



## School of Physics &amp; Astronomy

## PHS4200/PHS4021 Statistical Mechanics

## Lecture 8: The Ising Model

### 8.1 Introduction

The study of critical phenomena associated with the cooperative behaviour of a large number of interacting particles is a central theme in modern statistical mechanics - in particular, the study of phase transitions near a critical point. As the critical point is approached, the thermodynamic quantities exhibit divergent behaviour and the order parameter vanishes. There are numerous approximate methods for studying critical phenomena, most notably the Landau theory<sup>1</sup> of phase transitions; however, all these “mean field” models suffer from a major deficiency, namely, they are unable to correctly account for long range correlations near the critical point. A more sophisticated approach, based on the renormalisation group<sup>2</sup>, and codified within a field theoretic description of statistical mechanics, remedies the deficiencies of older phenomenological models - correctly accounting for scaling and universality associated with critical phenomena. We will return in a later lecture to discuss renormalisation group methods applied to critical phenomena.

An alternative approach to understanding phase transitions is based on lattice models, which provide a highly idealised description of a many-particle interacting system. There are only a handful of exactly solvable lattice models, and their scarcity makes them valuable as a basis of understanding salient aspects of cooperative phenomena. However, one must exercise care in extrapolating the predictions of exact models to real systems. In this lecture we discuss the celebrated Ising model, which has applications to a wide variety of model systems, including magnetism, order-disorder transitions, the helix-coil transition in DNA and neural networks for pattern recognition.

### 8.2 The Ising Model

Ferromagnetic materials, such as *Fe*, *Ni* and *Co*, exhibit a permanent magnetisation (in the absence of an external magnetic field). Ferromagnets display a phase transition at some characteristic temperature, known as the Curie temperature  $T_C$ . Below  $T_C$  the magnetic moments (spins) of the atoms become spontaneously aligned, giving rise to a macroscopic magnetisation,  $\mathbf{M}$ . Above  $T_C$  the spins are oriented randomly, producing zero magnetisation. As the temperature approaches the Curie point from above, a ferromagnet undergoes a phase transition, becoming spontaneously magnetised (in the absence of an external magnetic field). The appearance of long range order (magnetisation) is related to symmetry breaking, in which the discrete  $Z_2$  symmetry of the ground state ( $+\mathbf{M}$  or  $-\mathbf{M}$ ) is not the same as the rotational  $O(3)$  symmetry of the Hamiltonian. A simple idealised model of magnetism was proposed by Lenz in 1920 and solved

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<sup>1</sup> An introduction to the Landau theory of critical phenomena can be found at:

[https://en.wikipedia.org/wiki/Landau\\_theory](https://en.wikipedia.org/wiki/Landau_theory)

<sup>2</sup> A comprehensive discussion of the renormalisation group applied to critical phenomena can be found at:

<https://journals.aps.org/rmp/pdf/10.1103/RevModPhys.55.583>

by his student Ising in 1925. The Lenz-Ising model (known simply as the Ising model<sup>3</sup>) is one of a small number of lattice models that can be solved exactly. For example, the Ising model has exact solutions in one and two dimensions, and for the latter case it exhibits a phase transition; however, an exact solution in three dimensions has not been found<sup>4</sup>. In the Ising model we consider  $N$  spins on a  $D$ -dimensional periodic cubic lattice ( $D = 1, 2, 3$ ), and associate a spin variable with each lattice site. In the Ising model the spin variable  $S_i^z = \hbar \sigma_i^z / 2$  ( $i = 1, 2, \dots, N$ ) only adopts one of two values; namely the spin is either up ( $\sigma_i^z = +1$ ) or it is down ( $\sigma_i^z = -1$ ), with respect to the  $z$ -axis, which is defined by an external magnetic field. Henceforth we will omit the  $z$  label and denote the site on the  $i$ -th site simply by  $\sigma_i = \pm 1$ .

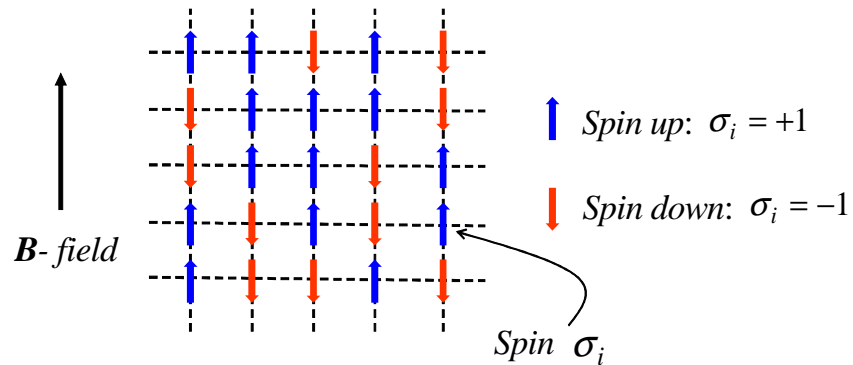
A given set of spins  $\{\sigma\} = \{\sigma_1, \sigma_2, \dots, \sigma_N\}$  specifies a configuration of the system. Figure 8.1 shows a spin configuration on a two-dimensional lattice. The energy (Hamiltonian) for the system is given by:

$$E(\{\sigma\}) = -\sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j - B \sum_{i=1}^N \sigma_i \quad (\sigma_i = \pm 1), \quad (8.1)$$

where  $\langle ij \rangle$  denotes a nearest-neighbour pair of spins and  $B$  is the external magnetic field. The interaction energy  $J_{ij}$  in Eq. (8.1) is defined by the exchange integral:

$$J_{ij} = \int \Psi_j^*(1) \Psi_i^*(2) V_{ij} \Psi_j(2) \Psi_i(1) d^3 \mathbf{r}_1 d^3 \mathbf{r}_2, \quad (8.2)$$

where  $V_{ij}$  is the interaction potential between the two electrons that give rise to the spin.



**Figure 8.1:** Spins on a two-dimensional lattice.

For simplicity we will assume that both  $J_{ij}$  and  $B$  are constants; for isotropic interactions between spins we set  $J_{ij} = J$ , and in this case the Ising model (8.1) simplifies to:

<sup>3</sup> Ising's original paper, "Beitrag zur Theorie des Ferromagnetismus", was published in Zeitschrift für Physik, **31**, 253-258 (1925). A translation of Ising's paper, titled: "Contribution to the Theory of Ferromagnetism", can be found at:

[http://www.hs-augsburg.de/~harsch/anglica/Chronology/20thC/Ising/isi\\_fm00.html](http://www.hs-augsburg.de/~harsch/anglica/Chronology/20thC/Ising/isi_fm00.html)

<sup>4</sup> In 2000 Sorin Istrail claimed that there was no exact solution to the three-dimensional Ising model. His paper, "Statistical Mechanics, Three Dimensionality and NP Completeness: I Universality of Intractability of the Partition Functions of the Ising Model across Non-planar Lattices", 32<sup>nd</sup> ACM Symposium on the Theory of Computing (ACM Press, 2000), pp. 87-96, can be found at:

<http://www.cs.brown.edu/~sorin/pdfs/Ising-paper.pdf>

$$E(\{\sigma\}) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - B \sum_{i=1}^N \sigma_i \quad (\sigma_i = \pm 1), \quad (8.3)$$

The case  $J > 0$  corresponds to ferromagnetism, in which the energy of the system is reduced when the spins are parallel ( $\uparrow\uparrow$  or  $\downarrow\downarrow$ ), i.e.,  $-J\sigma_i\sigma_j = -J < 0$ ; the case  $J < 0$  corresponds to antiferromagnetism, in which the spins are antiparallel ( $\uparrow\downarrow$  or  $\downarrow\uparrow$ ), i.e.,  $-J\sigma_i\sigma_j = +J > 0$ . We will only consider the case  $J > 0$ .

**Exercise 8.1:** Calculate the lowest energy of the Ising model where the spins are on a two-dimensional lattice. Assume  $J > 0$  and  $B = 0$ . Generalise the result to the case of a hypercubic lattice in  $D$  dimensions.

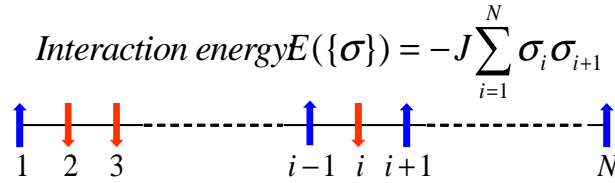
The thermodynamic properties of the Ising model are calculated from the canonical partition function, which is a sum over all states (i.e., over the  $2^N$  spin configurations):

$$\begin{aligned} Z(\beta, B, N) &= \sum_{\{\sigma=\pm 1\}} e^{-\beta E(\{\sigma\})} \\ &= \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1} \exp \left( \beta J \sum_{\langle ij \rangle} \sigma_i \sigma_j + \beta B \sum_{i=1}^N \sigma_i \right), \end{aligned} \quad (8.4)$$

where  $\beta = 1/k_B T$  is the inverse temperature defined in terms of Boltzmann's constant  $k_B$ . The interaction term couples the different spins so that the summations in Eq. (8.4) are “entangled”. In Sec. 8.2.1 we will solve the one-dimensional Ising model analytically and show that it does not exhibit a phase transition.

