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Fisher renormalization of phase transitions

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Critical Phenomena and Fisher Renormalization

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Abstract

This thesis offers a full background to the subject of phase transitions and critical phenomena through derivation and explanation of all relevant thermodynamic quantities, and the critical exponents and amplitudes that accompany them. Then, all universal quantities for ferromagnetic phase transition systems including scaling relations and amplitude relations are derived. Two paradigms of phase transition modeling - the one-dimensional and mean field Ising models - are fully evaluated. With a full background in place focus then turns to Fisher renormalization, where the critical exponents and amplitudes of a real system operating under constraint are derived from the ideal system. These exponents and amplitudes are then tested for involution, resulting in a discovery regarding the involutory nature of universal quantities that are fisher renormalized.

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1 Statistical Mechanics

As the name suggests, statistical mechanics is the application of statistical principles to the field of mechanics. When seeking to understand some of the thermodynamic properties of a real system, use of thermodynamics can be impractical due to the generalized nature of the subject. Similarly, using mechanics can prove to be equally impractical as one attempts to apply the microscopic molecular detail that mechanics requires to a real system spanning a macrostate of more than 10^{24} interacting molecules. Statistical mechanics can be used to bridge this gap between methods and provide real solutions to real problems, by essentially calculating the average properties of a mechanical system.

In these systems one has minimal control at best over the components, and is restricted to measuring some average properties of the system such as the magnetization, or temperature. Statistical mechanics looks to predict the relations between these properties of the macrostate, based on knowledge of the microscopic forces taking place between the components.

Another aspect to consider when concerning the value of statistical mechanics is entropy. For a thermodynamic system the entropy can only be derived through observation and experimentation. In statistical mechanics the entropy is a function of the distribution of the system and its microstates.

1.1 The Macrostate

The macrostate of a system refers to the thermodynamic state of the system. It is a specification of the thermodynamic properties, such that the thermodynamic state of the system can be defined. Unfortunately, it offers little more than this in terms of interactions between the components of the system.

A typical macrostate for a pure substance offers just the nature of the system, the quantity of the system, and some paired thermodynamic coordinates - such as pressure P and volume V , magnetization M and magnetic field H , etc. Other properties such as the internal energy e are then derived from these coordinates. Using statistical mechanics, one will be able to find the values of all properties from first principles.

The macrostates considered here will be isolated systems, such that the system is considered to be the entirety of its own universe. By doing this, the internal energy of the system remains constant throughout, as does the volume of the system. The quantity of the substance is the number of component particles, N , that it contains.

For an isolated system where N is large, the fluctuations in other properties such as the temperature, T are small, and it is possible to precisely determine T using the other

known elements (N, e, V) . The results of this macrostate can be used to evaluate the behaviour of any other macrostates of the system, such as the (N, P, T) macrostate.

1.2 The Microstate

The microstate concerns the microscopic properties of the N particles that make up the system, and their mechanical state. It is the most detailed specification of the system that can be produced, specifying the individual properties of every single particle (where it has been established that $N \geq 10^{24}$). The sheer quantity of information that is contained in one microstate is indigestible even using modern technology. This conundrum of dealing with such a quantity of information is then worsened by the fact that the microstate is constantly changing (one mole of gas changes its macrostate roughly 10^{32} times per second).

As a means of getting around this problem, some form of averaging method must be sought so as to reduce the quantity of information.

In order to do so, consider that while there are a large number of possible microstates for the macrostate to be in, the quantity of possibilities is finite. This number, Ω , plays an important part in the statistical process.

1.3 The Averaging Postulate

The key assumption made for statistical mechanics is

All accessible microstates are equally probable

This is a reasonable assumption as it is supported by the following arguments:

- Time-Averages. The act of measuring the microstate takes a non-zero time period, during which the system will shift between any number of the Ω microstates. Due to this, it is necessary to average over all the Ω microstates to compensate for the changing state of the system.
- Confession of Ignorance: It is unknown which of the Ω microstates the system is in at any given time, so averaging over all microstates includes all options. This is known as an ensemble average due to the way it includes all microstates.

This assumption requires a degree of uniformity amongst the microstates. The microstates cannot be identical, but for the assumption to work the microstates must be similar to each other.

1.4 Distributions

The problem posed by the averaging postulate is a matter of quantity. Consider that one wishes to average over all Ω microstates in a real-sized system, where each microstate is composed of $N \geq 10^{24}$ individual elements (a quantity already deemed incalculably large). This results in a total of $\Omega = N^N$ microstates, a quantity too large to comprehend. In light of this, an alternative approach to precise microscopic knowledge of the system must be considered.

Such an approach is provided by a distribution specification, whereby if the system is assumed to be composed of weakly-interacting particles and each of the N particles is assigned an individual energy, the total internal energy e of this composition can be expressed as the sum of the energies of the particles

$$e = \sum_{l=1}^N E(l). \quad (1.1)$$

where $E(l)$ represents the individual energy of particle l . This expression assumes that the interaction between particles is negligible, but some non-zero interaction must be present in order for equilibrium to be achieved (a requirement of a thermodynamic system).

Such restrictions on interaction strength prevent this method from being used for systems of liquids (which feature strongly-interacting particles). Similarly it would seem to prevent an examination of solid systems given their strong interactions between atoms, but this can be worked around by considering that the definition of a particle within a system is not limited to just atoms, but can instead be used for conduction electrons, phonons, or (in particular for this project) localized spins.

The term distribution is used to refer to the energies of the particles within the system. In all possible microstates of the system each particle is in an individual identifiable state. A distribution specification does not identify the state of every particle, but instead identifies the quantity of particles that are in each state and in doing so creates a “middle-ground” between the microstate and the macrostate.

Distributions are commonly defined as a *distribution of states*, where a set of numbers (n_1, n_2, \dots, n_j) represent the number of particles in the respective states $1, 2, \dots, j$, which have the energies (E_1, E_2, \dots, E_j) . By accounting for all possible states of the system it is often found that $j \rightarrow \infty$, creating an infinite set. This set of distribution numbers (n_1, n_2, \dots, n_j) can be rewritten as the shorthand $\{n_j\}$.

An alternative definition of distributions is used when dealing with gases. This *distribution in levels* is similar to a distribution in states, but the set of numbers (n_1, n_2, \dots, n_i) represent the number of particles in level i , with associated energy E_i and degeneracy g_i

(number of states in level i). This set is written as $\{n_i\}$ in shorthand. This definition is less detailed than a distribution in states, but is specialized to cater for cases where identical energies ($E_i = E_j$) exist.

1.5 The Statistical Method

Consider an isolated system of identical weakly interacting particles, where the macroscopic properties of internal energy e , volume V and number of particles N are all known. The statistical description of this macrostate can be determined through a four-step process, outlined below:

1. Solve the one-particle problem.
2. Find the number of possible distributions.
3. Assign microstates to the distributions.
4. Find the average distribution.

To aid explanation of the process, a worked example will be detailed following an explanation of each step. This example is a simple solid macrostate consisting of $N = 4$ distinguishable particles A to D with a total internal energy $e = 4E$.

1.5.1 The One-Particle Problem

One starts by observing a single particle within the system, and examining the states that this particles may occupy. This overcomes the problems earlier attributed to mechanical analysis as by focusing on a single particle there is no danger of an overload of information. All distinct states are assigned $j(= 0, 1, 2, \dots)$ with the corresponding energies for each state labeled E_j . When dealing with gases these E_j are dependent on the volume V , while for solids the energies depend on the volume per particle V/N .

In our example, the possible energies that any of the four particles can occupy are $j = \{0, E, 2E, 3E, 4E\}$, therefore one finds that $E_j = jE$.

1.5.2 Possible Distributions

Now one must consider the ramifications of the one particle problem when extrapolated to all particles. While any particle may potentially occupy any of the j states, the whole system may impose restrictions that invalidate certain combinations of states. There are two tests used to determine the validity of these distributions. The first,

$$\sum_j n_j = N \quad , \quad (1.2)$$

verifies that the number of particles in all states corresponds with the total number of particles (so, all particles within the system have a clearly defined state). The second test,

$$\sum_j n_j E_j = e \quad , \quad (1.3)$$

ensures consistency with Eq.(1.1) by checking that the total energy over all states is the same as the total internal energy of the system. Each distribution that satisfies these conditions is recorded, and the set of all valid distributions $\{n_j\}$ is compiled.

