THE ISING MODEL: PHASE TRANSITION IN A SQUARE LATTICE

ALEXANDRE R. PUTTICK

Abstract. The aim of this paper is to give a mathematical treatment of the Ising model, named after its orginal contributor Ernst Ising (1925). The paper will present a brief history concerning the early formulation and applications of the model as well as several of its basic qualities and the relevant equations. We proceed to prove the existence of a critical temperature in two dimensions that follows from the application of the model onto the square lattice. We then move on to a discussion of further breakthroughs concerning the model, providing the mathematical argument that leads to the calculation of the value of the critical temperature as well as a further discussion on the Ising model's continuing significance in an array of scientific fields.

Contents

1. Formulation and Brief History

In 1925 German physicist Ernst Ising formulated what is now called the Ising model as his doctoral thesis under the guidance of Lenz. His orginal aim was to provide a mathematical model for empirically observed qualities of ferromagnetism. Ising initally formulated the model on the points (1,2,...,n) arranged along the **Z**-line as shown:

At each site there is a dipole or spin with two possible orientations, "up" or "down."

Definition 1.1. A *random field* is a probability measure placed on the set of all possible spin configurations on a given lattice.

We place a random field on the model choosing $\Omega = \{\omega = \{\omega_0, \omega_1, ..., \omega_n\}\}$ as our sample space where each $\omega_j =$"+" or "-" where + indicates up spin and -

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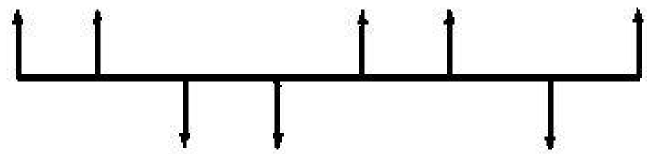

FIGURE 1. One-Dimensional Ising Model [2]

indicates down. We now consider a function σ_j : where $\sigma_j(\omega) = 1$ if $\omega_j = +$ and -1 if $\omega_j = -$.

Definition 1.2. Two indicies i and j are called *neighbor pairs* if they are exacly 1 unit apart.

Ising assigned a probability measure by assigning to each configuration an *energy function*:

$$U(\omega) = -J \sum_{i,j} \sigma_i(\omega)\sigma_j(\omega) - mH \sum_i \sigma_i(\omega) \tag{1.3}$$

We take the sum over all pairs (i, j) such that i and j are neighbor pairs. We call the first term the *interaction energy* which arises from the interactions between neighbor pairs. The second term represents energy due to magnetization where the sum just represents the difference in the number of up and down spins. It is important to note the assumption that only the interactions between neighboring pairs are significant.

In physics this total energy of the system is called the *Hamiltonian.* Here the constant J is a property of the material being considered, H describes the magnitude of the magnetic field with a signature that describes its direction and $m > 0$ is a constant that also depends on the material being considered. The situation in which $J > 0$ corresponds to the *attractive case*, where interaction tends to keep neighbors in the same orientation as opposed to $J < 0$, the *repulsive case*, in which opposite neighbor orientations are favored.

The next step is to assign probabilities proportional to

$$e^{\frac{1}{kT}U(\omega)} \tag{1.4}$$

where k is a universal constant (i.e. the *Boltzmann constant*) and T is the temperature. We then complete this to a probability function on Ω

$$P(\omega) = \frac{e^{\frac{1}{kT}U(\omega)}}{Z} \tag{1.5}$$

where

$$Z = \sum_\omega e^{\frac{1}{kT}U(\omega)} \tag{1.6}$$

which acts as a normalizing constant and is called the *partition function.* In Ising's initial employment of the one-dimensional model, he was primarily concerned with the 0 exterior field case. Even if the spins at each site were intitially random, it was thought that for sufficiently low temperatures the system would move toward a state of lower energy e.g. spins would align in mostly up or mostly down orientation.