### 8.2.1 The One-dimensional Ising Model

In the one-dimensional Ising model the interaction energy can be simplified to a summation over a single index (see Fig. 8.2); each of the  $N$  spins interact only with their two nearest neighbours and with an external magnetic field.



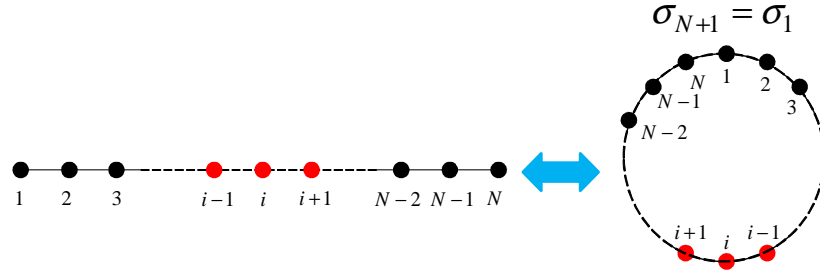
**Figure 8.2:** Spins in a one-dimensional lattice. In this case the interaction energy  $E(\{\sigma\})$  can be written as a sum over the index  $i$ .

The energy of the configuration of spins is given by:

$$E(\{\sigma\}) = -J \sum_{i=1}^N \sigma_i \sigma_{i+1} - B \sum_{i=1}^N \sigma_i. \quad (8.5)$$

We impose periodic boundary conditions, so that  $\sigma_{N+1} = \sigma_1$ , which makes the topology of the one-dimensional lattice equivalent to a circle  $S^1$  (see Fig. 8.3). The partition function (8.4) becomes:

$$Z(\beta, B, N) = \sum_{\{\sigma=\pm 1\}} e^{-\beta E(\{\sigma\})} = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1} \exp \left( \beta J \sum_{i=1}^N \sigma_i \sigma_{i+1} + \beta B \sum_{i=1}^N \sigma_i \right). \quad (8.6)$$



**Figure 8.3:** Imposing periodic boundary conditions ( $\sigma_{N+1} = \sigma_1$ ) makes the topology of the one-dimensional Ising lattice equivalent to a circle.

Before calculating the partition function for a system of interacting spins, let us first examine the simpler case where the spins are non-interacting ( $J = 0$ ). Consider a system of  $N$  non-interacting spins at temperature  $T$ , placed in an external magnetic field  $B$ . The partition function (8.6) becomes:

$$Z(\beta, B, N) = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1} \exp\left(\beta B \sum_{i=1}^N \sigma_i\right) = \prod_{i=1}^N \left( \sum_{\sigma_i=\pm 1} e^{\beta B \sigma_i} \right). \quad (8.7)$$

Because the spins are non-interacting we are able to factor the partition function into a product of  $N$  identical sums, each of which is evaluated to give:

$$\sum_{\sigma_i=\pm 1} e^{\beta B \sigma_i} = e^{\beta B} + e^{-\beta B} = 2 \cosh(\beta B). \quad (8.8)$$

The partition function (8.7) can now be evaluated to give:

$$Z(\beta, B, N) = \prod_{i=1}^N \left( \sum_{\sigma_i=\pm 1} e^{\beta B \sigma_i} \right) = 2^N \cosh^N(\beta B). \quad (8.9)$$

The probability of obtaining a particular spin configuration  $\{\sigma_i\}$  is given by:

$$Pr(\{\sigma\}) = \frac{e^{-\beta E(\{\sigma\})}}{Z(\beta, B, N)} = \frac{e^{-\beta E(\{\sigma\})}}{\sum_{\{\sigma=\pm 1\}} e^{-\beta E(\{\sigma\})}}. \quad (8.10)$$

The magnetisation in an external magnetic field  $B$  at absolute temperature  $T$  is calculated from the ensemble spin average (over all  $2^N$  spin configurations):

$$M(T, B) = \left\langle \sum_{i=1}^N \sigma_i \right\rangle = \sum_{\{\sigma=\pm 1\}} \left( \sum_{i=1}^N \sigma_i \right) Pr(\{\sigma\}) = \frac{\sum_{\{\sigma=\pm 1\}} \left( \sum_{i=1}^N \sigma_i \right) e^{-\beta E(\{\sigma\})}}{\sum_{\{\sigma=\pm 1\}} e^{-\beta E(\{\sigma\})}}. \quad (8.11)$$

The magnetisation defined by Eq. (8.11) can also be written as:

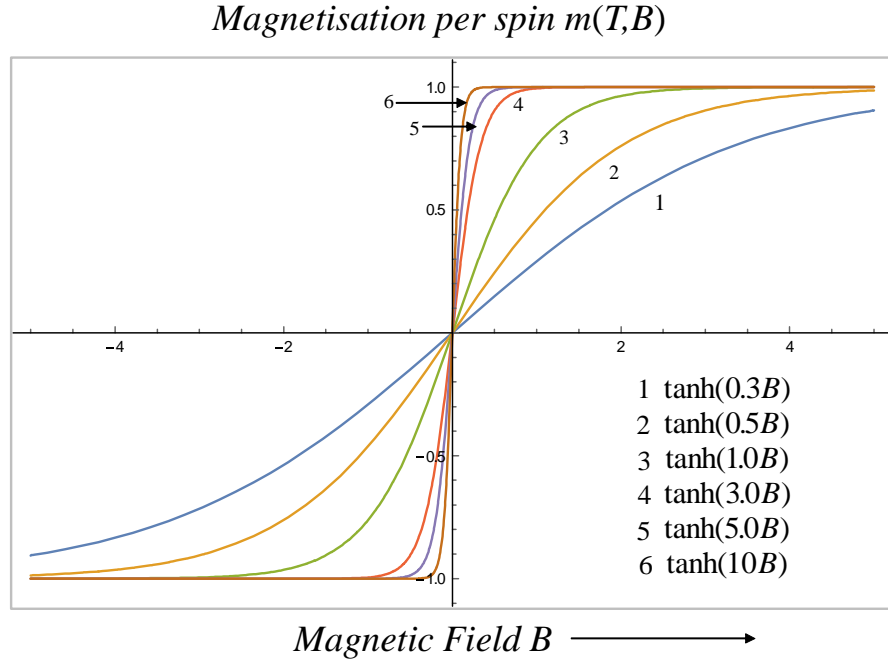
$$M(T, B) = \frac{1}{\beta} \frac{\partial}{\partial B} \ln Z(\beta, B, N). \quad (8.12)$$

It is common to evaluate the magnetisation per spin and take the thermodynamic limit in which  $N \rightarrow \infty$ . If we substitute the partition function (8.9) into the expression for the magnetisation (8.12) we obtain:

$$\begin{aligned} m(T, B) &= \lim_{N \rightarrow \infty} \frac{1}{N} M(T, B) = \frac{1}{\beta} \lim_{N \rightarrow \infty} \frac{1}{N} \frac{\partial}{\partial B} \ln Z(\beta, B, N) \\ &= \frac{1}{\beta} \lim_{N \rightarrow \infty} \frac{1}{N} \frac{\partial}{\partial B} \ln [2^N \cosh^N(\beta B)] \\ &= \tanh(\beta B). \end{aligned} \quad (8.13)$$

**Exercise 8.2:** Show that the magnetisation per spin is given by  $m(T,B) = \tanh(\beta B)$ .

Figure 8.4 shows the magnetisation per spin as a function of magnetic field for various values of  $\beta$  (i.e., inverse temperature). This shows that when the external field is zero the system is not magnetised at any temperature. This is indicative of a paramagnet, which only exhibits magnetisation in the presence of an external field.



**Figure 8.4:** Magnetisation per spin  $m(T,B)$  plotted against the magnetic field  $B$  for six values of the inverse temperature ( $\beta = 0.3, 0.5, 1.0, 3.0, 5.0$  and  $10.0$ ). Note that  $T = (k_B\beta)^{-1}$ , so that larger values of  $\beta$  correspond to lower temperatures.

