Phase Transition in the Ising Model

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Abstract

These are lecture notes for a talk based on "An Introduction to the Ising Model" by Barry Cipra. Available at `http://www.maa.org/programs/maa-awards/writing-awards/an-introduction-to-the-ising-model`. Some of the notation has been changed from the paper for clarity.

1 Introduction

Recall the Ising model. We have the following definitions, notation and conventions:

1. Lattice (graph) $G = (V, E)$ comprising sites (vertices) V and bonds (edges) E.
2. We let $N := |V|$, and assume that the graph is $2d$-regular (we typically assume it is the graph induced by the integer lattice in $\mathbb{R}^d$.)
3. We assume one of two things, whichever is more convenient at the time: boundary vertices have different degrees, or that there is no boundary, i.e. that the graph is on a d-torus.
4. Configuration: $\sigma \in \{\pm 1\}^N$.
5. Hamiltonian: $H = H(\sigma) = -\sum_{(i,j)\in E} K\sigma_i\sigma_j - \sum_{i\in V} J\sigma_i$, where K and J are constants.
6. Temperature t, inverse temperature $\beta = 1/kt$, k is the Boltzmann constant.
7. Partition function: $Z = Z(\beta, K, J, N) = \sum_\sigma e^{-\beta H(\sigma)}$.
8. We define a probability space on configurations by $\mathbb{P}(\sigma) = e^{-\beta H(\sigma))}/Z$.
9. Internal energy: $U = -\frac{d}{d\beta}\log Z$ (average Hamiltonian).
10. Free energy per lattice site: $F = F(\beta, K, J) = \lim_{N\to\infty} \frac{1}{N}\log Z$.

Remark 1.1. Recall from class that the partition function is equivalent to the cut polynomial of G under a change of variables and a one-to-two mapping between cuts and configurations.

Main problem of the Ising model: Find a closed-form, analytic expression for the function F (in β).

Why? We want to know whether a "phase transition" exists. These show up as discontinuities in F or its derivatives. Since F and its derivatives represent macroscopic properties of the system, this means that a small change in temperature (β) will lead to a large change in macroscopic properties.

What kind of phase transition are we interested in? The Ising model is most commonly used as a model for magnetism. We say that the lattice has *magnetization* if for some sites, there is a higher probability that it is one sign than the other. When there is no external field ($J = 0$), then by symmetry of $\mathbb{P}$, there is no magnetization. Conversely, there is magnetization when $J \neq 0$. We say that there is *spontaneous magnetization* if the the lattice still retains a degree of magnetization when external field is "turned off". We want to know if there is a phase transition with respect to the existence of spontaneous magnetization.

History: Ising computed F for $d = 1$, no phase transition (1925). Peierls showed that there is a phase transition for $d = 2$ (1936). Kramers and Wanniers showed that the phase transition occurs at $T_c = \sqrt{2} - 1$ (1941). Onsager computed the formula for F (1944). As of now (1987), nothing known about dimension $d \geq 3$.

2 Peierls' proof

We label the vertices with integer pairs, and try to compute $\mathbb{P}(\Omega_0)$, where Ω_0 denotes the the set of configurations for which $\sigma_0 = -1$, $0 = (0, 0)$. We model "turning off the magnetic field" as assuming $J = 0$, setting all $\sigma_i = 1$ on the boundary, and letting the boundary move off to infinity (i.e. $N \to \infty$). There is magnetization iff $\mathbb{P}(\Omega_0) \neq 1/2$. Note that by our boundary assumption, the partition function Z is now a sum over a subset of configurations $\Omega \subset \{\pm 1\}^N$.