This describes the phenomenon of *spontaneous magnetization.* Thus if we define *total magnetization* M as

$$M(w) = |\{\omega_j|\omega_j = +\}| - |\{\omega_i|\omega_i = -\}| \tag{1.7}$$

then M would have an expected distribution as shown in Figure 2. Ising remarked

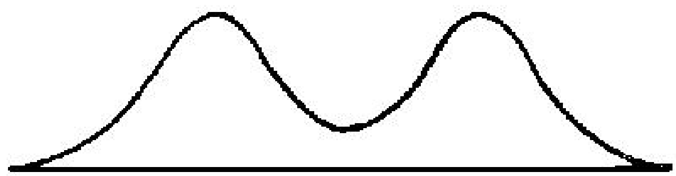

FIGURE 2. Distribution of Total Magnetization [2]

that this was not the case for the simple one-dimensional model. We give a simple proof of this fact later. Ising gave an argument for generalizing this result to the two-dimensional model and thus decided that it failed to successfully model magnetization. His model went virtually unnoticed for many years until the mid 1930s when Peierls (1936) developed an argument which showed that spontaneous magnetization does indeed occur in two-dimensions in the Ising model. We shall follow and flesh-out his argument in detail in section 3.

2. Characteristics of the Ising Model

Probabilities of the form in Equation 1.5 are known as Gibbs measures or Boltzmann Distributions. Such a measure demonstrates special probabilistic properties.

Definition 2.1. A probability measure is said to define a *Markov random field* if

$$P(\sigma_j = a \mid \sigma_k \; \forall k \neq j) = P(\sigma_j = a \mid \sigma_k \; \forall k \ni (k, j) \text{ is a neighbor pair}) \tag{2.2}$$

We state here without proof that the Gibbs Measure defined in Equation 1.5 defines a Markov random field– for full details see the result in Kindermann (1980). Probabilities of the form described in Equation 2.4 are called *local characteristics.* In this paper, we concern ourselves primarily with the two-dimensional lattice representation of the Ising model. In this scenario we consider finite $n \times n$ square lattices as shown in Figure 3. All the equations for this version of the model are identical though now when we sum over all neighbor pairs we include all four neighbors of interior points and the two or three for each point in the boundary. There is a simple way to eliminate the difference between the interior and boundary points by curling the square into a torus so that every site in the 1st column is associated with the analagous member in the nth column with the equivalent associations being made between the 1st and nth rows. Such a construction of the lattice is deemed to have a *periodic boundary.* We shall later discuss the implications of considering a periodic boundary later. However, we shall restrict our attention to the lattice with *fixed boundary* (Figure 4). We present as a lemma one important characteristic of the one-dimensional Ising model.

+	+	−	+	+	−	+
−	+	+	+	+	−	+
+	−	+	+	+	−	+
−	+	−	+	−	−	+
+	+	−	+	−	+	+
+	−	+	+	−	+	−
−	+	+	−	−	−	+

Figure 3. Two-Dimensional Ising Model

	+	+	+	+	+	
+	+	+	+	+	−	+
+	−	+	+	+	−	+
+	+	−	+	−	−	+
+	+	−	+	−	+	+
+	−	+	+	−	+	+
	+	+	+	+	+	

Figure 4. Lattice with Fixed Boundary

Lemma 2.3.

$$\lim_{n\to\infty} P(\sigma_n = 1|\sigma_0 = 1) = P(\sigma_n = 1|\sigma_0 = -1) \tag{2.4}$$