Let us now consider the one-dimensional Ising model with the interactions turned on, so that  $J \neq 0$ . The partition function (8.6) can be written as:

$$\begin{aligned}
 Z(\beta, B, N) &= \sum_{\{\sigma=\pm 1\}} e^{-\beta E(\{\sigma\})} \\
 &= \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1} \exp \left( \beta J \sum_{i=1}^N \sigma_i \sigma_{i+1} + \beta B \sum_{i=1}^N \sigma_i \right) \\
 &= \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1} \exp \left( \beta \sum_{i=1}^N [J \sigma_i \sigma_{i+1} + \frac{1}{2} B (\sigma_i + \sigma_{i+1})] \right).
 \end{aligned} \tag{8.14}$$

To evaluate the partition function (8.14) we introduce a  $2 \times 2$  transfer matrix defined by:

$$\mathbf{T} = \begin{pmatrix} \langle \sigma_i = +1 | \mathbf{T} | \sigma_i = +1 \rangle & \langle \sigma_i = +1 | \mathbf{T} | \sigma_i = -1 \rangle \\ \langle \sigma_i = -1 | \mathbf{T} | \sigma_i = +1 \rangle & \langle \sigma_i = -1 | \mathbf{T} | \sigma_i = -1 \rangle \end{pmatrix}, \tag{8.15}$$

where the matrix elements are given by:

$$\langle \sigma_i | \mathbf{T} | \sigma_{i+1} \rangle = \exp \left( \beta [J \sigma_i \sigma_{i+1} + \frac{1}{2} B (\sigma_i + \sigma_{i+1})] \right). \tag{8.16}$$

Using Eq. (8.16) allows us to construct the transfer matrix:

$$\mathbf{T} = \begin{pmatrix} e^{\beta(J+B)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)} \end{pmatrix}. \quad (8.17)$$

With these definitions we can re-write the partition function as:

$$\begin{aligned} Z(\beta, B, N) &= \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1} \exp \left( \beta \sum_{i=1}^N [J\sigma_i\sigma_{i+1} + \frac{1}{2}B(\sigma_i + \sigma_{i+1})] \right) \\ &= \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1} \langle \sigma_1 | \mathbf{T} | \sigma_2 \rangle \langle \sigma_2 | \mathbf{T} | \sigma_3 \rangle \dots \langle \sigma_{N-1} | \mathbf{T} | \sigma_N \rangle \langle \sigma_N | \mathbf{T} | \sigma_1 \rangle \\ &= \sum_{\sigma_1=\pm 1} \langle \sigma_1 | \mathbf{T}^N | \sigma_1 \rangle \\ &= \text{Tr} \mathbf{T}^N. \end{aligned} \quad (8.18)$$

In arriving at Eq. (8.18) we have exploited periodic boundary conditions and used the closure relation, i.e.,

$$\sum_{\sigma_i=\pm 1} |\sigma_i\rangle \langle \sigma_i| = \hat{\mathbf{I}}. \quad (8.19)$$

The trace is readily evaluated by diagonalising the transfer matrix, in which case the partition function is given by:

$$Z(\beta, B, N) = \text{Tr} \mathbf{T}^N = \lambda_+^N + \lambda_-^N. \quad (8.20)$$

where the two eigenvalues  $\lambda_{\pm}$  are calculated by evaluating the characteristic determinant:

$$\det(\mathbf{T} - \lambda \mathbb{I}_2) = \begin{vmatrix} e^{\beta(J+B)-\lambda} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)-\lambda} \end{vmatrix} = (e^{\beta(J+B)-\lambda})(e^{\beta(J-B)-\lambda}) - e^{-2\beta J} = 0. \quad (8.21)$$

Expanding Eq. (8.21) results in a quadratic equation in  $\lambda$ , i.e.,

$$\lambda^2 - 2\lambda e^{\beta J} \cosh \beta B + 2 \sinh 2\beta J = 0. \quad (8.22)$$

The eigenvalues are given by:

$$\lambda_{\pm} = e^{\beta J} \left[ \cosh \beta B \pm \sqrt{\cosh^2 \beta B - 2e^{-2\beta J} \sinh 2\beta J} \right]. \quad (8.23)$$

It is evident from Eq. (8.23) that  $\lambda_+ > \lambda_-$  for all values of  $B$ . In the thermodynamic limit where  $N \rightarrow \infty$ , only one of the eigenvalues contributes to the partition function, since:

$$\lim_{N \rightarrow \infty} \frac{1}{N} \ln Z(\beta, B, N) = \lim_{N \rightarrow \infty} \frac{1}{N} \ln (\lambda_+^N + \lambda_-^N) = \lim_{N \rightarrow \infty} \frac{1}{N} \ln \lambda_+^N \left[ 1 + \left( \frac{\lambda_-}{\lambda_+} \right)^N \right] = \ln \lambda_+. \quad (8.24)$$

**Exercise 8.3:** Reproduce the steps leading from Eq. (8.14) to Eq. (8.24).

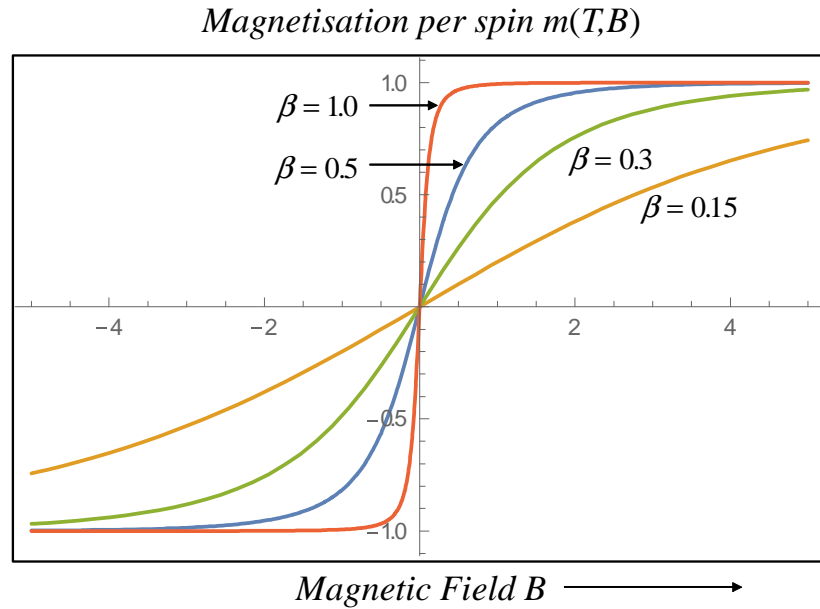
The magnetisation per spin is calculated from:

$$m(T, B) = \lim_{N \rightarrow \infty} \frac{1}{N} M(T, B) = \frac{1}{\beta} \lim_{N \rightarrow \infty} \frac{1}{N} \frac{\partial}{\partial B} \ln Z(\beta, B, N) = \frac{1}{\beta} \frac{\partial}{\partial B} \ln \lambda_+. \quad (8.25)$$

After a tedious calculation (or using Mathematica) we obtain:

$$m(T,B) = \frac{\sinh\beta B}{\sqrt{\cosh^2\beta B - 2e^{-2\beta J}\sinh 2\beta J}}. \quad (8.26)$$

Note that in the limit  $J \rightarrow 0$ , Eq. (8.26) reduces to  $m(T,B) = \tanh\beta B$ , which agrees with our earlier analysis [see Eq. (8.13)]. Figure 8.5 shows a plot of the magnetisation per spin for four different temperatures. It is evident that when  $B = 0$  the one-dimensional Ising model does not exhibit spontaneous magnetisation, i.e., for all  $T > 0$  we have  $m(T,B=0) = 0$ . The absence of a phase transition in the one-dimensional Ising model is due to the “competition” between the alignment of the spins in order to minimise the energy and the randomisation of the spins in order to maximise the entropy. In one-dimension there are not enough nearest neighbours to ensure that the tendency for alignment of spins dominates. However, in higher dimensions the Ising model does indeed exhibit a (ferromagnetic) phase transition. In Sec. 8.2.2 we discuss the two-dimensional Ising model.



**Figure 8.5:** Magnetisation per spin calculated for the one-dimensional Ising model. The exchange constant has been set to  $J = 1$  and  $m(T,B)$  is plotted for four different inverse temperatures  $\beta = 0.15, 0.3, 0.5$  and  $1.0$ . For all  $T > 0$  there is no spontaneous magnetisation at  $B = 0$ . Note that  $T = (k_B\beta)^{-1}$ , so that larger values of  $\beta$  correspond to lower temperatures.

### 8.2.2 The Two-dimensional Ising Model

In Sec. 8.2.1 we used the transfer matrix method to solve the one-dimensional Ising model. This method can also be applied to the two-dimensional Ising model, which was first solved analytically by Lars Onsager<sup>5</sup> in 1944. The Onsager solution represents a tour de force in

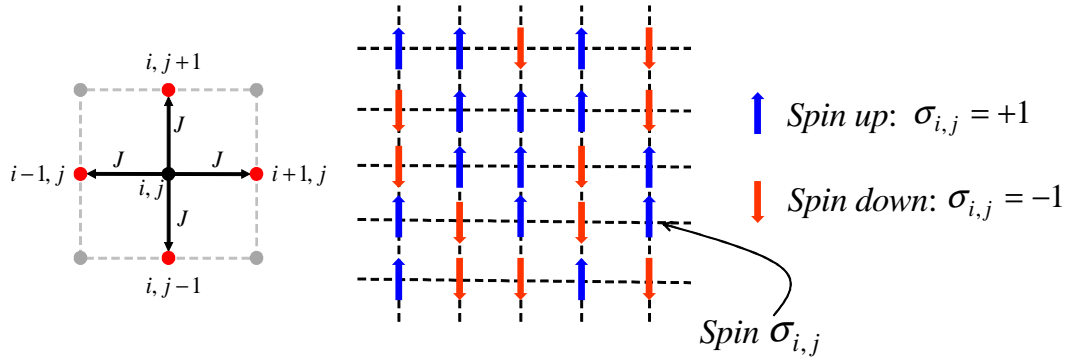
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<sup>5</sup> See Onsager, L., “Crystal Statistics I: A Two-dimensional Model with an Order-Disorder Transition”, Phys. Rev. **65**, 117 (1944). A pdf of the original paper can be found on the PHS4200 Moodle site, or downloaded from:

