, you can have that the $\lim_{i\to\infty} f_i(x)$ is not analytic even if all $f_i(x)$ are analytic functions. For example,

$$f_i(x) = \frac{x}{x^2 + 1/i^2}\,. \tag{57}$$

For any value of i, the function is analytic but

$$\lim_{i\to\infty} f_i(x) = \frac{1}{x}\,, \tag{58}$$

and this limit is not analytic! The function is singular at $x = 0$ and

$$\lim_{x\to 0^+} \lim_{i\to\infty} f_i(x) = +\infty \quad \text{and} \quad \lim_{x\to 0^-} \lim_{i\to\infty} f_i(x) = -\infty\,. \tag{59}$$

Similarly, $\langle M(B,N)\rangle$ is an analytic function for any finite N but the $N \to \infty$ may be singular with

$$\lim_{B\to 0^+} \lim_{N\to\infty} \langle M(B,N)\rangle \neq \lim_{B\to 0^-} \lim_{N\to\infty} \langle M(B,N)\rangle \tag{60}$$

This is what happens when you have phases which spontaneously break the symmetry.

2.5 Monte Carlo simulations of the two-dimensional Ising model

We will here summarize the Metropolis algorithm and the relevant equations. More detailed guidance will be given in the text of the exercises.

- We work with a square lattice and a total number of spins $N = L \times L$.
- We use the Metropolis algorithm to generate a sequence of configurations $\{S_0, S_1, \ldots\}$ sampled from the Boltzmann distribution. We will employ a very simple probability T to propose a move: we will flip one spin chosen at random (see Fig. 2).
- The "basic" Metropolis algorithm can be summarized as follows:

1. Initialize the spin configuration S_0
2. Propose a move: select a spin at random and flip it.

   You have obtained a new configuration S' (only differing from S_0 in one spin).
3. Compute $\Delta E = E(S') - E(S_0)$ and $p = \exp(-\beta\Delta E)$.
4. Accept or reject the move with probability p:

   If $\Delta E \leq 0$, $p \geq 1 \rightarrow$ accept the move and set $S_1 = S'$.

   If $\Delta E > 0$, $p < 1 \rightarrow$ pick a uniformly distributed random number $r \in [0,1]$.

   a) If $r < p$, move accepted $\rightarrow$ set $S_1 = S'$

   b) if $r > p$, move rejected $\rightarrow$ set $S_1 = S_0$
5. Update $M(S_1)$, $E(S_1)$, and other quantities needed in your averages.
6. Go back to 2) and iterate for N_{MC} times.
7. Visualize your data.
8. Throw away the first κ configurations. The measurements of physical observables are done after an equilibration time κ since the correct Boltzmann distribution is only approached after some time that depends on the initial configuration.
9. Collect the averages as

$$\langle M\rangle \approx \frac{1}{N_{\mathrm{MC}}} \sum_{k=1}^{N_{\mathrm{MC}}} M(S_k)\,.$$