Proof. Recall from Definition 2.3 that P defines a Markov random field. In this situation, we may regard the model as a *Markov chain* i.e. a Markov random field in which, since the sites lie on a line, we may look at each site as an independent time. In particular, this is a two-state (corresponding to the possible orientations at each site) Markov chain. This follows directly from Definition 2.3 in which the state at the next time depends only on the current state. Suppose that at each site the probability of the next site staying the same is given by p and the probability of changing is $(1-p)$. We can assume this p as the same for every site by the Markov property (def. 2.3). We can place this information in a *transition matrix* defined by $\begin{pmatrix} p & 1-p \\ 1-p & p \end{pmatrix}$ in which the top row and first column represent -, and the bottom row and second column represent $+$. Denote this matrix by $\mathbf{P}$. Suppose $\sigma_0 = -1$. We represent the spin at the 0 site by the column vector $v = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ Thus, because of the Markov property, repeated applications of this matrix to this vector will yield the probability distributions for far away spins. We wish to know

$$\lim_{n\to\infty} \mathbf{P}^n v \tag{2.5}$$

Since $\mathbf{P}$ is a 2×2 matrix, we calculate it characteristic polynomial as

$$f_P(t) = (t-p)^2 - (1-p)^2 \tag{2.6}$$

Thus we find the eigenvalues to be $\lambda_1 = 1$ and $\lambda_2 = 2p - 1$ with corresponding eigenvectors $(1/2, 1/2)$ and $(1/2, -1/2)$. P^n has eigenvalues λ_1^n and λ_2^n. We see from Equation 1.5 that so long as $J > 0$, $0 < 2p - 1 < 1$ since we are in the attractive case. Therefore, in the limit, $\lambda_2^n \to 0$. This shows that the probability distribution goes to $(1/2, 1/2)$ which is identical to the situation in which σ_0 has no effect on σ_n for far away n. $\square$

This signifies that the value of spins at one site has no effect on the spins at faraway sites. The goal is to show that this is not the case in two-dimensions i.e. that there exists a critical temperature T_c s.t. if we choose a point in the interior, it's orientation *is* affected by points in the boundary.

3. The Existence of a Critical Temperature on the Two-Dimensional Lattice

We now restrict ourselves to the attractive case with zero external field. The main idea of the proof is as follows. When we try to ascertain whether or not a system will achieve spontaneous magnetization we are really asking this: assume we have an exterior field H that aligns spins in the up direction. We want to know what the tendancy for each site to remain in the up position is after the field is removed. Thus we consider the fixed boundary model in which fixing the boundary at $+$ represents the effect of the external field. Recall that we are considering finite $n \times n$ lattices with fixed boundary. Letting $n \to \infty$ simulates reducing the field to 0^+. Thus we wish to know what the probability that $\sigma_o = -1$ as n gets arbitrarily large is where o is some point near the center of the lattice. If the influence of the boundary does not carry through to the center, $P(\sigma_o = -1) = 1/2$. We would like to show that for low enough temperatures $P(\sigma_o) < 1/2)$ no matter how far away the boundary points are. This shows that the effect carries through to the center as the field goes to zero and that spontaneous magnetization indeed does occur.

Theorem 3.1. *For the two-dimensional case, There exists a critical temperature, denoted by T_c s.t. $_c$, $P(\sigma_o = -1) < 1/2$ and $\forall\, T > T_c$, $P(\sigma_o = -1)_1/2$ where o is an arbitrary point near the center of the lattice.*

Proof. Let $\Omega_o \subset \Omega$ be the set of all configurations s.t. $\sigma_o = -1$. Then by Equation 1.5,

$$P(\sigma_o = -1) = \sum_{\omega \in \Omega_o} \frac{1}{Z} e^{\frac{1}{kT} U(\omega)} \tag{3.2}$$

Suppose we place another lattice over our initial lattice whose midpoints are the sites of the first lattice.

Definition 3.3. A closed curve is a *circuit* if it is a path constructed from drawing borders on our new lattice between odd pairs (i, j) i.e. pairs with opposite orientations, where $\sigma_i \neq \sigma_j$ (Figure 5)