<https://journals.aps.org/pr/abstract/10.1103/PhysRev.65.117>

mathematical physics; significantly, the two-dimensional Ising model displays a phase transition at a critical temperature  $T_c$ . The details of the Onsager solution are quite involved and we will not reproduce them in the current lecture (see Ref. [1]). However, for completeness we will summarise the salient features of the solution. We start with the energy of a two-dimensional ( $N \times N$ ) lattice of spins ( $\sigma_{i,j} = \pm 1$ ) in the absence of a magnetic field (see Fig. 8.6), and assume the interactions along the two orthogonal directions are isotropic ( $J_1 = J_2 = J$ ):

$$E(\{\sigma\}) = -J \sum_{i=1}^N \sum_{j=1}^N (\sigma_{i,j} \sigma_{i+1,j} + \sigma_{i,j} \sigma_{i,j+1}). \quad (8.27)$$



**Figure 8.6:** Two-dimensional Ising model with isotropic interactions between nearest neighbour spins.

In the thermodynamic limit (i.e.,  $N \rightarrow \infty$ ) the relevant thermodynamic functions are given by the following exact analytical expressions:

- (i) Internal energy per spin:

$$u(T, B=0) = -J \coth(2\beta J) \left( 1 + \frac{2}{\pi} \kappa' K_1(\kappa) \right), \quad (8.28)$$

where

$$\kappa = \frac{2 \sinh(2\beta J)}{\cosh^2(2\beta J)} \quad \text{and} \quad \kappa' = 2 \tanh^2(2\beta J) - 1, \quad (8.29)$$

and  $K_1(\kappa)$  denotes the complete elliptic integral<sup>6</sup> of the first kind:

$$K_1(\kappa) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - \kappa^2 \sin^2 \phi}}. \quad (8.30)$$

- (ii) Specific heat per spin:

$$c(T, B=0) = \frac{2}{\pi} [\beta J \coth(2\beta J)]^2 \left\{ 2K_1(\kappa) - 2E_1(\kappa) - (1 - \kappa') \left( \frac{\pi}{2} + \kappa' K_1(\kappa) \right) \right\}, \quad (8.31)$$

where  $E_1(\kappa)$  denotes the complete elliptic integral of the second kind:

$$E_1(\kappa) = \int_0^{\pi/2} \sqrt{1 - \kappa^2 \sin^2 \phi} d\phi. \quad (8.32)$$

<sup>6</sup> Mathematica can be used to evaluate elliptic integrals. A discussion of elliptic integrals (including complete elliptic integrals of the first and second kind) can be found at:

[https://en.wikipedia.org/wiki/Elliptic\\_integral](https://en.wikipedia.org/wiki/Elliptic_integral)



(iii) Magnetisation per spin:

$$m(T, B=0) = \begin{cases} \frac{(1 + z^2)^{1/4}(1 - 6z^2 + z^4)^{1/8}}{(1 - z^2)^{1/2}} & (T < T_c) \\ 0 & (T > T_c), \end{cases} \quad (8.33)$$

where  $z = e^{-2\beta J}$ .

As can be confirmed by using Mathematica, the complete elliptic integrals  $K_1(\kappa)$  and  $E_1(\kappa)$  have a singularity at  $\kappa = 1$ . From Eq. (8.29) this corresponds to:

$$\kappa = \frac{2\sinh(2\beta J_c)}{\cosh^2(2\beta J_c)} = 1 \quad \Rightarrow \quad \beta J_c = 0.44068679. \quad (8.34)$$

Equation (8.34) defines the critical temperature (or critical exchange constant), i.e.,

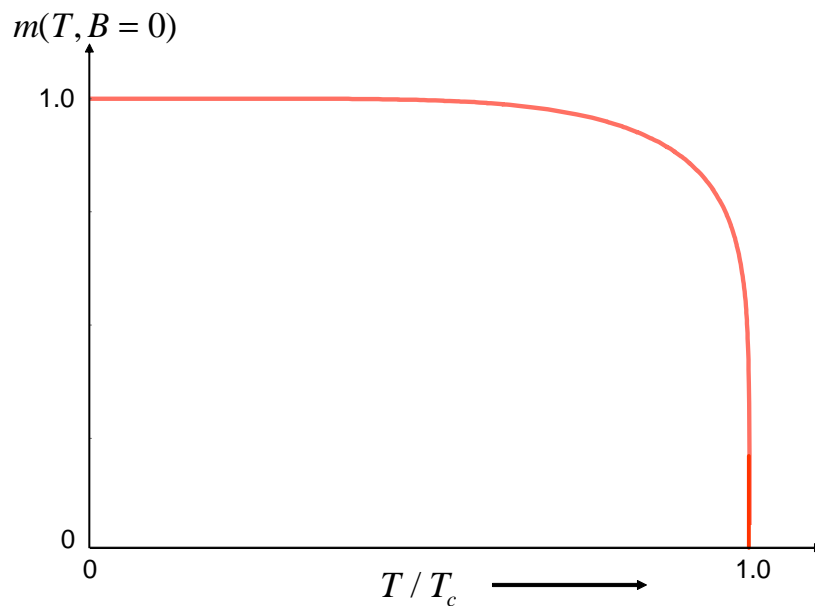
$$\beta J_c = 0.44068679 \quad \Rightarrow \quad T_c = 2.269185 \frac{J_c}{k_B}. \quad (8.35)$$

The appearance of a critical temperature (or critical exchange constant) is indicative of a phase transition in the thermodynamic functions. For example, Fig. 8.7 shows the spontaneous magnetisation per spin  $m(T, B=0)$ , which vanishes at a transition temperature  $T_c$  defined by  $z_c = \sqrt{2} - 1$ . Figure 8.8 shows the specific heat per spin  $c(T, B=0)$ , which displays a logarithmic singularity as  $T \rightarrow T_c$ .

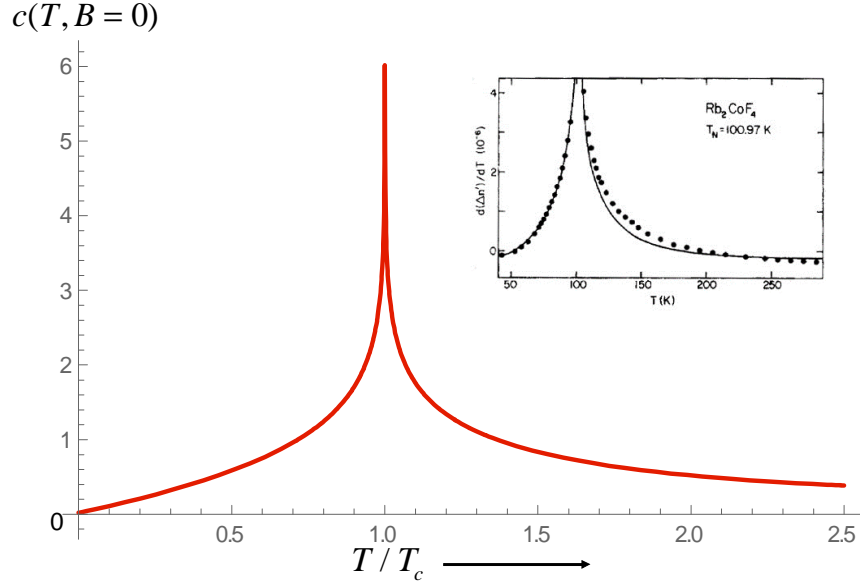
**Exercise 8.4:** Use the NSolve routine in Mathematica to solve Eq. (8.34).

**Exercise 8.5:** Use the Solve routine in Mathematica to show that  $m(T, B=0) = 0$  at  $z_c = \sqrt{2} - 1$ .

**Exercise 8.6:** Use the Plot routine in Mathematica to plot the specific heat per spin (8.31) and magnetisation per spin (8.33) as a function of  $\beta J$ , and show that these thermodynamic functions exhibit a phase transition.



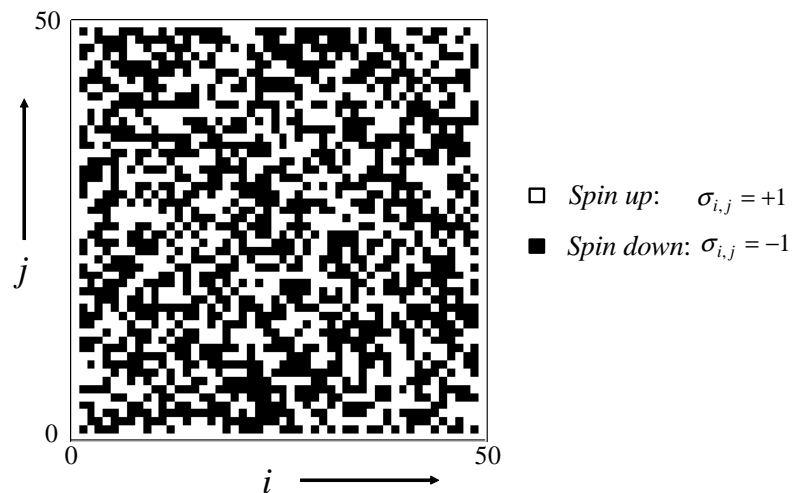
**Figure 8.7:** Magnetisation per spin of the two-dimensional Ising model. The exchange constant has been set to unity ( $J = 1$ ). Boltzmann's constant has also been set to unity. The model exhibits a phase transition at  $T = T_c$ .