In the case of our example, the conditions that must be satisfied are $\sum n_j = 4$ and $\sum n_j E_j = 4E$. Therefore in order to find the possible distributions one must determine how many combinations of four energies from the set $\{0, E, 2E, 3E, 4E\}$ can sum to $4E$. One can then simply deduce that there are five such distributions that meet these requirements, which are given below.

Distribution	n_0	n_1	n_2	n_3	n_4
D_1	3	0	0	0	1
D_2	2	1	0	1	0
D_3	2	0	2	0	0
D_4	1	2	1	0	0
D_5	0	4	0	0	0

1.5.3 Assigning Microstates

Given that one is aware of both the number of particles in the system, N , and the number of particles that are in each state j in each distribution $\{n_j\}$, one can now tackle the combinatorial problem of determining the quantity of microstates that correspond to each distribution. Call this number of microstates $t(\{n_j\})$. Observe that the sum of these t gives the total number of valid microstates for the system, i.e.

$$\sum t(\{n_j\}) = \Omega \quad (1.4)$$

In our example, one must now determine the number of microstates that can be formed from each of our five distributions. For instance, distribution D_3 has two particles with energy $2E$ and two with energy 0 . Via deduction or use of ${}_4C_2$ one finds that there are 6 combinations of four particles that can fulfill this requirement as explicitly stated below.

A	B	C	D
2	2	0	0
2	0	2	0
2	0	0	2
0	2	2	0
0	2	0	2
0	0	2	2

Thus, $t^{(3)} = 6$. Similarly, one finds $t^{(1)} = 4$, $t^{(2)} = t^{(4)} = 12$ and $t^{(5)} = 1$. Note that the distributions with the greater variance of values have the most microstates, and

thus will carry greater weight in the results. The total number of microstates can now be determined as $\sum t = 35$.

1.5.4 The Average Distribution

Given that the averaging postulate declared that all valid microstates must be equally probable, and that the quantity of valid microstates in each distribution is now known, the $t(\{n_j\})$ can be used as weightings of the distribution $\{n_j\}$. Thus, a weighted average over all possible distributions can be derived. This average distribution, $\{n_j\}_{\text{av}}$, describes the thermal equilibrium distribution where temperature remains constant.

This method is best explained via the provision of a worked solution to our example. Consider that the results gathered allow one to formulate a weighted average of the quantity of particles in a state with zero energy as thus:

$$\begin{aligned}(n_0)_{\text{av}} &= (n_0^{(1)}t^{(1)} + n_0^{(2)}t^{(2)} + n_0^{(3)}t^{(3)} + n_0^{(4)}t^{(4)}) / \Omega \\ (n_0)_{\text{av}} &= (3 \times 4 + 2 \times 12 + 2 \times 6 + 1 \times 12 + 0 \times 1) / \Omega = 60/35 = 1.71\end{aligned}$$

And similarly for the other states:

$$\begin{aligned}(n_1)_{\text{av}} &= (0 \times 4 + 1 \times 12 + 0 \times 6 + 2 \times 12 + 4 \times 1) / \Omega = 40/35 = 1.14 \\ (n_2)_{\text{av}} &= (0 \times 4 + 1 \times 12 + 2 \times 6 + 1 \times 12 + 4 \times 1) / \Omega = 24/35 = 0.69 \\ (n_3)_{\text{av}} &= (0 \times 4 + 1 \times 12 + 0 \times 6 + 0 \times 12 + 0 \times 1) / \Omega = 12/35 = 0.34 \\ (n_4)_{\text{av}} &= (1 \times 4 + 0 \times 12 + 0 \times 6 + 0 \times 12 + 0 \times 1) / \Omega = 4/35 = 0.11\end{aligned}$$

Therefore the average quantity of particles in each state can be summarized by the average distribution

$$\{n_j\}_{\text{av}} = (1.71, 1.14, 0.69, 0.34, 0.11)$$

1.6 Statistical Entropy and Microstates

The second law of thermodynamics states:

The total entropy of any isolated thermodynamic system never decreases over time.

In statistical mechanics, entropy is used in relation to probability whereby it is understood that while it is possible to revert a system to a previous state through performing the opposite of any procedure that increases the entropy of a system, it is almost infinitely improbable.

The statistical definition of entropy, S , for isolated systems is

$$S = k_B \ln \Omega \tag{1.5}$$

where $k_B = 1.38 \times 10^{-23} \text{JK}^{-1}$ is Boltzmann's constant, a constant that will be used frequently throughout this thesis. This definition was derived by famed physicist Ludwig

Boltzmann in the 19th century, extraordinary work considering that it occurred at a time when concepts like atoms and molecules were dismissed by most physicists as merely convenient theoretical constructs. This equation is engraved on Boltzmann's tombstone at the Vienna Zentralfriedhof.

This correlation between Ω and S provides an interesting interpretation of the third law of thermodynamics:

As temperature approaches absolute zero, the entropy of a system approaches an absolute minimum.

Consider that when $S = 0$ Eq.(1.5) yields the result $\Omega = 1$, suggesting that the reduction in temperature to absolute zero will provide an equilibrium to such systems, offering just a single accessible microstate.

1.7 Distinguishable Particles

With the statistical method outlined, the task remains to apply this procedure to realistic thermodynamic systems that contain a large quantity of N identical weakly-interacting particles. This study will focus on solid assemblies.

While the particles within the solid system remain identical, it is possible to identify individual particles by treating the solid formation of particles as a lattice, whereby each particle has an individual lattice location. This position will not change due to the nature of a solid assembly, so referring to any given lattice site will always correspond to the same individual particle.

The task is now to statistically describe this system of solid particles using the statistical method from section 1.5. This isolated system of N individual identifiable particles has a fixed volume V and internal energy e .

1.7.1 The One-Particle Problem

States are labeled $j = 0, 1, 2, \dots$ with corresponding energies E_j . We are dealing with a solid system so these energies are dependent on the volume per particle V/N , which is known as both V and N are known.

1.7.2 Possible Distributions

This follows as before, with a distribution in states $\{n_j\}$ used and then verified by Eq.(1.2) and Eq.(1.3).

1.7.3 Assigning Microstates

In this section the importance of distinguishability between the particles comes to the fore, as it allows the assignment of microstates to be seen as a combinatorial problem. There are N particles in the system, each of which must be assigned a state j in a valid microstate. So if the particles are split so that n_j particles are in each state j , the number of possible combinations that can be achieved will be the number of valid microstates

$$t(\{n_j\}) = N! / \prod_j n_j! . \quad (1.6)$$

1.7.4 The Average Distribution

The very large N value means that deducing the weighted averages becomes irrelevant, as it will become apparent that one of the distributions (referred to as $\{n_j^*\}$) will be much more likely than the others to the point where this distribution can be chosen as the average. This $\{n_j^*\}$ can clearly be observed to be the peak of $t(\{n_j\})$. This effectively reduces the problem into a case of maximizing $t(\{n_j\})$ such that $\sum_j n_j = N$ and $\sum_j n_j E_j = e$.

Also, consider the relationship between the total microstates within the system Ω , and the number of microstates per distribution, t . It should be apparent that

$$\Omega = \sum t(\{n_j\}) . \quad (1.7)$$

In practice, the domination of one distribution over all others allows them to be neglected, such that

$$\Omega \approx t(\{n_j^*\}) = t^* . \quad (1.8)$$

Note that this is not an exact reduction, but an approximate one. The dominant distribution is not representative of all microstates, but is close enough to doing so that it can be regarded as such.