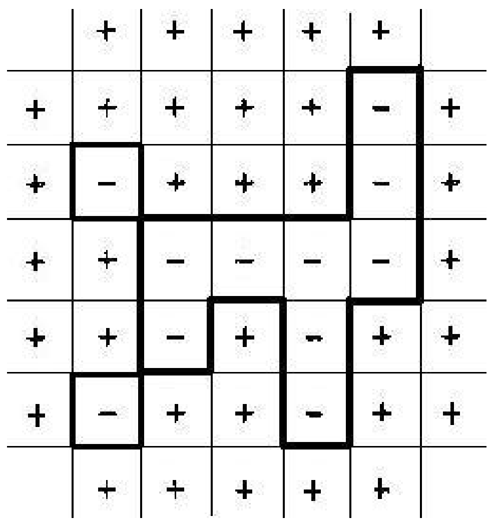

Figure 5. Two-Dimensional Lattice with Circuits

This is well-defined since no odd pairs exist on the boundary so that our path always closes. Furthermore, we see that the circuits define shapes whose interior consists of all "-". It is clear that the number of odd bonds is given by the total length of all circuits in the lattice. Let this number be denoted by $n_o(\omega)$. Since $\sigma_i(\omega)\sigma_j(\omega) = -1$ for all odd pairs and 1 for all even pairs, if we let $n_e(\omega)$ denote the number of even pairs, then

$$\sum_{i,j} \sigma_i(\omega)\sigma_j(\omega) = n_e(\omega) - n_o(\omega) \tag{3.4}$$

Let n_t equal the total number of pairs in the lattice. Note that n_t is constant. We have $l_e(\omega) = n_t - n_o(\omega)$. Thus we may rewrite Equation 1.5 in this situation as

$$P(\omega) = \frac{1}{Z} \exp(\beta(l_t - 2l_o(\omega))) = \frac{1}{Z' \exp(-2\beta(l_o(\omega))}$$

where $\beta = \frac{J}{kT}$ and Z has become a new constant Z'. For all $\omega \in \Omega_o$ o is contained in a circuit c. Let n denote the length of c and $\Omega_c \in \Omega_o$ be the set of all configuations containing the circuit c around σ_o. We associate with each $\omega \in \Omega_o$ an $\omega^{'}$ s.t. we change the values contained within c from "-" to "+." Then it is clear that

$$l_o(\omega^{'}) = l_o(\omega) - n \tag{3.5}$$

Let $\Omega^{'}$ be the set of all such ω'. We know that

$$P(c) = \frac{\sum_{\omega \in \Omega_c} e^{-2\beta l_o(\omega)}}{\sum_{\omega \in \Omega} e^{-2\beta l_o(\omega)}} \tag{3.6}$$

Where P(c) is the probability that the circuit c appears around o. Since each term in the sum is greater than zero, if we limit the number of terms in the denominator, we can only increase the fraction. Thus

$$P(c) \leq \frac{\sum_{\omega \in \Omega_c} e^{-2\beta l_o(\omega)}}{\sum_{\omega' \in \Omega'} e^{-2\beta l_o(\omega')}} = \frac{\sum_{\omega \in \Omega_c} e^{-2\beta l_o(\omega)}}{\sum_{\omega \in \Omega_c} e^{-2\beta (l_o(\omega) - n)}} \tag{3.7}$$

By factoring $e^{-2n\beta}$ from the bottom sum we attain

$$P(c) \leq e^{-2n\beta} \tag{3.8}$$

Let $c(n)$ = the number of circuits of length n around o. Then by Equation 3.9

$$P(\sigma_o = -1) \leq \sum_{n=4}^{\infty} c(n) e^{-2n\beta} \tag{3.9}$$

Suppose we take a random walk of length n on the the same lattice on which the circuits were drawn. The only random walks of this type that could close and form a circuit would be those that originate within a square of diagonal length n and side lengths $\frac{n\sqrt{2}}{2}$ as shown in Figure 6. We denote the number of such walks by $r(n)$. We know that $c(n) < \frac{1}{n} r(n)$ since for any generated path, a walk could have

