Interactive Potts Model

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Abstract

This document provides a qualitative explanation of critical phenomena involving the Potts model, which are showcased at https://farrenal.github.io/Potts. We first introduce the two-dimensional square lattice $q-$Potts model by relating it to the simpler Ising model with $q = 2$. We motivate and explain a Metropolis-Hastings algorithm to find the equilibrium lattice configuration for various temperatures and magnetising field strengths. Finally, we explain the showcased visuals with this background in mind.

Acknowledgments

We would like to thank Prof. Sinéad Ryan, who guided us during an independent reading project on statistical field theory. The meat of the introduction is our understanding of Prof. Tong's Part III notes on SFT. Our starting point for the code can be found here.

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1 Introduction to Criticality

To understand the idea of criticality in statistical physics, we will first review the Ising model. Armed with some familiarity with this toy model, we will generalise to the q-state Potts model [1]. This section follows [2] with some thermodynamic theory from [3].

1.1 The Ising model

Suppose we have a square lattice with N sites sitting in some heat bath with temperature T and external magnetic field H[1]. Fixed at each lattice site there is a magnetic dipole, which we view as a spin s_i, with values $+1$ or -1 corresponding to the two possible spin orientations; aligned or anti-aligned with the magnetic field. For each stationary dipole there is an associated potential energy related to the magnetic moment in the field, as well as a potential energy due the orientation of neighbouring dipoles. The Hamiltonian $\mathcal{H}$ of such a system has the form

$$\mathcal{H}(s) = -\sum_{\langle i,j\rangle} J_{ij} s_i s_j - \sum_{j=1}^{N} H_j s_j, \tag{1.1}$$

where the first term sums over neighbouring dipole interactions and the second term arises due to the dipoles' interaction with the external magnetic field. For simplicity, let us assume that the magnetic field is uniform in space such that $H_j = H$ for all $j = 1, \ldots,\ N$ and that the nearest neighbour coupling J_{ij} is the same between every pair of spins. Now the Hamiltonian is

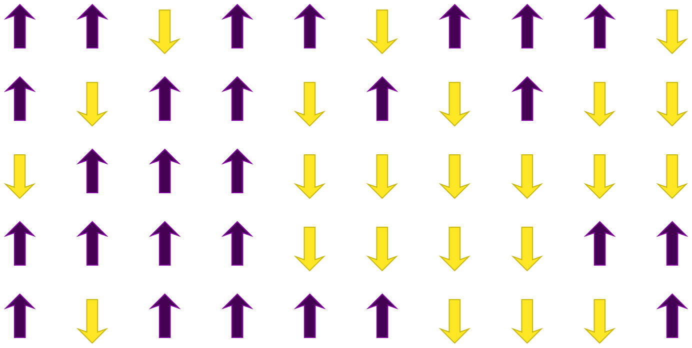

Figure 1. The 2D Ising model as a square lattice with two spin states.

$$\mathcal{H}(s) = -J\sum_{\langle i,j\rangle} s_i s_j - H\sum_{j} s_j. \tag{1.2}$$

By looking at the Hamiltonian (1.2), which corresponds to the energy of our system, we can make some distinction between regimes. If $J > 0$ then, to minimise the energy, neighbouring spins prefer to be pairwise aligned (ferromagnetism). If $J < 0$ then neighbouring spins prefer to be anti-aligned (anti-ferromagnetism). Going forward we will assume $J > 0$. The effect of the external magnetic field H is to cause dipoles/spins to preferentially align in its direction. Our Hamiltonian (1.2) assigns a minus sign to the term, which means that H points in the $s_i = +1$ direction (again to minimize $\mathcal{H}$).

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[1] Not to be confused with the magnetic field B. See [4] chapter 6.3.

We are working in a canonical ensemble, i.e. a heat bath with a conserved number of dipoles. The canonical partition function Z is given by

$$Z(T,J,H)=\sum_{\{s_i\}}e^{-\beta\mathcal{H}(s)} \tag{1.3}$$

where $\beta=1/k_{\mathrm{B}}T$ and we sum over all lattice configurations $\{s_i\}$. In statistical thermodynamics, this partition function arises as a normalisation factor for the probability distribution $p(E)$ for a system to have energy E in equilibrium with a heat bath of temperature T, where

$$p(E)=\frac{1}{Z}e^{\frac{E}{k_{\mathrm{B}}T}} \implies \langle X\rangle=\sum_E X(E)\;p(E)=\frac{1}{Z}\sum_{\{s_i\}}X\;e^{-\beta\mathcal{H}(s)}. \tag{1.4}$$

We discussed how spins tend to preferentially align due to neighbouring interactions or the magnetic field, but the temperature T of the system also plays an important role. At high temperatures, there are stronger thermal fluctuations, which randomly reorient the spins. At low temperatures, the effects of J and H are conversely far more influential. We are thus concerned with the *average* magnetisation density m of our spin lattice

$$m=\frac{1}{N}\Big\langle\sum_j s_j\Big\rangle\overset{(1.4)}{=}\frac{1}{N\beta}\frac{\partial\ln Z}{\partial H}. \tag{1.5}$$

In a completely disordered state where spins are randomly aligned, we expect there to be no magnetic character to the lattice, i.e. $m=0$. In the opposite case, when nearly all spins are aligned in the same direction, the net magnetisation of the lattice approaches N (all spins $s_i=+1$) or $-N$ (all spins $s_i=-1$) so that the magnetisation density approaches $m\pm1$. So because it details how ordered the spin lattice is, m is called the *order parameter* of our system.