**Figure 8.8** The specific heat per spin of the two-dimensional Ising model. The exchange constant has been set to unity ( $J = 1$ ). Boltzmann's constant has also been set to unity. The model displays a logarithmic singularity as  $T \rightarrow T_c$ . The inset shows experimental data for  $\text{Rb}_2\text{CoF}_4$ , which is a layered antiferromagnet. The solid line is a fit to the data based on the two-dimensional Ising model (from P. Nordblad et al., *Phys. Rev. B* **28**, 1983, 278-280).

### 8.2.3 Monte Carlo Simulation of the Two-dimensional Ising Model

In Sec. 8.2.2 we presented the analytical results for Onsager's solution to the two-dimensional isotropic Ising model. Currently there is no exact solution to the three dimensional Ising model, or indeed to most other lattice models.<sup>7</sup> However, we can exploit Monte Carlo techniques to numerically calculate the thermodynamic properties of a lattice model. Here we will apply the Monte Carlo method to the two-dimensional Ising model, in which the spin variables  $\{\sigma_{ij} = \pm 1\}$  are located on an  $N \times N$  square array, where  $(i, j)$  denotes the lattice coordinates. Figure 8.9 shows a random array of Ising spins on a  $50 \times 50$  lattice.



**Figure 8.9:** Random array of Ising spins on a  $50 \times 50$  lattice. Here a black square represents a down spin ( $\sigma_{ij} = -1$ ) and a white square denotes an up spin ( $\sigma_{ij} = +1$ ).

<sup>7</sup> A comprehensive treatment of lattice models can be found in Baxter, R. J., "Exactly Solved Models in Statistical Mechanics" (Academic Press, 1982). A pdf of this textbook is available at:

<https://physics.anu.edu.au/theophys/files/Exactly.pdf>

The energy of a two-dimensional  $N \times N$  configuration of spins  $\{\sigma = \pm 1\}$  for isotropic interactions is:

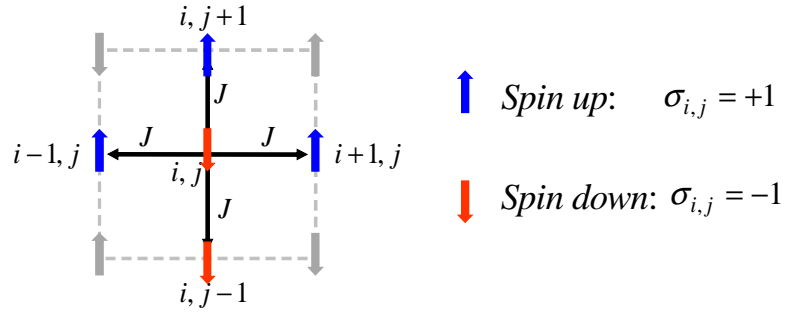
$$E(\{\sigma\}) = -J \sum_{i=1}^N \sum_{j=1}^N (\sigma_{ij} \sigma_{i+1,j} + \sigma_{ij} \sigma_{i,j+1}) - B \sum_{i=1}^N \sigma_{ij}. \quad (8.36)$$

The spin on the lattice site  $(i,j)$  is affected by the spins on the neighbouring sites, so that when  $J > 0$  the energy is lowest when all sites adopt the same values. We assume that only the four nearest neighbours can affect the spin at a given lattice site. The external magnetic field  $B$  tends to align the spins in the same direction. The energy of a pair of spins is given by:

$$E = -J \sigma_{ij} \sigma_{i+1,j} = -J \text{ (spins parallel) } \text{ or } +J \text{ (spins antiparallel)}. \quad (8.37)$$

Figure 8.10 shows the nearest neighbour interactions and the energy for a particular spin configuration (in the absence of an external magnetic field).

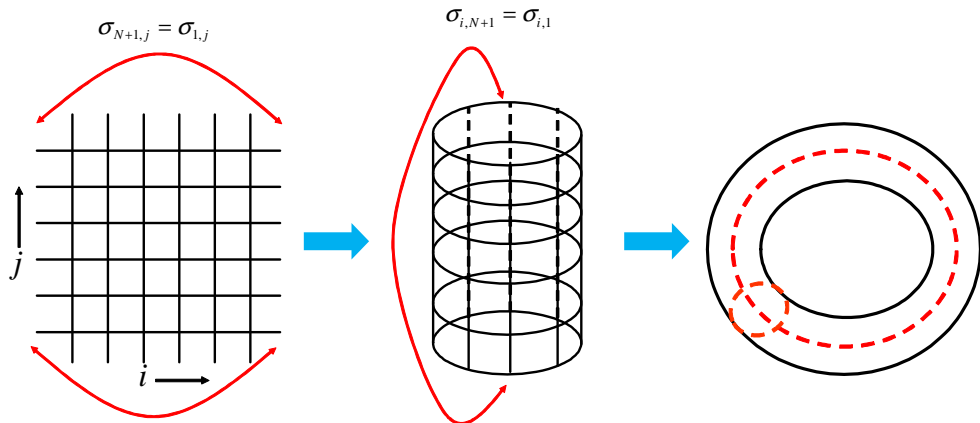
$$E = -J \sigma_{i,j} (\sigma_{i,j+1} + \sigma_{i+1,j} + \sigma_{i,j-1} + \sigma_{i-1,j}) = -J[(-1) + (-1) + (+1) + (-1)] = 2J$$



**Figure 8.10:** Schematic of the interactions between four nearest neighbour Ising spins. The total interaction energy in this case is  $2J$ .

As noted in Sec. 8.2.1 periodic boundary conditions are used to solve the Ising model. In two dimensions this makes the topology of the lattice toroidal (see Fig. 8.11):

$$\sigma_{N+1,j} = \sigma_{1,j} \quad \text{and} \quad \sigma_{i,N+1} = \sigma_{i,1}. \quad (8.38)$$



**Figure 8.11:** Periodic boundary conditions make the topology of the two-dimensional Ising lattice toroidal.

In order to calculate the thermodynamic properties of the two-dimensional Ising model it is first necessary to determine the partition function. However, even for a small lattice the total number of configurations makes the direct evaluation of the partition function intractable. For example,

consider a lattice of  $100 \times 100 = 10^4$  spins. The total number of configurations is  $2^{10^4} = 1.995 \times 10^{3010}$ . The Monte Carlo method allows us to generate configurations with a non-uniform probability density, or weight function, i.e., with a probability proportional to the Boltzmann factor  $\exp(-\beta E(\{\sigma\}))$ . Unfortunately even an ambitious Monte Carlo simulation will only sample a relatively small number of probable configurations (e.g.,  $10^{12}$ ); however, the vast majority of the  $10^{3010}$  configurations are improbable and contribute negligibly to the probability density. This is where the Metropolis<sup>8</sup> algorithm is exploited to sample those states that are statistically more important. This is achieved by systematically stepping through the lattice and deciding whether or not to flip a spin. To implement this algorithm we carry out the following:

- Start with a spin configuration  $\mathbf{S} = \{\sigma\}$  and make a trial step to a new spin configuration  $\mathbf{S}_T = \{\sigma^T\}$  by flipping one spin. Note that an arbitrary spin configuration can be used to start the algorithm.
- The trial step (of flipping the spin) is then accepted or rejected according to the ratio:

$$r = \frac{w(\mathbf{S}_T)}{w(\mathbf{S})} = \frac{e^{-\beta E(\{\sigma^T\})}}{e^{-\beta E(\{\sigma\})}} \quad (8.39)$$

- ▶ If  $r > 1$ , then the trial step is always accepted. In this case the spin is flipped and  $\mathbf{S} = \mathbf{S}_T$
- ▶ If  $r < 1$ , then the trial step is accepted with probability  $r$ . This step is accomplished by comparing  $r$  with a random number  $n$  uniformly distributed in the interval  $[0,1]$ , and accepting the step if  $n < r$ . If the trial step is not accepted it is rejected and the spin is not flipped.
- The process is then repeated as we step through the lattice.