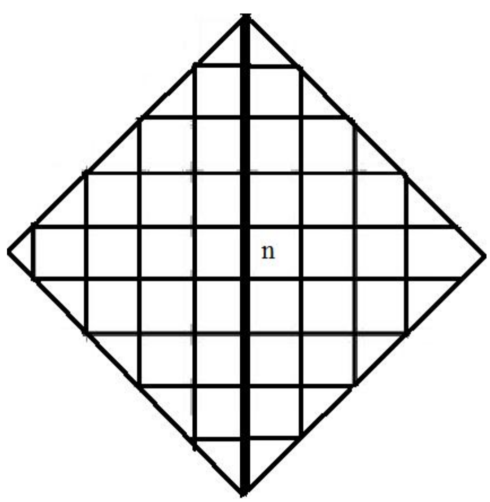

FIGURE 6. Possible Walk Starting Points

begun at any of the n points on the path. Additionally, within the square shown in Figure 6, the walk has $\frac{n^2}{4}$ possible staring points. From each staring point we have 4^n possible paths. Thus

$$c(n) < \frac{n4^n}{2} \tag{3.10}$$

Therefore we have by Equation 3.10

$$P(\sigma_o = -1) < \sum_{n=4}^{\infty} \frac{n4^n}{2} e^{-2n\beta} = \frac{1}{2} \sum_{n=4}^{\infty} n(4e^{-2\beta})^n \tag{3.11}$$

We know that $\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \forall x < 1$ and by differentiating we attain $\sum_{n=1}^{\infty} nx^{n-1} = \frac{x}{(1-x)^2}$. By letting $x = 4e^{-\beta}$ we see that for large enough β we have

$$P(\sigma_o = -1) < \frac{1}{2} \sum_{n=4}^{\infty} n(4e^{-2\beta})^n < \frac{1}{2} \sum_{n=1}^{\infty} n(4e^{-2\beta})^n = \frac{4e^{-2\beta}}{2(1-4e^{-2\beta})^2} \tag{3.12}$$

Since $\lim_{\beta\to\infty} \frac{4e^{-2\beta}}{2(1-4e^{-2\beta})^2} = 0$, we know that for β large enough, $P(\sigma_o = -1) < 1/2$. It's clear from the definition of P that it is monotonically increasing. Since increasing β is identical to raising T, we have proven the assertion that $P(\sigma_n = -1) < 1/2$. Now we need only show that as $T \to \infty$, $P(\sigma_n = -1) \to 1/2$. This follows easily from the fact that if we take any fixed lattice, letting $T \to \infty$ makes P tend to 1/2. This can be seen from (1.5). Since as T gets arbitrarily large the differences in each $U(\omega)$ contribute less and less, we eventually attain a measure in which each configuration occurs in equal probability. Since exactly 1/2 of the configurations have $\sigma_n = 1/2$ this proves the assertion. Thus we have proved the existence of T_c.

□

The matter of calculating the actual value of T_c, even in this simple case of the two-dimensional square-lattice, is a much more difficult question and was not discovered until 1944 by Norweigan-American chemical physicist Lars Onsager. This was only for the case of a two-dimensional lattice with 0 external field. The three-dimensional and non-zero field results are still unknown. We shall present Onsager's solution in full detail, but will provide an outline of the precise problem he had to solve.

4. The Onsager Transfer Matrix Solution of the Two-dimensional Model

Now we consider a slightly weaker form of the *periodic boundary* defined in section 1. The $n \times n$ lattice is wrapped in a cylinder so that if we denote the spin at the ith row jth column site by $\sigma_{i,j}$ then $\sigma_{i,n+1} = \sigma_{i,1}$ i.e. we have associated sites in the first and last columns as neighbor pairs. We can write the *Hamiltonian* of the system as

$$U(\omega) = -J \sum_{i=1}^{n-1} \sum_{j=1}^{n} \sigma_{i,j}\sigma_{i+1,j} - J \sum_{i=1}^{n} \sum_{j=1}^{n} \sigma_{i,j}\sigma_{i,j+1} - H \sum_{i=1}^{n} \sum_{j=1}^{n} \sigma_{i,j} \tag{4.1}$$