Free energy

According to (1.5), to find m we should know the partition function Z. We rewrite

$$Z=\sum_m\sum_{\{s_i\}|m}e^{-\beta\mathcal{H}(s)}=\sum_m e^{-\beta F(m)}, \tag{1.6}$$

where we first sum over all configurations $\{s_i\}$ with fixed average magnetisation m and then sum over all possible m. The average magnetisation lies between -1 and +1 and takes discrete values, quantised in units of $2/N$. Therefore in the thermodynamic limit when $N\gg1$, we may approximate the discrete sum (1.6) as an integral. This integral now implicitly defines a function $F(m)$ called the effective free energy. F depends on the average magnetisation m, the temperature T, and magnetic field strength H. This means

$$Z\approx\frac{N}{2}\int_{-1}^{+1}dm\;e^{-\beta F(m)}. \tag{1.7}$$

We further define the free energy per unit spin, $f(m)=F(m)/N$. Now our partition function is given by

$$Z\approx\frac{N}{2}\int_{-1}^{+1}dm\;e^{-\beta Nf(m)}. \tag{1.8}$$

In the thermodynamic limit $N\gg1$ while $\beta f(m)\sim1$. We may therefore make use of the saddle point approximation and evaluate the integral as the largest value of its integrand. The condition for steepest descent is

$$\frac{\partial f}{\partial m}(m_{\mathrm{eq}})=0. \tag{1.9}$$

where m_{eq} is the equilibrium value of the magnetisation, such that f is minimised. All in all, we have approximated our partition function to be

$$Z \approx e^{-\beta N f(m_{\text{eq}})}. \tag{1.10}$$

From thermodynamics we know that the Helmholtz free energy is given by $F_{\text{H}} = -\ln Z/\beta$ from which we see that the Helmholtz free energy can be viewed as the effective free energy evaluated at the saddle point in the thermodynamic limit, i.e. $F_{\text{H}} \approx F(m_{\text{eq}})$. This implies

$$m \overset{(1.5)}{=} \frac{1}{N\beta}\frac{\partial \ln Z}{\partial H} = -\frac{1}{N}\frac{\partial F_{\text{H}}}{\partial H}. \tag{1.11}$$

Mean field theory

We can get an estimate for the Hamiltonian of a lattice configuration by replacing each site's spin s_i with its mean value $\langle s_i \rangle = m$. We get

$$\mathcal{H} \approx \langle \mathcal{H} \rangle = -J \sum_{\langle i,j \rangle} m^2 - H \sum_{j} m \implies \frac{\langle \mathcal{H} \rangle}{N} \approx -\frac{1}{2} J Q m^2 - Hm, \tag{1.12}$$

where Q is the number of nearest neighbours per site[2]. This is a rather coarse approximation as it does not contain any dynamical information about the lattice. There is however the benefit of making the previous summations easier. All we need now do is count the number of configurations with magnetisation m to calculate

$$Z \approx \sum_{m} \sum_{\{s_i\}|m} e^{-\beta \langle \mathcal{H} \rangle} = \sum_{m} e^{-\beta \langle \mathcal{H} \rangle} \sum_{\{s_i\}|m} 1. \tag{1.13}$$

A system with magnetisation m with $N_{\uparrow}$ spins oriented up and $N_{\downarrow}$ oriented down has magnetisation

$$m = \frac{N_{\uparrow} - N_{\downarrow}}{N} = \frac{2N_{\uparrow} - N}{N}. \tag{1.14}$$

In statistical physics, a *microstate* is a specific configuration of the system realising energy E, volume V with N constituents in a microcanonical ensemble [3]. The number of microstates $\Omega(E, V, N)$ counts the total number of possible system configurations with such thermodynamic properties. For us, the number of microstates $\Omega(m)$ with magnetisation m is

$$\Omega(m) = \frac{N!}{N_{\uparrow}!(N - N_{\uparrow})!} = \binom{N}{N_{\uparrow}}. \tag{1.15}$$

This is because there are $\binom{N}{N_{\uparrow}}$ ways to choose $N_{\uparrow}$ sites from N to which we assign $s = +1$ while achieving a magnetisation m. (The rest must have $s = -1$.) In the thermodynamic limit, where $N \gg 1$, we can use Stirling's approximation[3] and some algebra to get

$$\frac{\ln \Omega(m)}{N} \approx \ln 2 - \frac{1}{2}(1+m)\ln(1+m) - \frac{1}{2}(1-m)\ln(1-m). \tag{1.16}$$

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[2] In $d = 1$ dimension, a square lattice has 2 nearest neighbours. In $d = 2$ dimensions, a square lattice has 4 nearest neighbours. In general, it's easy to see that a square lattice in d dimensions has $Q = 2d$ nearest neighbours. We must however divide Q by two in (1.12) to prevent double counting the same nearest neighbour pair.

[3] $\ln A! \approx A \ln A - A$ for very large $A \gg 1$.