For any configuration $\sigma \in \Omega_0$, we get a cut for the graph. Let $A(\sigma)$ be the connected component for 0 and let $\partial A(\sigma)$ denote its edge boundary. Notice that $\partial A(\sigma)$ is always a closed path in the dual lattice, where the vertices are half-integer pairs. Let

For a closed path in the dual lattice with 0 in its interior, we let Ω_S denote the set of configurations with $\partial A(\sigma) = S$. We define a bijective mapping $\sigma \mapsto \sigma'$ on Ω, by flipping the signs of all the vertices in the interior of S. Notice that for $\sigma \in \Omega_S$ and edge (i, j),

$$\sigma_i \sigma_j = \begin{cases} \sigma'_i \sigma'_j & (i, j) \notin S \\ -1 & (i, j) \in S. \end{cases}$$

As such, we have

$$\begin{aligned}-H(\sigma) &= K\sum_{(i,j)\in S}\sigma_i\sigma_j + K\sum_{(i,j)\notin S}\sigma_i\sigma_j\\ &= -K|S| + K\sum_{(i,j)\notin S}\sigma_i'\sigma_j'\\ &= -2K|S| + K\sum_{(i,j)\in E}\sigma_i'\sigma_j'\\ &= -2K|S| - H(\sigma').\end{aligned}$$

Let Ω_S' be the image of Ω_S under this mapping. This implies that

$$\begin{aligned}\mathbb{P}(\Omega_S) &= \frac{1}{Z}\sum_{\sigma\in\Omega_S}\exp(-\beta H(\sigma))\\ &= \frac{1}{Z}\sum_{\sigma'\in\Omega_S'}\exp(-2\beta K|S| - \beta H(\sigma'))\\ &= \exp(-2\beta K|S|)\mathbb{P}(\Omega_S')\\ &\le \exp(-2\beta K|S|).\end{aligned}$$

Since $\Omega_0 = \cup_S \Omega_S$, we can bound $\mathbb{P}(\Omega_0)$ by taking a union bound. For an integer n, let $s(n)$ be the number of closed paths around 0 of length n in the dual lattice with no self-intersections. We then have

$$\mathbb{P}(\Omega_0) \le \sum_S \exp(-2\beta K|S|) = \sum_{n=4}^{\infty} s(n)e^{-2\beta K n}.$$

It remains to bound the $s(n)$'s. Each such path has a vertex in a $2n$ by $2n$ square B_n centered at 0. Let $r(n)$ denote the number of walks originating in B_n, then $s(n) < r(n)$. On the other hand, we clearly have $r(n) = (2n)^2 \cdot 4^n$. Putting these together gives

$$\mathbb{P}(\Omega_0) \le \sum_{n=4}^{\infty}(4n)^2(4e^{-2\beta K})^n.$$

This quantity is clearly bounded away from 1/2 for β large enough, i.e. for T small enough. At high temperatures, it is "clear" that spontaneous magnetization does not happen. Hence, a phase transition occurs.

Remark 2.1. Let's see where the proof breaks down for $d = 1$. We can still define $A(\sigma)$ as before, but this time $\partial A(\sigma)$ is always 2 edges. We may continue to use the inversion trick to bound $\mathbb{P}(\Omega_S)$ for any two vertices S separating 0 from the boundary. However, the next step where we try to bound the number of S's of a given size falls apart, because there are arbitrarily many S's of size 2, and the inversion trick only gives $\mathbb{P}(\Omega_S) \le \exp(-4\beta K)$.

Remark 2.2. When $d > 2$, the proof will follow through if we can find a bound for the number of $d-1$-dimensional "edge surfaces" of size n that is $e^{O(n)}$. To see how this may done, with a slightly different formulation of the argument, see `https://arxiv.org/abs/1401.7894`.

3 Preliminary calculations for Z

Peirels proved the existence of a phase transition but does not locate it. We hence return to the main goal of finding a closed form expression for the average free energy function F. We now assume that the lattice is on a torus. Define $T = \tanh(\beta K)$, $U = \tanh(\beta J)$. Use formula

$$e^{\pm x} = \cosh x(1 \pm \tanh x)$$

to write

$$\begin{aligned} Z_{d,N} &= \sum_\sigma \exp\left(\sum_{(i,j)\in E} \beta K \sigma_i \sigma_j + \sum_{i \in V} \beta J \sigma_i \right) \\ &= \sum_\sigma \prod_{(i,j)\in E} (\cosh \beta K)(1 + \sigma_i \sigma_j T) \cdot \prod_{i\in V} (\cosh \beta J)(1 + \sigma_i U) \\ &= (2\cosh^d(\beta K)\cosh(\beta J))^N \tilde{Z}_{d,N} \end{aligned}$$

where

$$\tilde{Z}_{d,N} = \frac{1}{2^N} \sum_\sigma \prod_{(i,j)\in E} (1 + \sigma_i\sigma_j T) \cdot \prod_{i \in V} (1 + \sigma_i U).$$