The thermodynamic functions are calculated from a simulation as follows:

- (i) Internal energy per spin (expectation value of the total energy):

$$u = \frac{1}{N^2} U = \frac{1}{N^2} \langle E \rangle = \frac{1}{N^2} \sum_{\{\sigma\}} w(\{\sigma\}) E(\{\sigma\}). \quad (8.40)$$

- (ii) Specific heat per spin (at constant magnetic field):

$$c = \frac{1}{N^2} C = \frac{1}{N^2} \left( \sum_{\{\sigma\}} w(\{\sigma\}) E^2(\{\sigma\}) - \langle E \rangle^2 \right). \quad (8.41)$$

- (iii) Magnetisation per spin:

$$m = \frac{1}{N^2} M = \frac{1}{N^2} \sum_{\{\sigma\}} w(\{\sigma\}) \left( \sum_{ij} \sigma_{ij} \right). \quad (8.42)$$

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<sup>8</sup> See Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H., and Teller, E., “*Equation of State Calculations by Fast Computing Machines*”, J. Chem. Phys., **21**, 1087 (1953). A pdf of the original paper can be downloaded from:

<http://bayes.wustl.edu/Manual/EquationOfState.pdf>

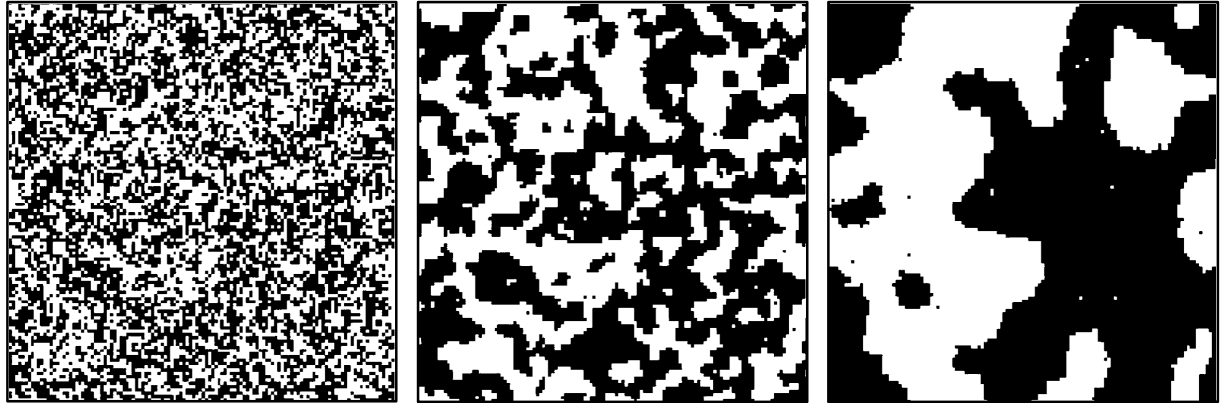
There is a nice history of this algorithm, written by Nick Metropolis, which can be found at:

<http://library.lanl.gov/cgi-bin/getfile?00326866.pdf>

(iv) Magnetic susceptibility per spin:

$$\chi = \frac{1}{N^2} \left( \sum_{\{\sigma\}} w(\{\sigma\}) \left( \sum_{ij} \sigma_{ij} \right)^2 - M^2 \right). \quad (8.43)$$

There are many resources available for simulating the two-dimensional Ising model<sup>9</sup>. Figure 8.12 shows an example of a simulation of the magnetisation based on a  $750 \times 750$  lattice. Here the exchange constant is fixed and the temperature is varied. At high temperatures the system is disordered with  $M = 0$ . As the temperature is lowered the model exhibits long range order, where larger clusters of spins emerge. These correspond to ferromagnetic domains.



**Figure 8.12:** *Simulation of the magnetisation of the two-dimensional Ising model on a  $750 \times 750$  lattice. As the temperature is lowered (from left to right) the model exhibits a phase transition in which the magnetisation is on average non-zero.*

**Exercise 8.7:** *Implement the Metropolis algorithm for the two-dimensional Ising model, using the following parameters:  $J = 1$ ,  $k_B = 1$  and  $B = 0$ . Use a lattice size of at least  $100 \times 100$  sites and vary the temperature from  $T = 5$  to  $T = 0$  in steps of  $0.2$ . Plot the magnetisation per spin and specific heat per spin using Eqs. (8.41) and (8.42). Look for evidence of a phase transition. Compare your results to the exact Onsager solution for an infinite lattice (see Sec. 8.2.2). Note that the finite lattice size smooths out the singularities in the thermodynamic functions.*

### 8.3 Applications of the Ising Model to Non-magnetic Systems

The Ising model has been applied to a wide variety of non-magnetic systems, including binary alloys, lattice gases, spin glasses, neural nets and DNA, to name but a few examples<sup>10</sup>. In applying the Ising model to these non-magnetic systems we map the Ising spins on the lattice to

<sup>9</sup> See for example:

<https://www.youtube.com/watch?v=PWUTBnvGegg>

<https://www.youtube.com/watch?v=kjwKgpQ-11s>

<http://demonstrations.wolfram.com/The2DIsingModelMonteCarloSimulationUsingTheMetropolisAlgorit/>

<sup>10</sup> Recently it has been shown that all spin models can be mapped to a simple universal model. See De las Cuevas, G. and Cubitt, T. S., “Simple Universal Models Capture all Classical Spin Physics”, *Science* **351**, 1180 (2016). A pdf of this paper is available at:

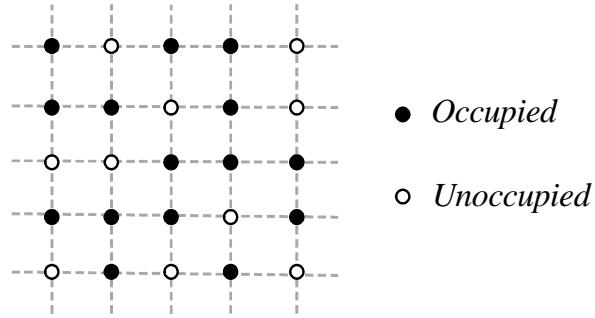
<http://science.sciencemag.org/content/sci/351/6278/1180.full.pdf>

the equivalent variables in the model system. Here we present a brief overview of three such systems; namely, the lattice gas, a binary alloy and the helix-coil transition in deoxyribonucleic acid (DNA).

### 8.3.1 The Lattice Gas

A lattice gas consists of a  $N$  lattice sites in which each site is either occupied or unoccupied by an atom. The total number of atoms is  $N_a$  and there are  $\gamma$  nearest neighbours for each lattice site (i.e., the coordination number is  $\gamma$ ). Figure 8.13 shows a two-dimensional lattice gas, where  $\gamma = 4$ . Each site has an occupation number defined by:

$$n_i = \begin{cases} 1 & (\text{occupied site}) \\ 0 & (\text{unoccupied site}) \end{cases} \quad (8.44)$$



**Figure 8.13:** A lattice gas consists of a  $N$  sites that are either occupied or unoccupied by atoms.

The energy of the lattice gas is given by:

$$E = -\epsilon N_{aa}, \quad (8.45)$$

where  $N_{aa}$  is the total number of nearest neighbour pairs of occupied sites in a given configuration of the lattice gas, and  $-\epsilon$  is the (constant) interaction energy for a pair of nearest neighbour atoms; hence a lattice gas interacts through a two-body potential, with the kinetic energy of the atoms neglected. The partition function of this system is:

$$Z(\beta, N_a, N) = \sum_{N_{aa}} g_N(N_a, N_{aa}) e^{\beta \epsilon N_{aa}}, \quad (8.46)$$

where  $g_N(N_a, N_{aa})$  is the number of distinct ways in which  $N_a$  indistinguishable atoms of the lattice gas can be distributed among the  $N$  sites, consistent with obtaining the value of  $N_{aa}$ . We can also formulate a lattice gas in terms of the grand canonical ensemble, i.e.,

$$\Xi(\beta, N, z) = \sum_{N_a=0}^N z^{N_a} Z(\beta, N_a, N). \quad (8.47)$$

The pressure  $p$  and the average number  $\langle N_a \rangle$  of atoms in the lattice gas are given by:

$$e^{\beta p N} = \sum_{N_a=0}^N z^{N_a} Z(\beta, N_a, N), \quad (8.48)$$

and

$$\langle N_a \rangle = \frac{N}{v} = \frac{z}{k_B T} \left( \frac{\partial p}{\partial z} \right)_T, \quad (8.49)$$

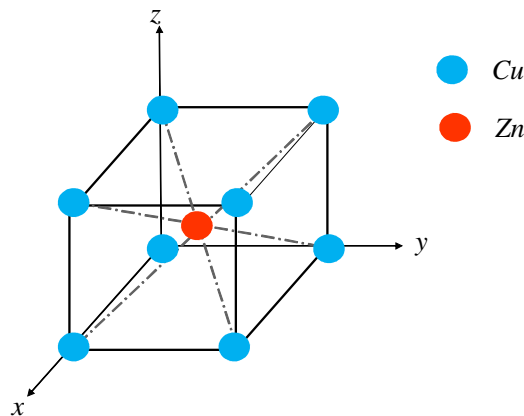
where  $v$  is the average volume per particle of the lattice gas. To establish a formal correspondence between the lattice gas and the Ising model we identify a spin up with an occupied site and spin down with an unoccupied site, i.e.,  $\sigma_i \Leftrightarrow n_i$ . Hence  $N_a$  is equivalent to the total number of up spins, i.e.,  $N_a = N_+$ . Table 8.1 summarises the correspondence between the relevant variables in the lattice gas and the Ising model. These correspondences allow one to translate the solution of the Ising model to that of a lattice gas. However, the lattice gas is an artificial system with limited applicability to actual physical systems; although it has been applied to model the melting of a crystal lattice.