According to (1.6), we have defined $f(m)$ such that

$$e^{\beta N f(m)} = \sum_{\{s_i\}|m} e^{-\beta\mathcal{H}} \approx e^{-\beta\langle\mathcal{H}\rangle} \sum_{\{s_i\}|m} 1 = \Omega(m) e^{-\beta\langle\mathcal{H}\rangle}. \tag{1.17}$$

Taking the natural log of both sides and substituting (1.16), we get the mean field free energy per site

$$f(m) \approx -Hm - \frac{1}{2}JQm^2 - k_{\mathrm{B}}T\big[\ln 2 - \frac{1}{2}(1+m)\ln(1+m) - \frac{1}{2}(1-m)\ln(1-m)\big] \tag{1.18}$$

Now we compute the mean field equilibrium magnetisation m_{eq} which satisfies (1.9), yielding

$$\beta(H + JQm_{\mathrm{eq}}) = \frac{1}{2}\log\left(\frac{1+m_{\mathrm{eq}}}{1-m_{\mathrm{eq}}}\right). \tag{1.19}$$

Rearranging gives us the self-consistency equation for the equilibrium magnetisation m_{eq},

$$m_{\mathrm{eq}} = \tanh(\beta H + \beta JQm_{\mathrm{eq}}). \tag{1.20}$$

We can interpret the argument of the hyperbolic tangent as an effective field $H_{\mathrm{eff}} = H + JQm_{\mathrm{eq}}$ which also encapsulates the neighbouring spin interactions' effect on each site. This H_{eff} is sometimes called the *mean field*, whence the name of this approximation.

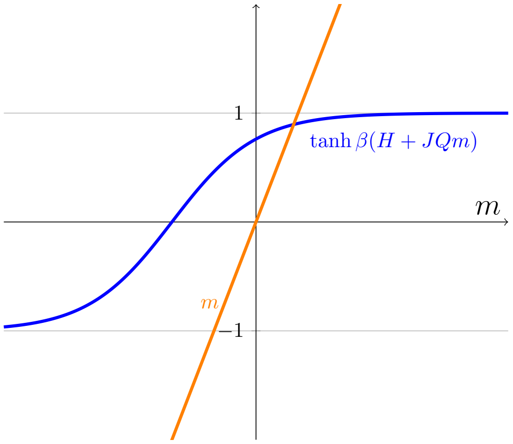


Figure 2. The self-consistency equation for m_{eq} is represented by the intersection of the two curves. We see that $m_{\mathrm{eq}} = 0$ is only a solution if $H = 0$ and $T \gg J$.

1.2 Phase transitions in the Ising model

In thermodynamics, a phase transition occurs when a certain quantity, the order parameter, changes discontinuously. By first order phase transitions, we then mean those characterised by a discontinuity in the first derivatives of F_{H} or the Gibbs free energy. We can extend this definition to second order phase transitions where the order parameter is a second derivative of the free energies and so on.

These derivatives are important because they detail the stability of a thermodynamic system. In particular, if the stability or equilibrium criteria are violated, by a discontinuity of a derivative, then we arrive at an unstable phase of matter which prompts a phase transition.

As we saw in (1.5), the order parameter for the Ising model is the average or equilibrium magnetisation m which is a first derivative of F_{H} as seen in (1.11). If instead of finding the equilibrium magnetisation m_{eq} for all regimes of m, we Taylor expand the free energy (1.18) around small m (which corresponds to a disordered state) we get the *Landau* mean field free energy

$$f(m) \approx -k_{\mathrm{B}}T\ln 2 - Hm + \frac{1}{2}(k_{\mathrm{B}}T - JQ)m^2 + \frac{1}{12}k_{\mathrm{B}}Tm^4 + \ldots \,. \tag{1.21}$$

The derivative of this approximation $\partial f/\partial m$ exhibits different behaviour in different regimes of J, T and H. We will consider now the critical behaviour of the Ising model in both the absence and presence of a magnetic field.

With $\boldsymbol{H = 0}$

Consider the mean field free energy $f(m)$ where there is no external magnetic field such that $H = 0$. From (1.21) we get

$$f(m) \propto \frac{1}{2}(T - T_c)m^2 + \frac{1}{12}Tm^4 + \ldots, \tag{1.22}$$

where we have defined the *critical temperature* $T_c = JQ/k_{\mathrm{B}} = 2dJ/k_{\mathrm{B}}$ in d dimensions and ignored the overall constant term $-k_{\mathrm{B}}T\ln 2$. The free energy minimum depends on the sign of the coefficient of the quadratic term as seen below.