As such,

$$F_d = \lim_{N\to\infty} \frac{1}{N} \log Z = \log(2\cosh^d(\beta K)\cosh(\beta J)) + \tilde{F}_d$$

where

$$\tilde{F}_d = \lim_{N\to\infty} \frac{1}{N} \log \tilde{Z}_{d,N}.$$

Since $\log(2\cosh^d(\beta K)\cosh(\beta J))$ is always analytic in β, it suffices to study $\tilde{F}_d$.

As before, we assume no external field, i.e. $J = 0$, in which case

$$\tilde{Z}_{d,N} = \frac{1}{2^N} \sum_\sigma \prod_{(i,j)\in E} (1 + \sigma_i\sigma_j T) = \sum_{n=4}^{dN} c_{d,N}(n) T^n.$$

What do the coefficients $c(n) = c_{d,N}(n)$ mean? Observe that for each σ, $P(\sigma) := \prod_{(i,j)\in E}(1 + \sigma_i\sigma_j T)$ is an element of the group ring $R\{\pm 1\}^N$ where $R = \mathbb{Z}[T]$. The operator $\frac{1}{2^N}\sum_{\sigma\in\{\pm 1\}^N}(-)$ is projection onto the trivial representation (i.e. onto constant terms). Hence we have

$$\sum_{n=4}^{dN} c_{d,N}(n) T^n = \text{constant term of } P(\sigma).$$

Now expand out the product $\prod_{(i,j)\in E}(1+\sigma_i\sigma_j T)$. Each term corresponds to a choice of 1 or $\sigma_i\sigma_j T$ for each $(i,j)\in E$. It contributes to the constant term if and only if all σ_i's are chosen an even number of times. As such, the number of contributing terms is equal to the number of even subgraphs (i.e. all vertices have even degree), and $c(n)$ is equal to the number of even subgraphs with exactly n edges.

Remark 3.1. This gives us a method for computing $c_{d,N}(n)$ explicitly. Using the power series of log, we can hence compute the coefficients for $\frac{1}{N}\log\tilde{Z}_{d,N}$. For $d=2,3$, the paper shows that the first few of these are independent of N for N large enough.

4 Locating the phase transition for $d=2$

We return to the $d=2$ case, and present Kramers amd Wanniers' proof for locating the phase transition at $T_c=\sqrt{2}-1$. The main idea is to develop a functional equation for $\tilde{Z}_2$ to show that singularities come in pairs. Since the "physics" tells us that there is a unique singularity, this forces it to be a specific value.

Because we are working with the torus model, the lattice is isomorphic to its dual lattice $\hat{G}=(\hat{V},\hat{E})$ (in the sense of graph theory). For each integer n, for N large enough, there is a one-to-two map between even subgraphs of the primal graph with n edges and subgraphs of the dual graph with boundaries of length n. Furthermore, subgraphs of the dual graphs are in bijection with configurations on the dual graph. As such, we have

$$\sum_{n=4}^{dN} c(n)T^n \cong \frac{1}{2}\sum_{\tau} T^{n(\tau)}$$

where the second sum is over configurations $\tau\in\{\pm 1\}^N$ of the dual graph, $n(\tau)$ denotes the length of the boundary of $A=\{i \mid \tau_i=1\}$, and $\cong$ means that the coefficients of T^n of both expressions agree for N large enough.