1.7.5 The Most Probable Distribution

The thermal equilibrium distribution can now be found through derivation of t^* and the corresponding $\{n_j^*\}$. This is made easier by using the properties of logarithms. Consider Eq.(1.6)

$$\begin{aligned} t(\{n_j\}) &= N! / \prod_j n_j! \\ \ln(t) &= \ln \left(N! / \prod_j n_j! \right) \\ \ln(t) &= \ln(N!) - \ln \left(\prod_j n_j! \right) \end{aligned}$$

$$\ln(t) = \ln(N!) - \sum_j \ln n_j! \quad . \quad (1.9)$$

We are dealing with large numbers in both logarithms here, which allows the use of Stirling's Approximation for large factorials

$$\begin{aligned} \ln(X!) &= X \ln(X) - X \\ \ln(t) &= (N \ln(N) - N) - \sum_j (n_j \ln(n_j) - n_j) \quad . \end{aligned} \quad (1.10)$$

The maximum value of t can now be found by finding the zero point of the derivative of Eq.(1.10), where $\partial \ln t = 0$. First, consider the derivative of Stirling's approximation

$$\frac{\partial}{\partial y} \ln(X!) = \frac{\partial X}{\partial y} \ln(X) + \frac{\partial X}{\partial y} - \frac{\partial X}{\partial y} = \frac{\partial X}{\partial y} \ln(X)$$

applying this to Eq.(1.10) gives

$$d \ln(t) = 0 = - \sum_j dn_j (\ln(n_j)) = - \sum_j \ln n_j^* dn_j \quad . \quad (1.11)$$

Here, dn_j represent allowable changes - those that keep N and U consistent with the distribution. Further, note that a lack of independence between dn_j s allows for the derivatives of Eqs.(1.2)and(1.3) to be used as additional restrictions

$$dN = \sum_j dn_j = 0 \quad (1.12)$$

$$de = \sum_j dn_j E_j = 0 \quad . \quad (1.13)$$

Given that the three previous equations are all equal to zero, the sum of arbitrary multiples of these three equations will also be equal to zero. Therefore it is possible to combine the three into one equation of the form

$$\sum_j \left(-\ln(n_j^*) + \alpha + \beta E_j \right) dn_j = 0 \quad (1.14)$$

where α and β are arbitrary constants.

Consider that the nature of these constants allows the above equation to be further simplified, as by selecting certain values of α and β will allow every term within the sum to be zero. Therefore the dominant distribution becomes

$$-\ln(n_j^*) + \alpha + \beta E_j = 0 \quad , \quad (1.15)$$

which can then be rearranged to make n_j^* the subject

$$n_j^* = \exp(\alpha + \beta E_j) \quad . \quad (1.16)$$

This is known as the Boltzmann distribution of this system.

1.7.6 Interpretation of α and β

Recall that α and β here are Lagrange multipliers applied to the conditions of Eqs.(1.2)-(1.3). As such, their values are derived from the number of particles N and the energy e of the system respectively. α is known as the “potential for particle number” and β is known as the “potential for energy”.

1. Determination of α

Consider Eq.(1.2), the condition for the number of particles. It is possible for Eq.(1.16) to be substituted into Eq.(1.2) by taking the dominant distribution as the only distribution $n_j^* = n_j$.

$$N = \sum_j n_j^* = \sum_j \exp(\alpha + \beta E_j) = e^\alpha \sum_j e^{\beta E_j} \quad (1.17)$$

The e^α part of this equation operates independent of j , so can be seen as a normalization constant, present to ensure that the distribution satisfies the requirement for the correct number of particles. If this constant is labeled A and the $\sum e^{\beta E_j}$ part is defined as the partition function, Z (an important quantity for this research that will be covered more fully at the end of this chapter), then the Boltzmann distribution from Eq.(1.16) can be rewritten in the form

$$n_j = A e^{\beta E_j} = (N/Z) e^{\beta E_j}. \quad (1.18)$$

2. Determination of β

To find the value of β , substitute n_j from Eq.(1.18) into the energy condition Eq.(1.3) to find

$$e/N = \frac{\sum_j E_j e^{\beta E_j}}{\sum_j e^{\beta E_j}}. \quad (1.19)$$

This equation cannot be rearranged to make β the subject, but given that the left hand side is a known constant (the internal energy per particle), it is possible to find a specific value for β that satisfies this equation. This equation is sufficient to describe β fully for a (e, V, N) macrostate and the correlation shown between β and (e/N) allows the equation to be described as a “potential for energy”.

It turns out that β can be written in terms of just one thermodynamic function, without the presence of any of e , V , or H . In fact, it is merely inversely proportional to the temperature of the system, T

$$\beta = \frac{1}{k_B T}. \quad (1.20)$$

where Boltzmann’s constant $k_B = 1.3807 \times 10^{-23} \text{Jk}^{-1}$ (sometimes written without subscript B).

The partition function is an important normalization function when dealing with thermodynamic phase transition systems. It is given by

$$Z(T) = \sum_s e^{\frac{1}{k_B T} E_j} = \sum_s e^{\beta E_s}. \quad (1.21)$$

The partition function can be used to provide a weighted average (or expectation value) of various quantities pertaining to the system. If X is any observable such as the magnetization or energy of a configuration, its expectation value is given in statistical mechanics as

$$\langle X \rangle = \frac{1}{Z} \sum_s X e^{\beta E_s}. \quad (1.22)$$

Further uses for the partition function will become clear in later chapters.

2 Phase Transitions

2.1 Background

A phase transition is classically defined as “the transformation of a thermodynamic system from one ‘phase’ to another”, where a phase is defined as a state of the system where all physical properties of the phase are essentially uniform. The transition occurs due to a change in one of the system’s intensive variables (variables that are independent of the quantity of material in a system, such as temperature).

The critical point is the required combination of pressure and temperature that one must subject a system to in order to induce a phase transition. The term critical phenomena stems from the “phenomenal” changes that a system goes through at the critical point - be it large-scale statistical changes in terms of measurable quantities, or physically observable alterations to systems.

For example, consider the phase transitions for the compound H_2O (water). Under standard atmospheric pressure (which is assumed throughout this thesis unless otherwise stated), at temperatures less than $0^\circ C$ pure H_2O is in a solid state (as ice), but between temperatures of $0^\circ C$ to $100^\circ C$ it is in a liquid state (as water). As the temperature passes $0^\circ C$, an observable phase transition occurs where the system goes through a physical metamorphosis and many measurable properties of the system (such as the density) change drastically. Though such an everyday occurrence may be regarded as ordinary, if one takes a moment to consider the almost absurdness that an ice cube at absolute zero $-273^\circ C$ bears no physical or statistical difference (other than the measurable temperature) to one at $-1^\circ C$, yet a further increase of just $1^\circ C$ causes a complete transformation of the entire system then perhaps the phenomenal activity occurring can be greater appreciated.

Phase transitions are not limited to solid-liquid-gas transformations. Consider the shift of ferromagnetic materials from magnetized to non-magnetized states, which will be covered in detail in section 2.2. Also, the creation of the universe itself - the big bang - can be defined as a phase transition [13]. The concept of phase transitions can also be applied to processes that are not temperature-driven, such as traffic flow [14].

There are many acceptable ways to change a phase transition system so that the partition function can be evaluated, each with their own pros and cons. Generally, these methods can be categorized into two strategies: models and approximations.

Models involve replicating the real system into an idealized model, whereby an assuming an ideal characteristic makes the system solvable. This generally involves simplifying the equation for the Energy in the system $E(S)$ to an extent where it can be calculated exactly. This can provide qualitative information on the behaviour of the system, though with this comes a loss of information regarding the thermodynamic functions of the real

system. No three-dimensional model has been fully solved, but exact solutions have been found for some simpler one and two-dimensional models, such as the Ising model.

Approximations simplify the behaviour of the real system, so that a smaller quantity of data is considered. There are a variety of different methods that can be considered approximations, a such as computer calculations of large microscopic systems that do not approach macroscopic size (i.e. a system comprised of a few hundred atoms). This method uses statistical sampling to derive the partition function, so is subject to statistical errors. Or, Cell/Cluster approximations that extrapolate the data from a small group of components within the system and apply it to the behaviour of the whole system. Approximations are made for the interactions occurring between this “cell” and the rest of the system. Mean field theory is one such method of approximating the real system.

2.2 Ferromagnetism

A ferromagnet is defined as any material that can exhibit a spontaneous magnetization. For this to occur, the ferromagnetic must first be placed in an external field parallel to its axis, then displays a non-zero magnetization once the external field is removed. This spontaneous magnetization then reverts to zero at high temperatures when the ferromagnetic system undergoes a phase transition to a paramagnetic state, as displayed by Fig1. The critical point at which these ferromagnetic phase transitions occur is known as the Curie temperature.