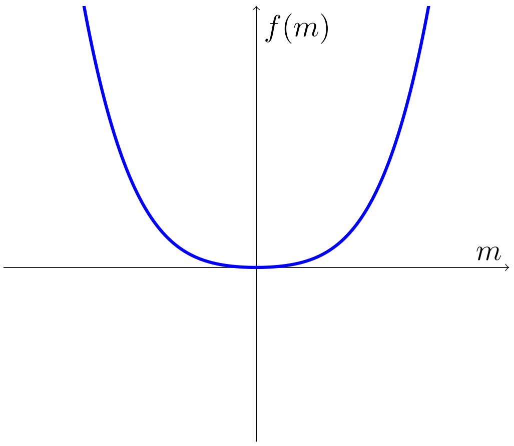


Figure 3. Free energy $f(m)$ for $T > T_c$

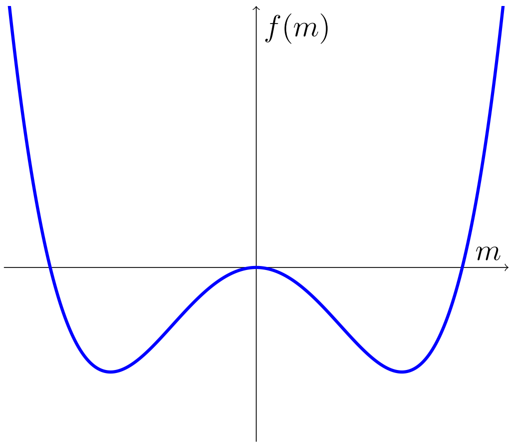


Figure 4. Free energy $f(m)$ for $T < T_c$

Computing $f'(m_{\mathrm{eq}})$ gives us, truncating from $\mathcal{O}(m^6)$,

$$(T - T_c)m_{\mathrm{eq}} + \frac{1}{3}Tm_{\mathrm{eq}}^3 = 0 \implies m_{\mathrm{eq}}\big(m_{\mathrm{eq}}^2 - \frac{3(T_c - T)}{T}\big) = 0. \tag{1.23}$$

We see from Figure 3 that when $T > T_c$ the minimum corresponds to $m_{\mathrm{eq}} = 0$, while for $T < T_c$ Figure 4 tells us that $m_{\mathrm{eq}} = \pm\sqrt{3(T - T_c)/T}$. But this Landau mean field expression for $f(m)$ is only valid for small m, which happens around $T \approx T_c$ according to what we just discussed. (The equilibrium m_{eq} is most likely to be measured on the lattice, so we can talk about it 'happening'.)

When m is not small enough to truncate at order $\mathcal{O}(m^6)$, i.e. when T is not close enough to T_c we need to look at our self-consistency equation (1.20) again

$$m_{\text{eq}} = \tanh(\beta H_{\text{eff}}), \qquad H_{\text{eff}} = k_{\text{B}} T_c m_{\text{eq}}. \tag{1.24}$$

For $T \approx 0$, $\beta H_{\text{eff}} \to \pm\infty$ so we see from Figure 2 that $\tanh \beta H_{\text{eff}} \to \pm 1$ for all m_{eq} depending on the sign of H_{eff}. This means $m_{\text{eq}} = \pm 1$. We can visualise this on the following sketch of a phase diagram.

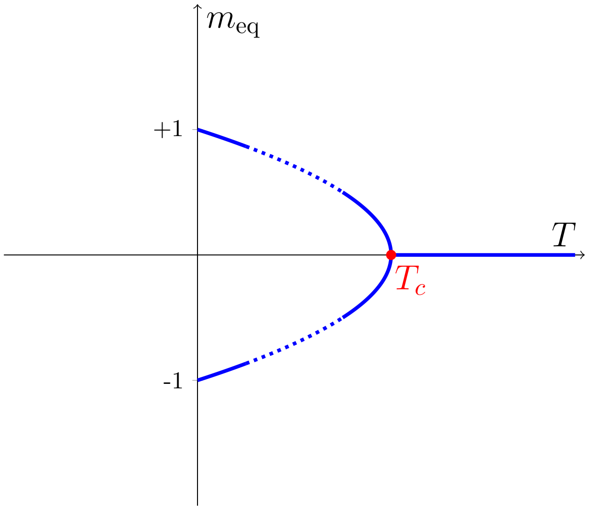


Figure 5. Phase diagram for the Ising model with order parameter being the equilibrium magnetisation m_{eq} of the lattice.

At low temperatures, far below T_c, the equilibrium magnetisation takes values ± 1 as the alignment effect of the magnetic field overwhelms the random alignment caused by thermal fluctuations. At high temperatures, above T_c, the opposite happens and spins tend to be randomly aligned overall, which results in a vanishing magnetisation. Meanwhile, at T_c the magnetisation switches on or off abruptly. Since m is smooth, this is a continuous (so second order) phase transition of the spin lattice from a disordered state $m = 0$ when $T > T_c$ to an ordered state $m \to \pm 1$ when $T < T_c$.

There is however an ambiguity in the latter case when the lattice has to 'decide' between spin orientations. m_{eq} is determined by the sign of H_{eff} which is circularly determined by itself.

With $H \neq 0$

Just like with $H = 0$, the minimum of $f(m)$ in (1.21) will depend on whether T is above or below T_c. However this time, when $T < T_c$, such that the quadratic term is negative and creates those two dips, one dip will be lowered by the linear term $-Hm$.