**Table 8.1:** Correspondence between the lattice gas and the Ising model.

Lattice Gas	Ising Model
$N_a, N - N_a$	$N_+, N - N_+ = N_-$
$\epsilon$	$4J$
$z$	$e^{2\beta(\gamma J - B)}$
$p$	$-\left(\frac{F}{N} + \frac{1}{2}\gamma J - B\right)$
$\frac{\langle N_a \rangle}{N} = \frac{1}{v}$	$\frac{\langle N_+ \rangle}{N} = \frac{1}{2}\left(\frac{M}{N} + 1\right) \quad (M = N_+ - N_-)$

### 8.3.2 Binary Alloy

Order-disorder phase transitions are observed in some alloys, such as the binary alloy  $\beta$ -brass, which is a body centred cubic lattice comprised of  $Zn$  and  $Cu$  atoms (see Fig. 8.14). At low temperatures the  $Zn$  and  $Cu$  atoms in  $\beta$ -brass are sited in a well ordered manner in different sub-lattices. However, above the phase transition temperature ( $T_c = 738 \text{ K}$ ) the  $Zn$  and  $Cu$  atoms are randomly distributed on the lattice sites.



**Figure 8.14:** The structure of the binary alloy  $\beta$ -brass consists of  $Cu$  and  $Zn$  atoms on a body centred cubic lattice.

A model of a binary alloy, such  $\beta$ -brass, considers two types of atoms, 1 and 2, with  $N_1$  atoms of type 1 and  $N_2$  atoms of type 2. A configuration is characterised by the number of nearest neighbours pairs of atoms, of which there are three types (11), (12) and (22);  $N_{11}$  denotes the number of nearest neighbours of type (11),  $N_{12}$  is the number of nearest neighbours of type (12) and  $N_{22}$  is the number of nearest neighbours of type (22). Note that we do not differentiate between (12) and (21), so that  $N_{12} = N_{21}$ . We require:

$$N_1 + N_2 = N. \quad (8.50)$$

Denoting the coordination number by  $\gamma$ , i.e., the number of nearest neighbours for each lattice site, we also have:

$$\gamma N_1 = 2N_{11} + N_{12}, \quad (8.51)$$

and

$$\gamma N_2 = 2N_{22} + N_{12} \quad (8.52)$$

Using Eqs. (8.50) - (8.52) allows us to write:

$$N_{12} = \gamma N_1 - 2N_{11}, \quad (8.53)$$

and

$$N_{22} = \frac{1}{2}\gamma N + N_{11} - \gamma N_1. \quad (8.54)$$

The energy of a configuration of atoms in the binary alloy can be written as:

$$E = \epsilon_{11}N_{11} + \epsilon_{12}N_{12} + \epsilon_{22}N_{22}, \quad (8.55)$$

where  $\epsilon_{11}$ ,  $\epsilon_{12}$  and  $\epsilon_{22}$  are the (constant) interaction energies of the three different nearest neighbour pairs of atoms in the binary alloy. Using Eqs. (8.53) and (8.54) we can also write the configurational energy as:

$$\begin{aligned} E &= \epsilon_{11}N_{11} + \epsilon_{12}(\gamma N_1 - 2N_{11}) + \epsilon_{22}(\frac{1}{2}\gamma N - \gamma N_1 + N_{11}) \\ &= \frac{1}{2}\gamma\epsilon_{22}N + \gamma(\epsilon_{12} - \epsilon_{22})N_1 + (\epsilon_{11} + \epsilon_{22} - 2\epsilon_{12})N_{11}. \end{aligned} \quad (8.56)$$

We can now establish a correspondence between a binary alloy and a lattice gas (see Table 8.2).

**Table 8.2:** Correspondence between a lattice gas and a binary alloy.

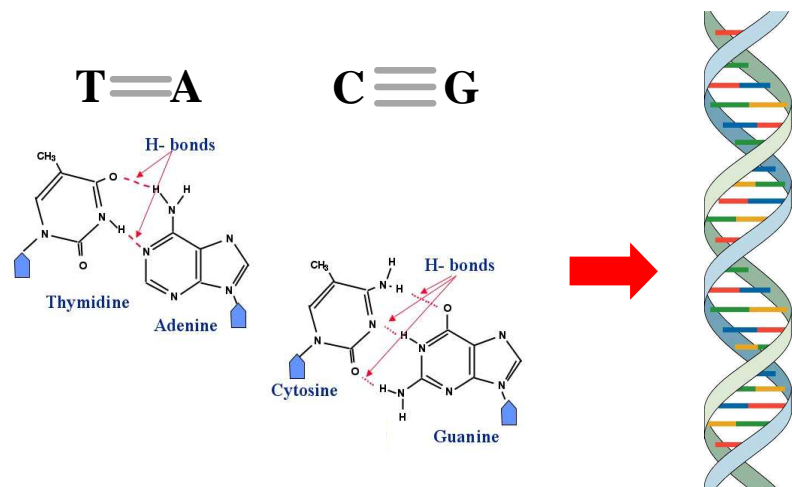
Lattice Gas	Binary Alloy
$N_a, N - N_a$	$N_1, N - N_1 = N_2$
$-\epsilon$	$\epsilon_{11} + \epsilon_{22} - 2\epsilon_{12}$
Helmholtz free energy $F$	Helmholtz free energy $F - \frac{1}{2}\gamma\epsilon_{22}N - \gamma(\epsilon_{12} - \epsilon_{22})N_1$



**Exercise 8.8:** Establish the correspondence between a binary alloy and the Ising model.

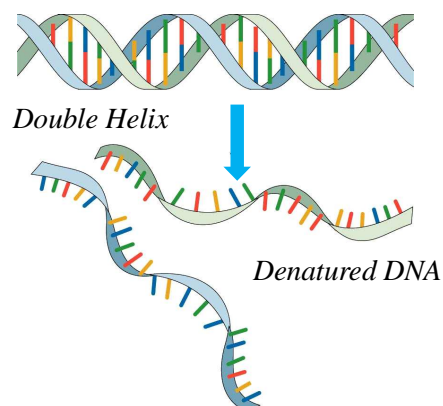
### 8.3.3 The Helix-Coil Transition of DNA

Our final example of the Ising model applied to a non-magnetic system is the helix-coil transition of DNA. The deoxyribonucleic acid (DNA) molecule consists of long chains of relatively simple molecules called nucleotides. The nucleotides consist of three parts - a phosphate group, minus one oxygen atom (hence the prefix “deoxy”), a sugar called ribose, and a base. The base alone distinguishes one nucleotide from another and the four bases which occur in DNA are composed of purines (adenine: A and guanine: G) and pyrimidines (cytosine: C and thymine: T). A single strand of DNA consists of many nucleotides, which form the covalent backbone of DNA. Two single strands, or coils, are coupled through relatively weak hydrogen bonds, which connect the nucleotides (specifically the bases) to form a double helical structure. Each base in one strand faces a complementary base in the other strand; thus A always pairs with T, and C always pairs with G. This situation is represented schematically in Fig. 8.15.

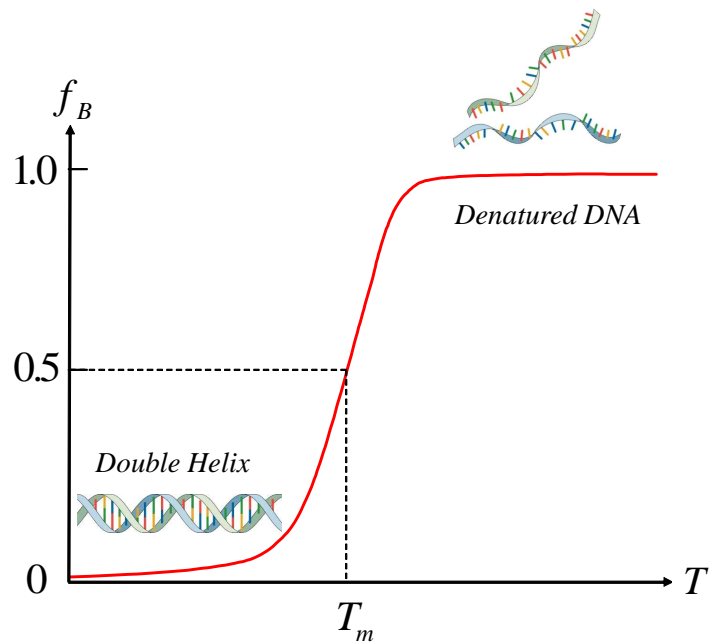


**Figure 8.15:** Schematic representation of the double helical structure of DNA. The four bases are connected via hydrogen bonds, with A always pairing with T, and C always pairing with G.

The inter-strand bonding is quite weak compared to the strong covalent bonds along the backbone, and the stability of the DNA structure is found to be sensitive to its environment. Under treatment by heat or pH changes from the neutral value, the double-helical structure transforms into two separate strands (coils). This configuration transition (denaturation) is known as the helix-coil transition (see Fig. 8.16) and is observed in the melting curves of DNA (see Fig. 8.17 and Ref. [3]).