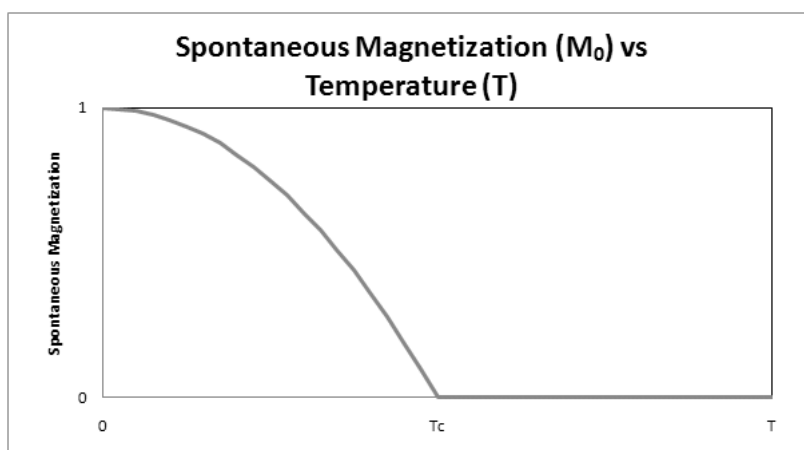


Figure 1: The effect of increase in temperature on the magnetization of a ferromagnet

An example of a ferromagnetic material is Iron, which displays a spontaneous magnetization at low temperatures in the absence of an external magnetic field, but makes the ferromagnetic phase transition from magnetized to demagnetized at the critical temperature of 770°C . Other ferromagnetic materials include cobalt (1130°C) and nickel (358°C).

Consider a ferromagnetic system, which has the thermodynamic variables tempera-

ture T , magnetization M , and the external magnetic field H . These variables are not independent, but rather are related through the equation of state of the system

$$\mathcal{F}(T, M, H) = 0 . \quad (2.1)$$

This equation describes a two-dimensional surface within the three-dimensional (T, M, H) space. Consider the effect this has on the graph of M against H . At temperatures $T \geq T_c$, this is a simple continuous graph. But at temperatures below the critical temperature T_c , this graph will display a discontinuity inside the region of the equation of state (i.e. when $H = 0$) as displayed by fig2.

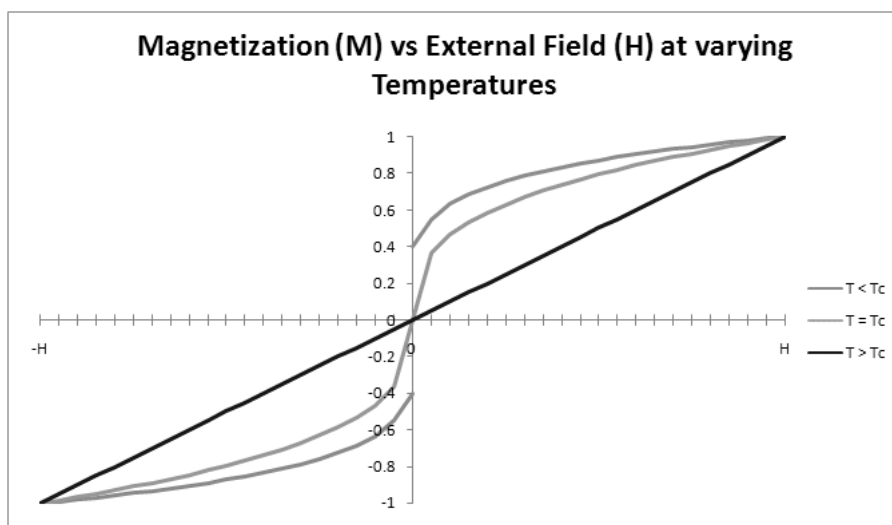


Figure 2: Phase Transitions in the MH plane

When considering critical phenomena, it is convenient to introduce a variable for the temperature relative to the critical temperature. This is known as the reduced temperature, and is defined as

$$t = \frac{T - T_c}{T_c} . \quad (2.2)$$

For temperatures below the critical temperature, the spontaneous magnetization M_0 takes different values for different temperatures (while above the critical temperature $M_0 = 0$). In fact, the spontaneous magnetization can be characterized as some power of the temperature

$$M_0 \propto |T - T_c|^\beta \quad T \rightarrow T_c^- .$$

Using the reduced temperature instead of one may write

$$M = B|t|^\beta \quad t \rightarrow 0^- \quad (2.3)$$

Here β is a critical exponent and B is a critical amplitude.

Critical exponents are quantities that can be used to characterize a continuous phase transition. These exponents vary depending on the system and material at hand. Through evaluation of all the critical exponents one can determine what is happening to a system during a phase transition. Note that the spontaneous magnetization is an example of an order parameter - a property of the system that is zero in one phase and non-zero in the other.

Critical amplitudes allow for a full explanation of the equation. With a critical exponent alone one would just have knowledge of the scaling behaviour of the thermodynamic function in question, but when a critical exponent is used in tandem with a critical amplitude the thermodynamic function can be expressed fully.

The critical exponents and critical amplitudes will be covered fully in section 4.

3 The Ising Model

3.1 The Nearest Neighbour Ising Model

The Ising model is a popular model used to apply the processes of statistical mechanics to the study of ferromagnets. The model simplifies the structure of a real system to the extent that it can be solved in one and two dimensions (a full solution to the three dimensional model has yet to be derived).

Consider that the atomic structure of a solid ferromagnet is such that all particles within the system lie rigidly in place, in ordered rows and columns equidistant to the neighbouring particle in each dimension. This structure can be seen mathematically as a lattice of N particles identifiable via their location, labeled $i = 1, \dots, N$.

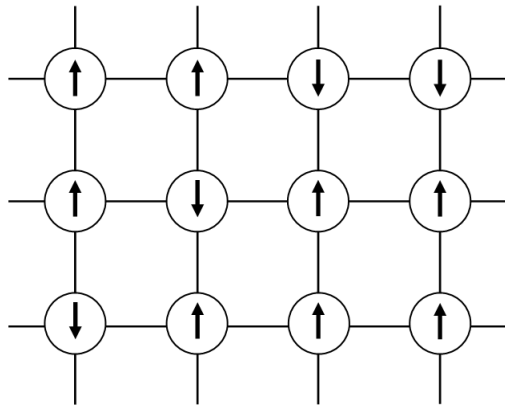


Figure 3: The Ising model lattice in 2 dimensions

Consider also that this system of particles could be seen as not one ferromagnetic entity, but as an amalgamation of individual particles that all operate as ferromagnets themselves. Each of these particles must have a magnetic alignment, an orientation on which their magnetism lies. In a real system these orientations (known as "spins") could be in any direction independent of each other, but in the Ising model they are restricted to all lying on a single line as shown in Fig.3. The restrictions imposed on these "spins" by the model mean that their magnetization is now a binomial quantity - each spin is either fully positive or fully negative along one line. Therefore each "spin" S_i has a value of ± 1 to signify its full magnetization in either direction. The set of all spins, S can be defined as

$$S = \{S_1, \dots, S_N\}.$$

The spins within the system interact with each other, and the energy associated with the interaction between any two neighbouring spins i and j can be defined as

$$E_{ij} = -JS_iS_j = \pm 1 \tag{3.1}$$

This energy = -1 when the spins are parallel (both up or both down), and $+1$ when they are not. Here J is a coupling constant representing the strength of the interactions.

The Ising model has continued to be relevant in the study of phase transitions due to universality. The critical exponents don't depend on the details of the model used but on the dimensionality and inherent symmetries of the system, which allows a relatively simple system like the Ising model to provide results for the exponents that are just as accurate as much more complex systems. This property means that an Ising model where all particles interact with each other is equally effective at summarizing the behaviour of the system as a much simpler model where only the nearest neighbours interact. On this basis it is preferable to use this "nearest neighbour" model to garner results for the system.

Bearing in mind that there are two possible values for each S_i , it is clear that there are 2^N possible configurations for the set S , where each of the 2^N configurations specifies a single state of the system. The configurations will not necessarily have identical energies, as shown by Fig.4.

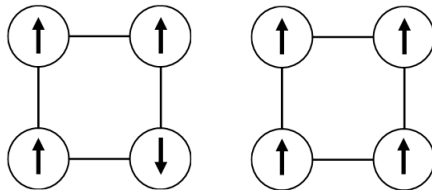


Figure 4: Two configurations of spins with differing energies

The total energy for one such configuration of spins is

$$E = -J \sum_{\langle i,j \rangle} S_i S_j \quad (3.2)$$

where $\langle i,j \rangle$ denotes that the two spins i and j are nearest neighbours (spins immediately adjacent to each other in any direction on the lattice), and J is defined as the interaction strength.