We denote a column configuration by $\sigma_j = (\sigma_{1,j}, \sigma_{2,j}, ..., \sigma_{n,j})$. Observe that there are 2^n possible configurations for each column. Next we write

$$U(\omega) = \sum_{j=1}^{n} [V_1(\sigma_j) + V_2(\sigma_j, \sigma_{j+1})] \tag{4.2}$$

where

$$V_1(\sigma_j) = -J \sum_{i=1}^{n-1} \sigma_{i,j}\sigma_{i+1,j} - H \sum_{i=1}^{n} \sigma_{i,j} \tag{4.3}$$

which gives the total interaction energy within the jth column, and

$$V_2(\sigma_j, \sigma_{j+1}) = -J \sum_{i=1}^{n} \sum_{j=1}^{n} \sigma_{i,j}\sigma_{i,j+1} \tag{4.4}$$

Which gives the interaction energy between the jth and (j+1)th column. We now have a partition function given by

$$\begin{gathered} Z_n = \sum_{\omega} e^{-bU(\omega)} = \\ \sum_{\sigma_1, \sigma_2, \ldots, \sigma_n} \exp[-b(\sum_{j=1}^{n} [V_1(\sigma_j) + V_2(\sigma_j, \sigma_{j+1})] = \\ \sum_{\sigma_1, \sigma_2, \ldots, \sigma_n} \prod_{j=1}^{n} L(\sigma_j, \sigma_{j+1}) \end{gathered} \tag{4.5}$$

where $b = 1/kT$ and

$$L(\sigma_i, \sigma_j) = \exp[-b(V_1(\sigma_j)] \exp[V_2(\sigma_j, \sigma_{j+1})] \tag{4.6}$$

In the last term, we observe a sum that has the form of a matrix product. Note that we sum over all possible configurations of σ_1. If we define $L^n(\sigma, \sigma)$ as the (σ, σ) component of the $2^n \times 2^n$ matrix obtained by raising L to the nth power, we have

$$Z_n = \sum_{\sigma_1} L^n(\sigma_1, \sigma_1) \tag{4.7}$$

Now we see that the trace of L^n is equal to the partition function. Since the trace of a matrix is equal to the sum of its eigenvalues, we have

$$Z_n = \sum_{j=1}^{2^m} \lambda_j^n \tag{4.8}$$

where $\lambda_1 \geq \lambda_2 ... \geq \lambda_{2^n}$ are eigenvalues.

Definition 4.9. The free energy per spin ψ in the thermodynamic limit by

$$-\frac{\psi}{kT} = \lim_{n\to\infty} n^{-2} \log Z_n \tag{4.10}$$

We state here without proof that if this function is analytic there is no phase transition, otherwise a singularity appears at the boundary temperature [**?**]. In this situation

$$-\frac{\psi}{kT} = \lim_{n\to\infty} n^{-1}\log\lambda_1 + \lim_{n\to\infty}[n^{-2}\log(1+\sum_{j=2}^{2^n}(\frac{\lambda_j}{\lambda_1})^n)] = \lim_{n\to\infty} n^{-1}\log\lambda_1 \tag{4.11}$$

Thus the problem is reduced to solving for λ_1 Onsager's result was

$$\lambda_1 = (2\sinh 2v)^{n/2}\exp[\frac{1}{2}(\gamma_1+\gamma_3+...+\gamma_{2n-1}] \tag{4.12}$$

. The derivation of this result is quite complicated, and even showing that this λ_1 leads to a non-analytic ψ is quite difficult– for full details see Thompson (1979). The same transfer matrix argument can be applied to higher dimensions but has never lead to a successful solution except for the two-dimensional case.

5. Concluding Remarks

There is much to be understood about the Ising model. We've discussed already the Ising model's original use in modeling ferromagnetism. Forms of the Ising model have been analyzed and/or applied in many fields. Most notable are certain combinatoric approaches as well as applications in biological systems. Examples can be seen in analyzing hemoglobin, allosteric enaymes and DNA. Surely the Ising model will enjoy continued significance in both the mathematical and scientific realm for years to come.

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