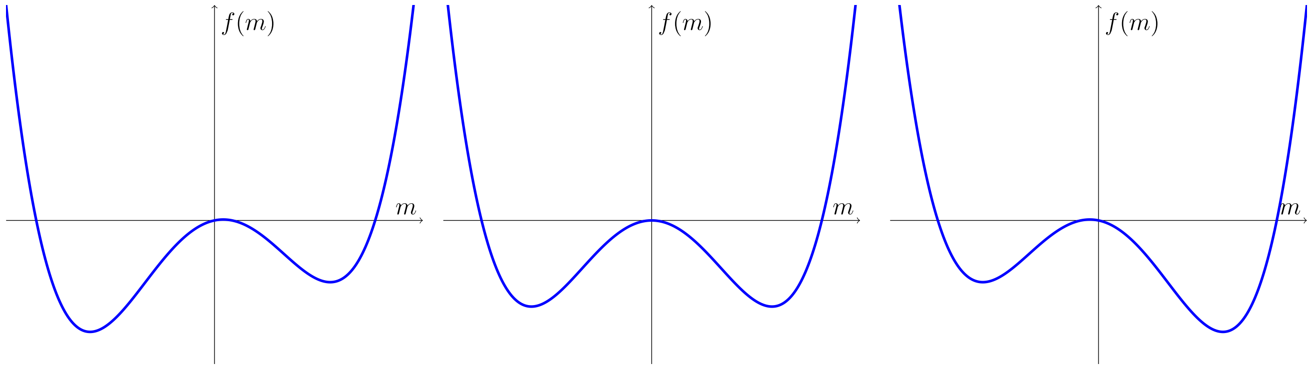


Figure 6. $T < T_c$ and $H < 0$, $T < T_c$ and $H = 0$, $T < T_c$ and $H > 0$.

Looking at (1.23), time at high temperatures the magnetisation smoothly asymptotes to 0 as $m \to H/T$. At low temperatures, the magnetisation asymptotes smoothly to ± 1, where there is no ambiguity this time. For $H \neq 0$, there is no phase transition as a function of T. However, if we kept T fixed with $T < T_c$, then looking at Figure 6, there is a discontinuous first order phase transition as m switches from -1 to 0 to $+1$ as we increase the magnetic field from a negative value.

Critical temperature

We have seen how the phase behaviour of the Ising model depends on T, H and $T_c \propto J/k_{\mathrm{B}}$. However, our expression $T_c = 2dJ/k_{\mathrm{B}}$ taken from the Landau mean field approximation (1.21) does not agree with the exact result (1.25) for $d = 2$ and $H = 0$, which is found using *Kramers–Wannier duality* [5, 6]. This duality exploits an elegant symmetry in statistical physics which relates the partition function of a low temperature to a high temperature Ising model. In turns out that, for a square lattice where the nearest-neighbour interaction is isotropic (horizontal and vertical interactions are equivalent), we have

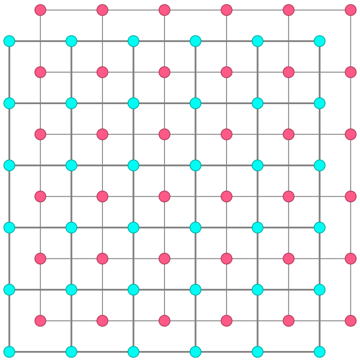


Figure 7. A square lattice is self-dual, which is used in Kramers–Wannier duality.

$$T_c = \frac{2}{\ln\left(1+\sqrt{2}\right)} \frac{J}{k_{\mathrm{B}}} \approx 2.269 \frac{J}{k_{\mathrm{B}}}. \tag{1.25}$$

To learn how this number pops out of a polygon-counting problem, watch this video that A. Farren and M. Whelan created on the subject, or alternatively read [5] from which our presentation followed.

1.3 The Potts model

The q-Potts model generalises the Ising model to higher spin systems. Beyond the ability of the Potts model to emulate spin systems it is equally useful in modelling lattice gases, binary (tertiary and beyond) alloys and superconductors [5, 6]. The model's critical behaviour (and numerical accessibility) is what motivated us to undertake this project.

We first replace the $s_i s_j$ term in the Ising model Hamiltonian (1.1) with $\delta(s_i, s_j) = (1 + s_i s_j)/2$ and ignore the constant term which does not play a role as it does not contribute to the Hamiltonian's variational behaviour. In doing so we obtain the Potts model Hamiltonian

$$\mathcal{H}(s) = -2J \sum_{\langle i,j \rangle} \delta(s_i, s_j) - H \cdot \sum_j s_j, \tag{1.26}$$

where sites have spin orientations s_i which now take discrete values $0, 1, \ldots,\ q-1$. The meaning of $H \cdot s_j$ in the Hamiltonian (1.26) is that only the spins parallel to H contribute.