An aspect to consider when dealing with the Ising model is the boundary conditions under which the system operates. Consider that for any real, physical system there must exist start and end points that separate the system from the rest of the universe, in the form of edges, corners, and faces. In a nearest-neighbour model, these "boundary particles" will interact with fewer particles than those within the system, and one must make assumptions on the behaviour of the boundary particles in order to find a solution. Some commonly-used boundary conditions are detailed below:

If one defines the lattice as $\Lambda \subset \mathbb{Z}^d$, the boundary conditions can be formally expressed as the fixation of the spins in its infinite complement $\Lambda^c = \mathbb{Z}^d / \Lambda$

Periodic boundary conditions are where each spin interacts with the same number of neighbours, so there are no edges. The last particle in any direction of the lattice does not stay as an edge, but instead becomes neighbour with the first particle in that direction. A useful property of this is that it means that the model is translationally invariant, so the energy from interaction between spins on a one-dimensional Ising model will be identical at every site. This also has the advantage of allowing the average energy of each spin $\langle S_i \rangle$ to be independent of the spin i , as with fixed boundary conditions the spins along the boundary would display a differing energy to their neighbours lying within the interior of the system. This system can be visualized in the form of two-dimensional model spanning the surface of a three dimensional edgeless shape, such as the surface of a sphere or a torus. Under periodic boundary conditions, the spin configuration in Λ^c consists of repeated copies of the spin configuration in Λ . I.e.,

$$s(n_1 + m_1L, n_2 + m_2L, \dots, n_d + m_dL) = s(n_1, n_2, \dots, n_d), \quad (3.3)$$

i.e.,

$$s(0, n_2, \dots, n_d) = s(L, n_2, \dots, n_d), \quad s(L + 1, n_2, \dots, n_d) = s(1, n_2, \dots, n_d), \quad (3.4)$$

for all sites $(n_1 + m_1L, n_2 + m_2L, \dots, n_d + m_dL) \in \Lambda$ and integers m_1, m_2, \dots, m_d .

Open (also known as free) boundary conditions are where the system is considered to have clear defined boundaries along the edges of the system, with no restrictions placed on the values of the boundary particles. These spins on the edges of the system will interact with fewer neighbours than those that are not on the edges. As such, these boundary conditions create a model that is not translationally invariant. As there are no restrictions imposed on the spins it is possible for a system to tend to either a fully + or fully - state at temperatures below T_c , and this openness of possibilities can create a “bottleneck” where both outcomes vie for dominance. This period where the final state of the system is indeterminate is known as the “mixing time” When modeling open boundary conditions, the complement Λ^c is empty in the sense that the spins outside Λ are fixed to zero. For nearest neighbour interactions this is,

$$s(0, n_2, \dots, n_d) = s(L + 1, n_2, \dots, n_d) = 0, \quad (3.5)$$

and similar for the remaining directions.

Fixed boundary conditions are similar to open boundary conditions in that they both have clearly defined boundaries, but here the values of these boundary particles are defined and unchanging. Typical cases involve all spins along a boundary being fixed to the same value, i.e. all + or all -. By doing so, one reduces the possible phases that a system may occupy and leads to the system approaching a configuration with uniform spins more quickly when $T < T_c$. Consider that if a boundary is fixed at +, the possibility of a system entering an all - state has been removed. Thus, the system tend to the remaining possible uniform state sooner than periodic or free systems.

Fixed conditions are preferable to use under circumstances where the region surrounding the boundary is stable, and the change in a system is focused on the center with little impact on the boundary.

This study will focus on systems with periodic boundary conditions. The translational invariance of these conditions will offer simpler calculations, and given the scale of realistic systems (of more than 10^{24} particles) the proportion of particles lying on an open boundary will be statistically insignificant to the extent where one may to disregard their impact on the results. The restrictions imposed on a system with fixed boundaries suggest that it would better be examined for a specific study, rather than the broader background to phase transition systems offered by this thesis.

3.2 The Free Energy and its Derivatives

Given the multitude of possible configurations of spins that the system can adopt, average properties of thermodynamic functions over all these configurations must be taken. The magnetization of a single configuration of spins is

$$M = \sum_{i=1}^N S_i \quad (3.6)$$

and by using Eq.(1.22) the average (or expectation value) of the magnetization is

$$\langle M \rangle = \frac{\sum_{\{S_i\}} M e^{-\beta E}}{\sum_{\{S_i\}} e^{-\beta E}} \quad (3.7)$$

where $\sum_{\{S_i\}}$ symbolizes the sum over all configurations.

By examining the denominator of Eq.(3.7) it is clear that this corresponds to the partition function of Eq.(1.21). Therefore the partition function for the isolated system is

$$Z = \sum_{\{S_i\}} e^{-\beta E} . \quad (3.8)$$

An external magnetic field H is now introduced to the system, operating parallel to the orientation of the spins. The energy due to this field is

$$E_1 = -H \sum_i S_i = -HM , \quad (3.9)$$

so the total configurational energy of the system from Eq.(3.2) becomes

$$E_{\text{total}} = E + E_1 = -J \sum_{\langle i,j \rangle} S_i S_j - HM , \quad (3.10)$$

and by using the reduced external field, defined as

$$h = \beta H = \frac{H}{k_B T} , \quad (3.11)$$

the partition function from Eq.(3.8) becomes

$$Z(\beta, h) = \sum_{\{S_i\}} e^{-\beta E_{\text{total}} + hM} . \quad (3.12)$$

After the partition function, the next most fundamental quantity in statistical mechanics is the free energy, F . The total free energy of the system is

$$F(\beta, h) = -\frac{1}{\beta} \ln(Z) , \quad (3.13)$$

and the free energy per site is

$$f(\beta, h) = -\frac{1}{N} \frac{1}{\beta} \ln(Z(\beta, h)) . \quad (3.14)$$

Consider the derivative of $-f$ with respect to H

$$\begin{aligned} -\frac{\partial f}{\partial H} &= -\frac{\partial f}{\partial h} \frac{\partial h}{\partial H} = -\beta \frac{\partial f}{\partial h} \\ -\frac{\partial f}{\partial H} &= \frac{1}{N} \frac{1}{Z} \frac{\partial Z}{\partial h} , \end{aligned} \quad (3.15)$$

then by using Eq.(3.30) and the definition of the partition function from Eq.(3.12), one finds

$$-\frac{\partial f}{\partial H} = \frac{1}{N} \frac{1}{Z} \sum_{\{S_i\}} M e^{-\beta E + hM} = \frac{1}{N} \langle M \rangle$$

therefore

$$m = -\frac{\partial f}{\partial H} = -\beta \frac{\partial f}{\partial h} . \quad (3.16)$$

The magnetization per site is proportional to the derivative of the free energy per site with respect to the reduced external field.

Through a similar process, further thermodynamic functions can be shown to be proportional to derivatives of the free energy per site. Consider the derivative of βf with respect to β , using Eq.(3.14)

$$\frac{\partial(\beta f)}{\partial \beta} = -\frac{1}{N} \frac{\partial \ln(Z)}{\partial \beta} = -\frac{1}{N} \frac{1}{Z} \frac{\partial Z}{\partial \beta} ,$$

then by using

$$\frac{\partial Z}{\partial \beta} = - \sum_{\{S_i\}} E e^{-\beta E} \quad (3.17)$$

one obtains

$$= \frac{1}{N} \frac{1}{Z} \sum_{\{s_i\}} E e^{-\beta E} = \frac{1}{N} \langle E \rangle ,$$

therefore

$$\frac{\partial(\beta f)}{\partial \beta} = e , \quad (3.18)$$

the internal energy of the system is proportional to the derivative of the free energy with respect to β .