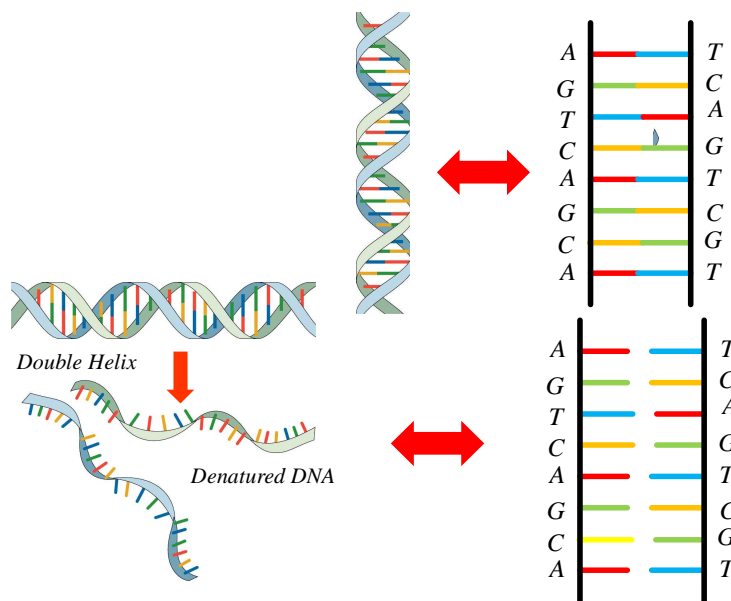


**Figure 8.16:** Under treatment by heat or pH, the hydrogen bonds between base pairs are broken, and DNA undergoes a helix-coil transition. The denatured DNA consists of two separate strands (coils).



**Figure 8.17:** *Melting curve for homopolymeric DNA. Here the fraction of broken nucleotides  $f_B$  is plotted against the temperature. The melting temperature  $T_m$  represents the temperature at which 50% of the base pairs are broken [3].*

The one-dimensional Ising model can be used to describe the melting curves of DNA. As we noted in Fig. 8.15, the double helical DNA structure is stabilised through bonding between the sequences of AT base pairs and GC base pairs. A bonded complex between opposite nucleotides includes, in addition to hydrogen bonding, contributions from other cooperative interactions (e.g., electrostatic and hydrophobic interactions). A bonded complex is considered to play a role analogous to a spin up configuration and a broken complex to a spin down configuration. The state of the DNA molecule is then specified by the configuration of broken and intact complexes, where the DNA structure is represented schematically as a ladder whose “rungs” are identified as the complexes joining the base pairs (see Fig. 8.18).



**Figure 8.18:** *The DNA structure is modelled as a ladder in which the rungs are formed by base pairs, i.e., A with T and G with C, held together by two or three hydrogen bonds. As the temperature increases and the DNA molecule denatures, the double helix transforms into two separate coils, represented by broken rungs on the ladder.*

We now introduce a parameter  $\sigma_i$  for each complex, so that:

$$\sigma_i = \begin{cases} +1 & \text{if the } i\text{-th complex is broken} \\ -1 & \text{if the } i\text{-th complex is intact} \end{cases} \quad (8.57)$$

The state of bonding of the DNA molecule comprising  $N$  base pairs is denoted by:

$$\{\sigma\} = \{\sigma_1, \sigma_2, \sigma_3, \dots, \sigma_{N-1}, \sigma_N\}. \quad (8.58)$$

In a particular configuration  $\{\sigma\}$  the number of broken complexes is given by:

$$N(\{\sigma\}) = \sum_{i=1}^N \frac{1}{2}(1 + \sigma_i) \quad (8.59)$$

If  $P(\{\sigma\})$  is the probability distribution for the configuration  $\{\sigma\}$ , the average number of broken complexes is given by:

$$\langle N \rangle = \sum_{\{\sigma\}} N(\{\sigma\})P(\{\sigma\}) = \frac{1}{2}N + \frac{1}{2}\left\langle \sum_{i=1}^N \sigma_i \right\rangle, \quad (8.60)$$

where the angular brackets indicate an average over the  $2^N$  configurations (or states) of the DNA molecule. In magnetic language  $\langle N \rangle = \frac{1}{2}N(1 + m)$ , where  $m$  is the magnetisation per spin. Based on an Ising model with nearest neighbour interactions we can write the probability distribution as:

$$P(\{\sigma\}) = \frac{1}{Z(\beta, N)} \exp\left(\sum_{i=1}^N \beta(J\sigma_i\sigma_{i+1} + B\sigma_i)\right), \quad (8.61)$$

where  $J$  specifies the strength of the nearest neighbours interaction between complexes and  $B$  is a parameter associated with a bonding complex. These parameters can be estimated from thermal denaturation data (see [3]). The partition function is defined by:

$$Z(\beta, N) = \sum_{\{\sigma = \pm 1\}} \exp\left(\sum_{i=1}^N \beta(J\sigma_i\sigma_{i+1} + B\sigma_i)\right), \quad (8.62)$$

where periodic boundary conditions are assumed, i.e.,  $\sigma_{N+1} = \sigma_1$ , which makes the topology of the molecule circular (see Sec. 8.2.1). These boundary conditions have no effect on the thermodynamic properties of the system.

We can immediately apply the results of the one-dimensional Ising model (see Sec. 8.2.1) to calculate the fraction of broken complexes as a function of temperature, i.e.,

$$f_B = \frac{\langle N \rangle}{N} = \frac{1}{N\beta} \frac{\partial}{\partial B} \ln Z(\beta, N) = \frac{1}{2} + \frac{1}{2}m(T, B), \quad (8.63)$$

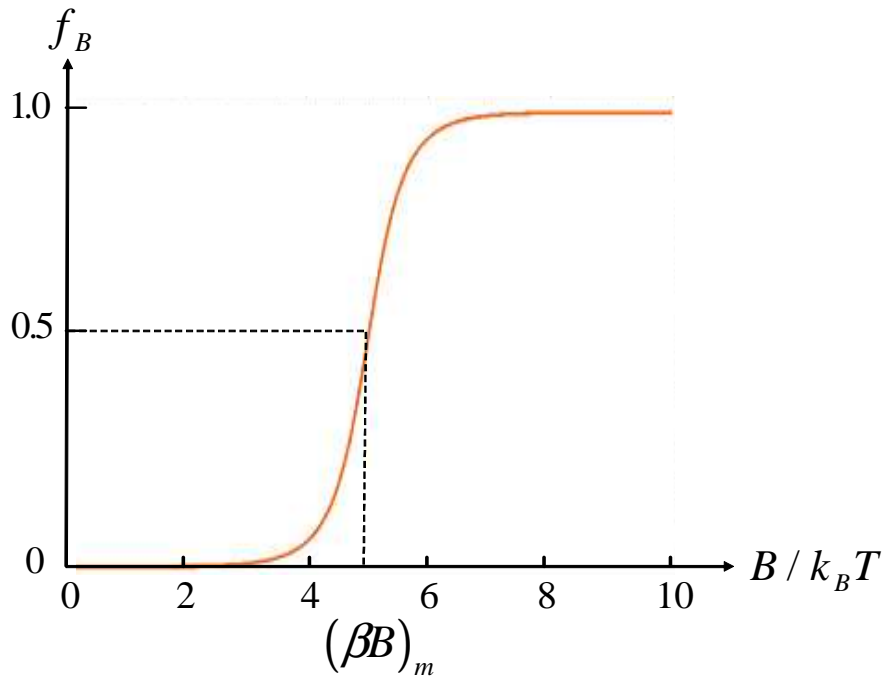
where  $m(T, B)$  is given by Eq. (8.26):

$$m(T, B) = \frac{\sinh \beta B}{\sqrt{\cosh^2 \beta B - 2e^{-2\beta J} \sinh 2\beta J}}. \quad (8.64)$$

It should be evident that Eqs. (8.63) and (8.64) reproduce the ideal melting curves for homopolymeric DNA (see Fig. 8.17). For completeness, in Fig. 8.19 we plot a “typical” melting curve based on the Ising model. In concluding it is important to emphasise that although the Ising model affords insight into the denaturation process, there are many influences<sup>11</sup> that effect the helical stability of the DNA molecule, e.g., binding ligands, histones, repressors, promoters, etc.

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<sup>11</sup> See e.g., <http://www.atdbio.com/content/53/DNA-duplex-stability>



**Figure 8:19:** The melting curve of DNA calculated from the Ising model of the helix-coil transition. Here we have set  $\beta J = 0.25$  and plotted the fraction of broken complexes  $f_B$  as a function of the ratio  $\beta B = B/k_B T$ .

## References

- [1] Huang, K., *Statistical Mechanics* (2<sup>nd</sup> Edition, John Wiley and Sons, 1987). Chapters 14 and 15. Onsager's solution to the two-dimensional Ising model is discussed in Chapter 15.
- [2] Sethna, J. P., *Statistical Mechanics: Entropy, Order Parameters, and Complexity* (Oxford University Press, 2006). Chapter 8. A pdf of this textbook is available at: <http://pages.physics.cornell.edu/~sethna/StatMech/EntropyOrderParametersComplexity.pdf>
- [3] Lando, D. Y., *et al.*, "Determination of Melting Temperature and Temperature Melting Range for DNA with Multi-peak Differential Melting Curves", *Analytical Biochemistry*, **479**, 28-36 (2015).