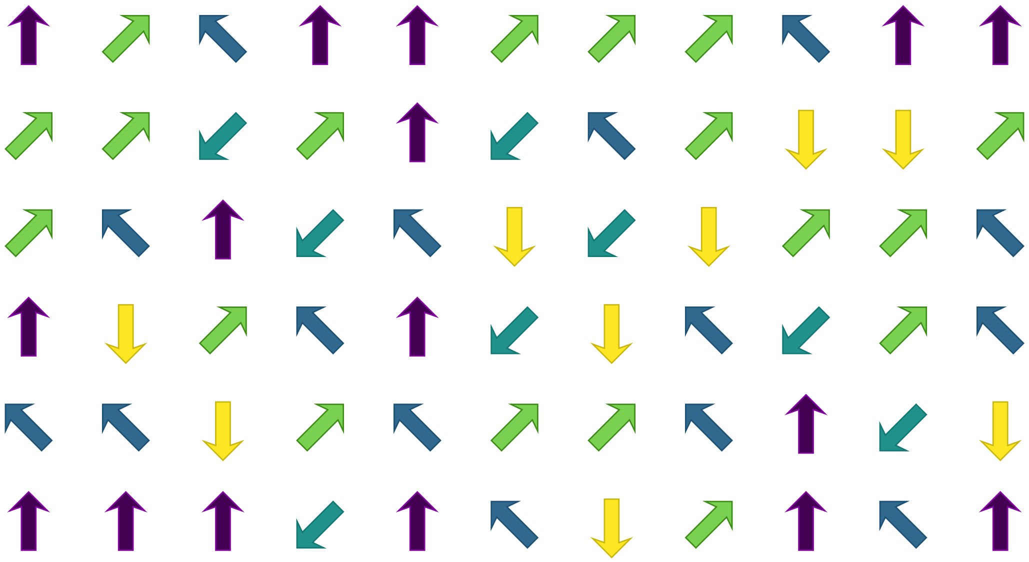


Figure 8. The 2D q-Potts model as a square lattice with q spin states.

There are various shapes of lattices and conventions for how to define ‘spin orientation’. For the purposes of this project we will stick with the standard two-dimensional square lattice existing in $q-1$ dimensional space so that the spins are all orthogonal [7]. This means that only one spin direction is parallel to the magnetic field H. As in the Ising model, it is also possible to consider multi-site interactions, or beyond-nearest-neighbour interactions which we will forego to keep it easy-peasy. The definition of magnetisation is not so obvious anymore as we would need to specify how to ‘add’ spins and find an analog to the net alignment to the magnetising field.

For a discussion of the Potts model with various definitions, see the seminal review by Wu [7].

2 Numerical Simulation of the Potts Model

Our objective is to numerically display how the equilibrium configuration of the Potts model lattice depends q, T and H values. We will see how to implement a Metropolis-Hastings algorithm, which is a Markov chain Monte Carlo method, to reflect the physical factors influencing the evolution of a lattice site (e.g. thermal fluctuations, magnetic field alignment). This section will take from [6, Ch. 7].

2.1 Metropolis Hastings algorithm

Initialisation

We start by randomly initialising a `width`×`height` lattice with site spins `state[i][j]` taking values $0,\ 1, \dots,\ q-1$ where `i`≤`width` and `j`≤`height`. This is the *current* configuration which is stored in a two-dimensional array `state`.

```
import numpy as np
import random

### Initialise lattice with width and height for some q value
    state = np.zeros((width, height))
    state=[[random.randint(0,q-1) for i in range(width)] for i in range(height)]
    state=np.array(state)
```

Listing 1. A snippet of the code found here.

Random flip

Once the lattice is initialised, a lattice site (m, n) with spin $s(m, n) =$`state[m][n]` is randomly selected, where $m \in \{1, \dots,$ `width`$\}$ and $n \in \{1, \dots,$ `height`$\}$. Its four nearest neighbours

$$\mathcal{N} = \{(m-1, n),\ (m+1, n),\ (m, n-1),\ (m, n+1)\} \tag{2.1}$$

and their spin values are identified by looking left, right, above and below the (m, n) site all the while imposing boundary conditions. This explicitly means $s(a, b) = s(a+\texttt{width}, b) = s(a, b+\texttt{height})$. Once this site and its neighbours are identified, we suggest a random flip of the (m, n) site's spin, i.e.

$$s(m, n) \xrightarrow{?} \tilde{s}$$

where $\tilde{s}$ is randomly chosen from $\{0, 1, \dots, q-1\}$. Accepting this flip defines the *proposed* configuration.

```
### Pick random lattice site
    m=random.randint(0, height-1)        # row
    n=random.randint(0, width-1)         # column

    next=random.randint(0,q-1)           # suggested flip
    current=state[m][n]                  # store current state

### Identify neighbours of (m,n)
    left   = state[m][(n - 1 + width) % width]
    right  = state[m][(n + 1) % width]
    top    = state[(m - 1 + height) % height][n]
    bottom = state[(m + 1) % height][n]
```

Listing 2. Suggested change of randomly selected site and identifying neighbours.

The associated change in energy comes only from terms in (1.26) which involve the site (m, n), i.e.

$$\begin{aligned}\Delta E = \mathcal{H}_{\text{proposed}} - \mathcal{H}_{\text{current}} &= -2J \sum_{i \in \mathcal{N}} \delta(s_i, \tilde{s}) - H \cdot \tilde{s} + 2J \sum_{i \in \mathcal{N}} \delta(s_i, s(m,n)) + H \cdot s(m,n) \\ &= 2J \sum_{i \in \mathcal{N}} \Big(\delta(s_i, s(m,n)) - \delta(s_i, \tilde{s}) \Big) + H \cdot \Big(s(m,n) - \tilde{s} \Big). \qquad (2.2)\end{aligned}$$

where we sum over the four nearest neighbours and only account for magnetising field contributions where the spin is aligned with the direction of H. (Unlike the Ising model, the spins are not either aligned or anti-aligned as assumed in (1.1) which has $H \cdot s_j = \pm H$)

```
### Computing change of energy associated with suggested spin flip
    # summing over horizontal and vertical neighbours' contributions
    dleft   = (left==current)-1*(left==next)
    dright  = (right==current)-1*(right==next)
    dtop    = (top==current)-1*(top==next)
    dbottom = (bottom==current)-1*(bottom==next)
    dE=2*J*(dleft+dright+dtop+dbottom)+H*((Hdirection==current)-1*(Hdirection==next))
```

Listing 3. Code implementation of (2.2) with `current` representing $s(m,n)$ and `next` representing $\tilde{s}$. Boolean logic is used for Kronecker deltas.