This result for the internal energy can be used to find an equation for the specific heat with regards to the internal energy. Consider that by using the substitution $Z'_\beta = \frac{\partial Z}{\partial \beta}$, it is possible to write

$$e = -\frac{1}{N} \frac{1}{Z} Z'_\beta ,$$

so by differentiating both sides with respect to β

$$\frac{\partial e}{\partial \beta} = -\frac{1}{N} \frac{\partial}{\partial \beta} [Z^{-1} Z'_\beta] ,$$

and via the product rule for differentiation

$$\frac{\partial e}{\partial \beta} = -\frac{1}{N} [Z^{-1} Z''_\beta - Z^{-2} Z'_\beta Z'_\beta] = -\frac{1}{N} \left[\frac{Z''_\beta}{Z} - \left(\frac{Z'_\beta}{Z} \right)^2 \right] . \quad (3.19)$$

Given Eq.(3.8) and (3.17), it becomes apparent that

$$\frac{Z'_\beta}{Z} = -\langle E \rangle$$

and a second differentiation of the partition function with respect to β yields

$$Z''_\beta = \sum_{\{s_i\}} E^2 e^{-\beta E}$$

$$\frac{Z''_\beta}{Z} = \langle E^2 \rangle .$$

Using these, Eq.(3.19) becomes

$$\frac{\partial e}{\partial \beta} = -\frac{1}{N} [\langle E^2 \rangle - \langle E \rangle^2] . \quad (3.20)$$

Section 3.3 will show that this variance of energies displayed by the right hand side of Eq.(3.20) is equivalent to the specific heat, such that one finds

$$c = k_B \beta^2 \frac{\partial e}{\partial \beta} = \frac{\partial e}{\partial T} , \quad (3.21)$$

the specific heat is proportional to the derivative of the internal energy with respect to T . If one then takes into account Eq.(3.18), the specific heat can be written in terms derivatives of the free energy:

$$c = k_B \beta^2 \frac{\partial^2(\beta f)}{\partial \beta^2} = -T \frac{\partial^2 f}{\partial T^2} . \quad (3.22)$$

Focus now turns to the connection between the magnetization and isothermal susceptibility. Consider that by Eq.(3.15) one finds

$$m = -\frac{1}{N} \frac{\partial Z}{\partial h} . \quad (3.23)$$

Via the substitution $Z'_h = \frac{\partial Z}{\partial h}$ and use of the product rule, the derivative of Eq.(3.23) with respect to h can be written

$$\frac{\partial m}{\partial h} = -\frac{1}{N} \left[Z^{-1} Z''_h - Z^{-2} Z'_h Z'_h \right] ,$$

which can be simplified to

$$\frac{\partial m}{\partial h} = -\frac{1}{N} \left[\frac{Z''_h}{Z} - \left(\frac{Z'_h}{Z} \right)^2 \right] . \quad (3.24)$$

Using Eq.(3.12) the second derivative of the partition function with respect to h is

$$\frac{\partial^2 Z}{\partial h^2} = \sum_{\{S_i\}} M^2 e^{-\beta E + hM} , \quad (3.25)$$

i.e.

$$\frac{Z''_h}{Z} = \langle M^2 \rangle$$

so one may express Eq.(3.24) as

$$\frac{\partial m}{\partial h} = -\frac{1}{N} \left[\langle M^2 \rangle - \langle M \rangle^2 \right] . \quad (3.26)$$

Consider that one can rearrange part of this equation into a variance of the magnetization

$$\langle M^2 \rangle - \langle M \rangle^2 = \langle (\langle M \rangle - M)^2 \rangle ,$$

This allows one to write Eq.(3.26) in the form

$$\frac{\partial m}{\partial h} = -\frac{1}{N} \left[\langle (M - \langle M \rangle)^2 \rangle \right] . \quad (3.27)$$

As will be covered in section 3.3, the isothermal susceptibility is traditionally defined as the variance of the magnetization, allowing one to state

$$\chi = \beta \frac{\partial m}{\partial h} = \frac{\partial m}{\partial H} \quad (3.28)$$

The isothermal susceptibility of the system is the derivative of the magnetization per site with respect to the external field. Then, by considering Eq.(3.16) the susceptibility can be defined in terms of derivatives of the free energy as

$$\chi = -\beta^2 \frac{\partial^2 f}{\partial h^2} = -\frac{\partial^2 f}{\partial H^2} \quad (3.29)$$

The various factors which multiply the derivatives here, to give the thermodynamic functions, do not play a crucial role in what follows so they are dropped for simplicity. They may be reinstated by referring to this section. Furthermore, although these thermodynamic functions are given as derivatives of the free energy with respect to T , β , or H , they are henceforth more loosely written as derivatives with respect to the reduced temperature t or reduced field h , for clarity.

3.3 Thermodynamic Functions

Consider that by Eq.(1.22) the average magnetization can be written

$$\langle M \rangle = \frac{1}{Z} \sum_{\{S_i\}} M e^{-\beta E} . \quad (3.30)$$

Using this, if there are N sites in the system then the magnetization per site of one configuration is $\frac{M}{N}$. It follows that the magnetization per site over all configurations, m , is

$$m = \frac{1}{N} \frac{1}{Z} \sum_{\{S_i\}} M e^{-\beta E}$$

$$m = \frac{1}{N} \langle M \rangle . \quad (3.31)$$

Through application of Eq.(3.6) this becomes

$$m = \frac{1}{N} \left\langle \sum_i^N S_i \right\rangle = \frac{1}{N} \sum_i^N \langle S_i \rangle . \quad (3.32)$$

One assumes that $\langle S_i \rangle$ is independent of i due to the translational invariance of the system. This then gives

$$m = \frac{1}{N} \langle S_i \rangle \sum_i^N 1 = \langle S_i \rangle . \quad (3.33)$$

The internal energy of the system, e , is defined in a similar manner to the magnetization

$$e = \frac{1}{N} \langle E \rangle . \quad (3.34)$$

Another thermodynamic function, the reduced isothermal susceptibility of the system χ , is defined as the variance of the magnetization

$$\chi_{\text{red}} = \frac{1}{N} \langle (\langle M \rangle - M)^2 \rangle . \quad (3.35)$$

By examining this variance it can be written as

$$\chi_{\text{red}} = \frac{1}{N} [\langle M^2 \rangle - \langle M \rangle^2] . \quad (3.36)$$

This definition of the reduced susceptibility is similar to the traditional definition of susceptibility such that one can state

$$\chi = \frac{\beta}{N} [\langle M^2 \rangle - \langle M \rangle^2] = \beta \chi_{\text{red}} \quad (3.37)$$

using β from Eq.(1.20).

The reduced specific heat is defined as the variance of the configurational energy of the system

$$c_{\text{red}} = \frac{1}{N} \langle (E - \langle E \rangle)^2 \rangle , \quad (3.38)$$

then via the equivalence of

$$\langle (E - \langle E \rangle)^2 \rangle = \langle E^2 \rangle - \langle E \rangle^2$$

observe that this can be rewritten, giving

$$c_{\text{red}} = \frac{1}{N} [\langle E^2 \rangle - \langle E \rangle^2] . \quad (3.39)$$

This can be shown to correspond to the traditional definition for the specific heat by

$$c = k_B \beta^2 c_{\text{red}} = \frac{k_B \beta^2}{N} [\langle E^2 \rangle - \langle E \rangle^2] . \quad (3.40)$$

3.4 History

The term “critical point” was first used by Irish chemist Thomas Andrews (1813-1885), who investigated phase transitions when studying the Liquefaction of gases in the 1860’s.

Liquefaction is a process by which the correct combination of pressure and temperature to turn a gas into a liquid is derived, so Andrews was essentially researching phase transitions. He defined the point at which a liquid-gas transition occurs as a “critical

point”, a term which has gone on to be used for all higher-order phase transitions. Andrews also produced graphs of pressure against temperature for various substances to show how the two quantities affect the critical point.

Prior to Andrews’ work on critical points, French physicist Baron Charles Cagniard de la Tour (1777-1859) discovered the critical point at which superfluid phase transitions occur when he conducted experiments using cannons in 1822. This work showed that a point exists that when surpassed all phases of a substance have equal densities and become indistinguishable from one another. The Baron dubbed this critical point “etat particulier” (the particular state), and found the temperature at which water could not be converted from a gaseous state back to liquid regardless of the pressure to be 362°C .

The Ising model was first proposed by Wilhelm Lenz (1888-1957) in 1920 [10]. Lenz then supervised Ernst Ising (1900-1998), who studied the model for his dissertation in 1924 [4]. This dissertation looked at the case of what is now known as the one-dimensional nearest-neighbour Ising model, where spins on the one-dimensional chain can only spin up or down, and only interact with their nearest neighbours. This dissertation showed that the spontaneous magnetization of ferromagnets cannot be explained using the one-dimensional model. The lack of a phase transition in the one-dimensional model led Ising to falsely believe that there would not be a phase transition in models of higher dimensions, and he dismissed his work as an unimportant contribution to the field. Ising himself then drifted away from work in phase transitions in the following years and became a teacher, but his work was continued by others (his lack of involvement in the scientific community thereafter was such that in 1949 he was surprised to discover that his paper had become so widely-used) [7].

The term “Ising model” stems from Sir Rudolf Peierls (1907-1995) whose paper “on Ising’s Model of Ferromagnetism” [15] argued that a spontaneous magnetization must be present in this model. Work on the model was continued by the likes of Michael Ellis Fisher (1931-) [9] and many others.