Next, observe that

$$n(\tau)=\sum_{(i,j)\in\hat{E}} 1_{\tau_i\neq\tau_j},$$

and

$$\begin{aligned} T^{1_{\tau_i\neq\tau_j}} &= \frac{1}{2}((1+T)+\tau_i\tau_j(1-T)) \\ &= \frac{1+T}{2}\left(1+\tau_i\tau_j\left(\frac{1-T}{1+T}\right)\right). \end{aligned}$$

Hence,

$$T^{n(\tau)}=\left(\frac{1+T}{2}\right)^{2N}\prod_{(i,j)\in\hat{E}}\left(1+\tau_i\tau_j\left(\frac{1-T}{1+T}\right)\right).$$

Putting everything together, we get

$$\tilde{Z}_{d,N}(T) \cong \frac{1}{2}\sum_{\tau}\left(\frac{1+T}{2}\right)^{2N}\prod_{(i,j)\in\hat{E}}\left(1+\tau_i\tau_j\left(\frac{1-T}{1+T}\right)\right)$$
$$= \frac{1}{2}\left(\frac{(1+T)^2}{2}\right)^{N}\tilde{Z}_{d,N}\left(\frac{1-T}{1+T}\right).$$

Now take logarithms, divide by N and let N go to infinity. Then, assuming the limit exists, we get

$$\tilde{F}_d(T) = \log\left(\frac{(1+T)^2}{2}\right) + \tilde{F}_d\left(\frac{1-T}{1+T}\right).$$

Recall that $T = \tanh(\beta K)$ takes values between 0 and 1, and notice that $t \mapsto \frac{1-T}{1+T}$ is a bijection on the unit interval. This tells us that if $T = \tanh(\beta K)$ is a singularity for $\tilde{F}_d$, so is $\frac{1-T}{1+T}$, which means that there are two singularities unless $T = \frac{1-T}{1+T}$. Solving this, we get $T = \sqrt{2}-1$.

5 Formula for $\tilde{F}_1$

In 1944, Onsager computed the formula for $\tilde{F}_2$ for the zero magnetic field case. The formula is

$$\tilde{F}_2(T,0) = \frac{1}{2}\int_0^1\int_0^1 \log\big((T^2+1)^2 - 2T(1-T^2)(cos(2\pi x)+cos(2\pi y)\big)dxdy.$$

Unfortunately, the proof is (supposedly) hard, so we will give Ising's proof for $\tilde{F}_1$ instead. Here, we do not need to assume $U=0$, and we work with the non-torus model. The main idea of the proof is to decompose $\tilde{Z}_N = \tilde{Z}_{N,+} + \tilde{Z}_{N,-}$, where $\tilde{Z}_{N,\pm}$ is the partition function over the set of configurations for which $\sigma_N = \pm 1$. We are then able to obtain a recursion relation as follows:

$$\begin{bmatrix}\tilde{Z}_{N,+}\\ \tilde{Z}_{N,-}\end{bmatrix} = M\cdot\begin{bmatrix}\tilde{Z}_{N-1,+}\\ \tilde{Z}_{N-1,-}\end{bmatrix},$$

where

$$M = \frac{1}{2}\begin{bmatrix}(1+U)(1+T) & (1+U)(1-T)\\ (1-U)(1-T) & (1-U)(1+T)\end{bmatrix}$$

This is for $N \geq 3$, so we have the formula

$$\tilde{Z}_N = \begin{bmatrix}1 & 1\end{bmatrix}\cdot M^{N-2}\cdot\begin{bmatrix}\tilde{Z}_{2,+}\\ \tilde{Z}_{2,-}\end{bmatrix}.$$

One may compute the value of $\tilde{Z}_{2,\pm}$, but it is not necessary since we are taking limits. We compute the eigenvalues of M as

$$\lambda_{\pm} = \frac{1+T\pm\big((1+T)^2-4T(1-U^2)\big)^{1/2}}{2}.$$

These are real, since $0 < T, U < 1$, so we get

$$\tilde{F}_1(T,U) = \log \lambda_+ = \log\left(\frac{1 + T + \big((1+T)^2 - 4T(1-U^2)\big)^{1/2}}{2}\right).$$