If this resulting spin flip is energetically favourable, with $\Delta E < 0$ such that it decreases the energy, then the flip is accepted immediately and we redefine $s(m, n) = \tilde{s}$. If $\Delta E > 0$, then we give the change a second chance which is more or less forgiving depending on the relative likelihood of the new configuration. In particular, we look at the ratio of probability distributions (1.4) between the current spin lattice and the proposed one

$$\frac{p_{\text{current}}}{p_{\text{proposed}}} = \frac{e^{-\beta \mathcal{H}_{\text{current}}}/Z}{e^{-\beta \mathcal{H}_{\text{proposed}}}/Z} = e^{-\beta \Delta E} = e^{-\Delta E / k_{\text{B}} T}, \qquad (2.3)$$

which necessarily lies between 0 and 1 for $\Delta E > 0$. A uniformly random number $r \in [0, 1)$ is chosen to compare with $\exp(-\Delta E / k_{\text{B}} T)$. We finally then impose the following condition; if $r < \exp(-\Delta E / k_{\text{B}} T)$, then we accept the proposed configuration and $s(m.n) = \tilde{s}$, otherwise we dismiss the change. To see that this makes sense, let us think about how the exponent behaves for different regimes.

- **Low temperatures** $k_{\text{B}} T \ll \Delta E$ The spin lattice is rigid with respect to thermal fluctuations. We expect neighbouring spin sites to lock each other in aligned orientations for $J > 0$. This also agrees with the change condition since the exponent tends to 0 and no random spin changes are allowed unless energetically favourable, i.e. $\Delta E < 0$, which corresponds to aligned neighbours.
- **High temperatures** $k_{\text{B}} T \gg \Delta E$ Thermal fluctuations are now stronger and random spin flips are more frequent, the exponent tends to 1. It then makes sense that the random change tends to be always accepted since $r < 1$.

```
### Conditional acceptance of suggested flip
    dE*=1/(2*J)                         # to work with T in right units
    if dE<=0: state[m][n] = next        # immediately accept change if favourable
    else:
        r=np.random.uniform()           # generate random number
        if dE>0 and r < np.exp(-dE/T):  # where T in units of J/kB
            state[m][n] = next
```

Listing 4. To work with temperature in natural units of J/k_{B}, we normalise the energy change before proceeding with checking the acceptance conditions for the Metropolis-Hastings algorithm described above.

Rinse and repeat

After initialising the lattice and performing a step (considering a random flip), we start with whatever configuration is leftover, whether or not we ended up accepting the change. This configuration becomes the current configuration and we perform another random flip as outlined above.
After enough proposed changes are considered and either accepted or rejected, the overall properties of the lattice will stop changing. This is because no configuration is more energetically favourable and thus more likely. This is the definition of thermodynamic equilibrium, which has thus been achieved. We can now relate our analysis of section 1 to a suitably chosen output of this iterated Metropolis-Hastings algorithm. (To us a *suitably chosen* final lattice does not show any sign of changing over a few hundred random flips, which usually occurs after $\sim 10^5$ steps for our code.)