The Ising model was solved exactly in two dimensions under a zero external field by Norwegian theoretical physicist Lars Onsager (1903-1976) in 1944 [11], during his time as associate professor at Yale University.

While there have been numerous claims to a fully-worked solution to the three dimensional Ising model, none have been widely accepted by the scientific community.

Aside from work in real dimensions, approximations have been used to obtain results of effectively-infinite dimensional models. Mean Field theory was introduced by William L. Bragg and Evan J. Williams in 1934 [16], and numerous other methods of such an approximation have been developed since.

3.5 Classification of Phase Transitions

The original classification method for phase transitions was devised by Paul Ehrenfest (1880-1933), whose interest in the subject grew when he studied under Ludwig Boltzmann at the University of Vienna. The Ehrenfest classification method states that the order of a phase transition is the lowest derivative of the free energy of the system that displays a discontinuity. Thus, phase transitions were defined as first order, second order, etc.

Consider the definition of the internal energy from Eq.(3.18).

$$e = \frac{\partial(\beta f)}{\partial \beta} \sim \frac{\partial f}{\partial t} \quad (3.41)$$

In a first order phase transition the behaviour of this internal energy resembles Fig.5(A).

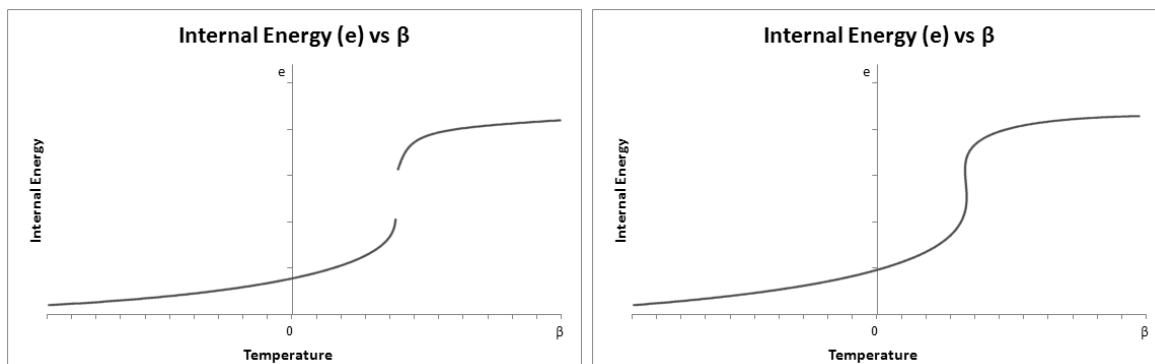


Figure 5: Behaviour of the internal energy at a first (A) and second (B) order phase transition

For a second-order phase transition, the internal energy will not display a discontinuity like Fig.5(B), but the specific heat defined using Eq.(3.21) as

$$c = \frac{\partial^2 f}{\partial \beta^2} \sim \frac{\partial^2 f}{\partial t^2} \quad (3.42)$$

will be discontinuous, as shown by Fig.6.

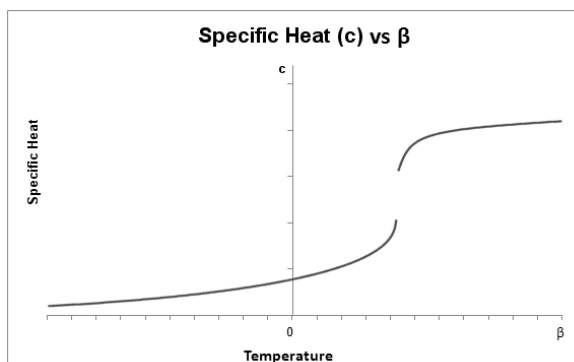


Figure 6: The specific heat of a second order phase transition

For field-driven phase transitions such as the Ising model the behaviour of the magnetization and isothermal susceptibility must also be considered, as they form the first and second derivatives of the free energy with respect to the reduced external magnetic field h .

$$M \sim \frac{\partial f}{\partial h} \tag{3.43}$$

$$\chi \sim \frac{\partial^2 f}{\partial h^2} \tag{3.44}$$

Through consideration of Fig.2 it is apparent that for temperatures below the critical point the magnetization will display a discontinuity, identifying a first-order phase transition. However, if no discontinuity occurs then the isothermal susceptibility χ falls into consideration.

Discoveries in the field have led to a need for an updated classification method. Following Lars Onsager's solution to the two-dimensional Ising model it has been discovered that divergences can occur within these graphs, as well as discontinuities. Subsequently, it has been found that divergences occur much more commonly than the typical discontinuities.

The modern classification scheme for phase transitions takes both discontinuities and divergences into account, such that the order of a phase transition is defined as the lowest derivative of the free energy that displays non-analyticity. A key difference between the discontinuities is that while divergences are characterized by critical exponents, discontinuities are not. Janke, Johnston and Kenna have proved that first order divergent phase transitions do not exist (2007) [5]. Thus far, no phase transitions of order 3 or higher have been found to naturally occur, but there is no physical reason why they cannot exist.

4 Critical Exponents and Critical Amplitudes

From Fig.2 at the critical point $T = T_c$ the magnetization is a continuous curve that passes through the origin. In fact, this is empirically well described by

$$m(0, h) \sim |h|^{\frac{1}{\delta}} \quad h \rightarrow 0$$

or

$$m(0, h) = D|h|^{\frac{1}{\delta}} \quad (4.45)$$

where δ is another critical exponent, and D is the corresponding critical amplitude to this equation.

The isothermal susceptibility of the system, χ , is defined by Eq.(3.28)

$$\chi(t, h) = \frac{\partial m(t, h)}{\partial h}. \quad (4.46)$$

This is just the equation of the tangent of the curves in Fig2. This curve diverges as $h \rightarrow 0$, and behaves in different ways depending on whether the temperature approaches the critical temperature from above or below. Thus, two critical exponents are in principle needed to explain the behaviour.

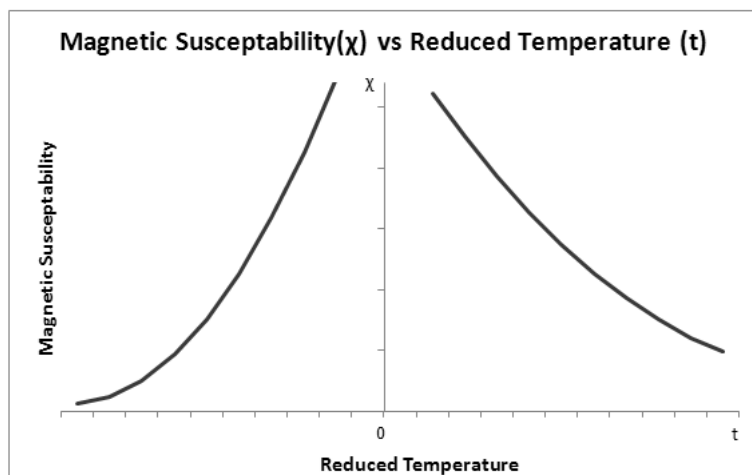


Figure 7: Divergence of Isothermal Susceptibility around critical temperature

When a high temperature is lowered to the critical temperature, $t \rightarrow 0^+$, the behaviour of the susceptibility is

$$\chi(t, 0) \sim t^{-\gamma^+} \quad t \rightarrow 0^+. \quad (4.47)$$

Similarly, for the divergence when a low temperature rises toward the critical temperature, $t \rightarrow 0^-$, the susceptibility is given by

$$\chi(t, 0) \sim (-t)^{-\gamma^-} \quad t \rightarrow 0^-. \quad (4.48)$$

However, through experimentation these critical exponents are found to be identical, and one usually has $\gamma_+ = \gamma_- = \gamma$ and writes

$$\chi(t) = \Gamma_{\pm}|t|^{-\gamma} \quad t \rightarrow 0. \quad (4.49)$$

The equality of γ_+ and γ_- also paves the way for a universal critical amplitude ratio. While the isothermal susceptibility is derived from the second derivative of the free energy of the system with respect to temperature, the specific heat is given by the second derivative of the free energy of the system with respect to the external field

$$c = \frac{\partial^2 f(t, h)}{\partial t^2}. \quad (4.50)$$

The specific heat (or heat capacity) of the system, c , can be viewed as a counterpart of sorts to the isothermal susceptibility. While the isothermal susceptibility is derived from the second derivative of the free energy of the system with respect to temperature, the specific heat is given by the second derivative of the free energy of the system with respect to the external field

$$c = \frac{\partial^2 f(t, h)}{\partial t^2}. \quad (4.51)$$

Examining the behaviour of the specific heat at a phase transition reveals another divergence where $C \sim \infty$ at $T = T_c$.