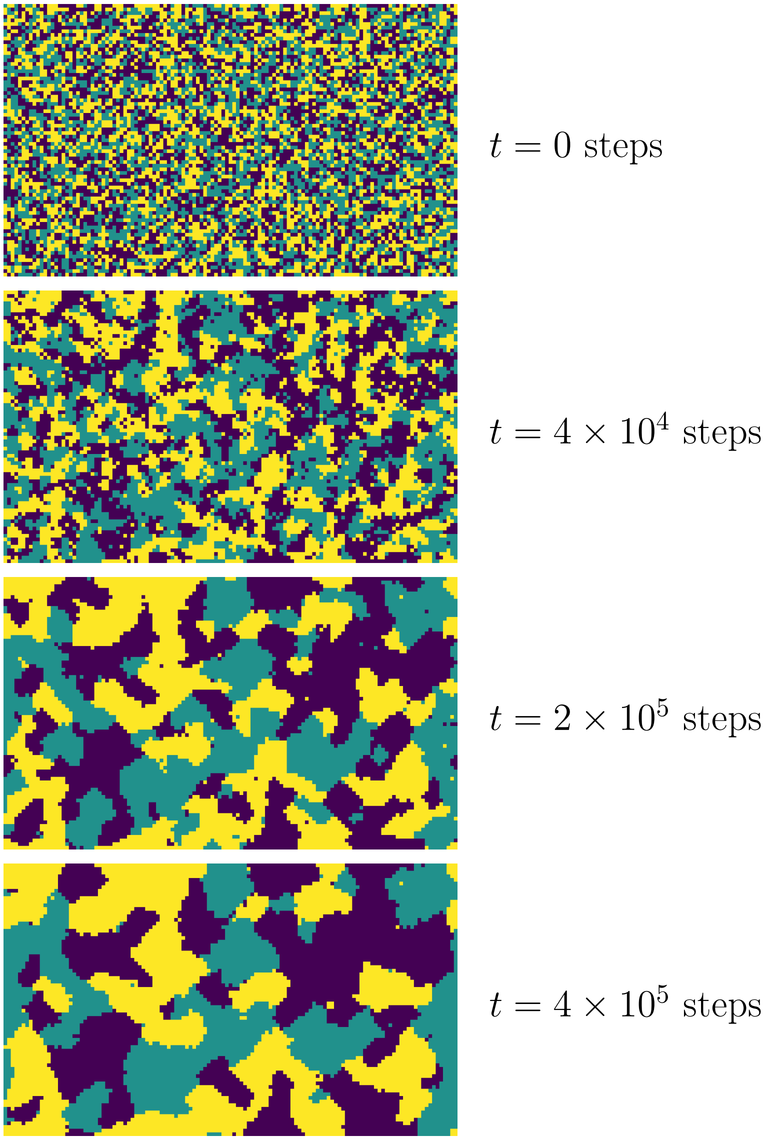


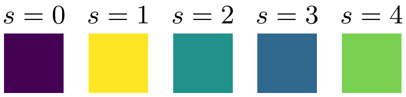
Figure 9. Time evolution of a $q = 3$ lattice in the absence of H with $T = 2J/k_{\rm B}$.

3 Explanation of the Visuals

In this section we use what we learned to explain the behaviour of the visuals shown here. The lattice is initialised to a random configuration and then evolved over 'time', which is the number of iterations of the Metropolis-Hastings algorithm (see Figure 9). Eventually, different thermodynamic equilibria are reached for different q, T and H values. Let's explore how each of these variables affect the evolution of the Potts model[4].

3.1 Choosing q

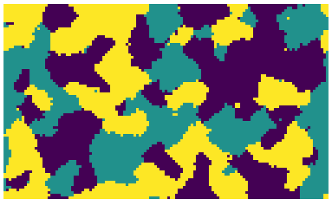
The q-Potts model has sites which can take q values. For us these values will be represented by colours instead of arrows as in Figure 8, where sites' spin orientation can take values $0,\ 1, \dots,\ q-1$. Specifying q then amounts to choosing how many different colours a site of the square lattice can be in. Of course, $q = 2$ corresponds to the Ising model. The colour scheme we employ is below.



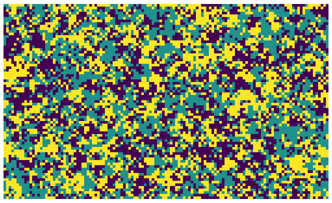
3.2 Choosing T

The spin lattice is in a heat bath at temperature T, which induces more or less thermal fluctuations depending on how T compares to the spin coupling J. At low temperatures, the lattice displays configurations with *domains* which are regions in which all sites have the same colour (or spin orientation). The size and uniformity of these domains is determined by the neighbouring spin interaction and the temperature.

- **Low temperatures**
  The spin lattice is stable with respect to thermal fluctuations. For energy to be minimised, neighbouring spins tend to lock each other in aligned orientations which favours the creation of domains.



- **High temperatures**
  Thermal fluctuations are stronger and random spin flips are more frequent. Domains are never created as regions with uniform spin orientation are now susceptible to being broken by thermal behaviour.



Between the two extremes of low and high temperatures, there is a critical point around which features of both regimes are present. Just below the critical temperature, we expect to see remnants of domains while just above we expect to see far fewer. We can view this as the phase transition described in section 1.2 generalised to the Potts model.

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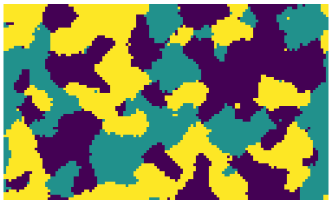
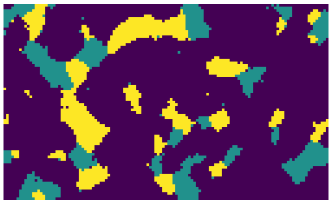
[4] In the final code, we actually incorporated nearest-nearest-neighbour interaction to achieve rounder domains. This does not affect the subsequent discussion and makes the visuals much prettier.

3.3 Choosing H

Our lattice is also in a magnetic field with strength H and direction parallel to the $s = 0$ direction.



- $\boldsymbol{H = 0}$
  If there is no magnetic field, then only the above considerations of temperature are relevant in explaining the evolution of the lattice over time.



- $\boldsymbol{H \neq 0}$
  As the magnetic field strength is dialed up, the spin orientation which is parallel to the direction of the field (here $s = 0$) is more energetically favoured. For any temperature the $s = 0$ orientation will be more abundant than others. And, for strong H, even the randomness of high-temperature thermal fluctuations is subdued and replaced with an ordered configuration.

For each q value chosen, the critical temperature and what it means for a magnetic field to be 'strong' varies. Seeking to show only the qualitative dependence of the phase behaviour of the q-Potts model on T and H, we played around with the numerical values and took note of what temperatures seemed to be critical and what magnetic fields seemed to be strong. Here are those numerical values.

q	T values in J/k_B	H values in spin moments
2	0.5, 2.0, 2.5, 5.0	0, 1, 5, 10
3	0.5, 1.5, 2.0, 4.0	0, 3, 8, 15
4	0.5, 1.5, 2.0, 3.5	0, 5, 10, 25
5	0.5, 1.5, 2.0, 3.0	0, 5, 15, 35

The dynamical GIFs were generated using `matplotlib.animation` for the user to select on the page.

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