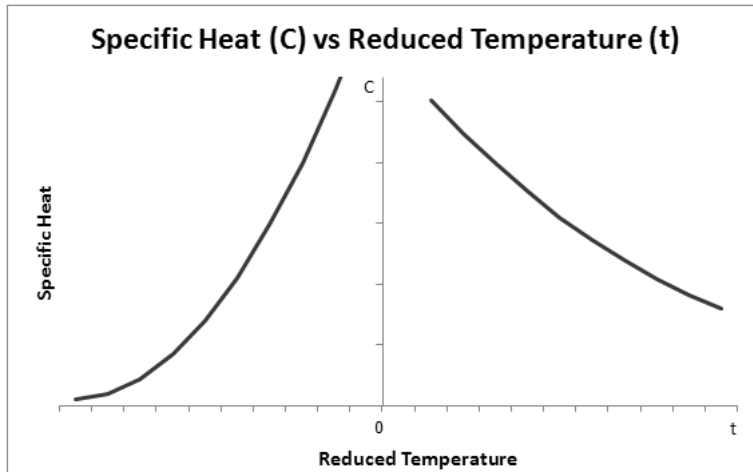


Figure 8: Divergence at the critical temperature for specific heat

This is a power-law relationship where

$$c \sim \frac{1}{|T - T_c|^\alpha} \sim |T - T_c|^{-\alpha}$$

which using the reduced temperature becomes

$$c = C_{\pm} + A_{\pm}|t|^{-\alpha} \quad (4.52)$$

(again, both an α_+ and an α_- exist depending on the direction that the critical point is approached from, but through experimentation it can be shown that $\alpha_+ = \alpha_- = \alpha$). Thus, another universal amplitude ratio concerning A_{\pm} is found

$$\frac{A_+}{A_-} \text{ is universal .} \quad (4.53)$$

A further critical exponent is associated with the correlation function. Consider that the correlation between two spins at sites i and j , defined as

$$G(i, j) = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle \quad . \quad (4.54)$$

Given the translational invariance of spin energies, it can be assumed that the only variable on which the correlation function will depend on is the distance between the sites. If the positions of the sites are defined x_i and x_j respectively then the distance between them is

$$r_{ij} = |x_i - x_j| \quad (4.55)$$

so the correlation function can be written as $G(i, j) = G(r_{ij})$. It is expected that away from T_c the correlation between spins will decrease exponentially as the distance between them increases, reaching zero as the distance between spins approaches infinity

$$G(r) \rightarrow 0 \quad \text{as} \quad r \rightarrow \infty \quad ,$$

in fact, it has been shown via experimentation that there are two solutions for $G(r)$, depending on whether the system is at a critical state.

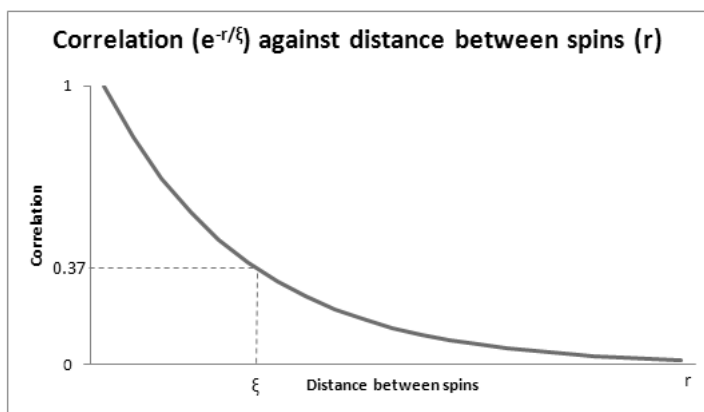


Figure 9: Correlation against spin length

Away from the critical point, the exponential decay of the correlation function behaves as

$$G(r) \sim \frac{e^{-\frac{r}{\xi}}}{r^{d-2+\eta}} \quad (4.56)$$

where d represents the dimensionality of the system, and η is another critical exponent that characterizes the behaviour of the system.

Consider Fig.9, the graph of the behaviour of the numerator of the correlation function of Eq.(4.56) against the distance between spins. It can be seen that if $r = \xi$ then $e^{-r/\xi} = e^{-1} \approx 0.37$, around one third of its starting value.

At the critical point, the correlation length ξ becomes infinite. Under this condition the numerator of Eq.(4.56) will become 1. Then the scaling behaviour of the equation can be replaced by the critical amplitude Θ , leaving

$$G(r) = \frac{\Theta}{r^{d-2+\eta}} \quad t = 0 . \quad (4.57)$$

The correlation length, ξ , is a measurement of the distance over which the spins are correlated. It turns out that in a second-order phase transition, the behaviour of this correlation length with respect to temperature takes the form of Fig.10.

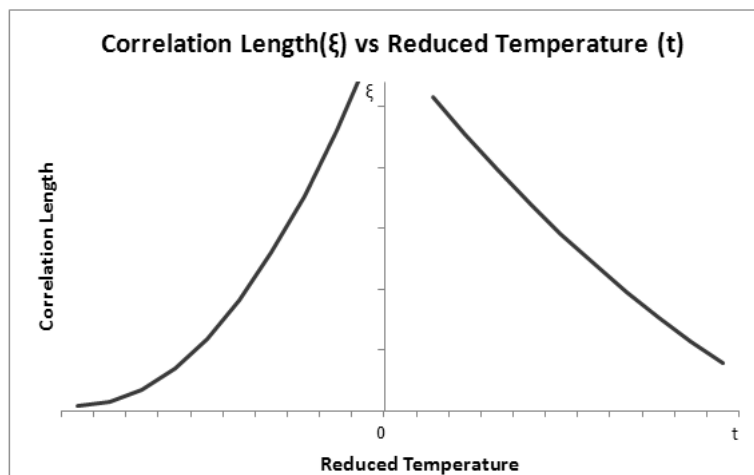


Figure 10: Divergence at the critical temperature for Correlation Length

This divergence of the correlation length allows for it to be defined by critical exponents, which differ depending on the direction from which the critical temperature is approached.

$$\xi \sim t^{-\nu_+} \quad t \rightarrow 0^+ \quad (4.58)$$

$$\xi \sim (-t)^{-\nu_-} \quad t \rightarrow 0^- \quad (4.59)$$

The two exponents are found to be identical, $\nu = \nu_{\pm}$, so the two equations are commonly combined to

$$\xi = N_{\pm}|t|^{-\nu} \quad (4.60)$$

giving the universal amplitude ratio

$$\frac{N_+}{N_-} \text{ is universal .} \quad (4.61)$$

Thus, all critical exponents and critical amplitudes have been defined. The goal of sections 6 and 7 is to discover the numerical values of these exponents for two forms of the Ising model.

5 Scaling Relations

It has been hypothesized that the thermodynamic inequalities for the critical exponents seem to be satisfied experimentally as equalities. This applies to exponents calculated in many models.

It will be shown in this chapter that if the potential of a system is a generalized homogeneous function (so it satisfies some simple scaling relation), the exponents will be expressed in terms of a smaller set of parameters such that they satisfy the thermodynamic inequalities as equalities. These free parameters cannot be calculated so this process will not lead to numerical solutions to the critical exponents, but the assumed scaling property of the thermodynamic potential gives specific predictions for the equation of state which also seems to be supported by experiments.

5.1 Homogeneous Functions

A function $F(x)$ is said to be homogeneous if

$$F(\lambda x) = g(\lambda)F(x) \quad (5.1)$$

for any λ . Consider then that

$$\begin{aligned} F(\lambda\mu x) &= F(\lambda(\mu x)) \\ &= g(\lambda)F(\mu x) \end{aligned}$$

by application of Eq.(5.1). Repeating this process yields

$$F(\lambda\mu x) = g(\lambda)g(\mu)F(x) . \quad (5.2)$$

Consider, on the other hand, a single application of Eq.(5.1) as

$$\begin{aligned} F(\lambda\mu x) &= F((\lambda\mu)x) \\ &= g(\lambda\mu)F(x) , \end{aligned}$$

comparing this with Eq.(5.2) yields

$$g(\lambda)g(\mu) = g(\lambda\mu) . \quad (5.3)$$

Differentiating both sides of this with respect to μ ,

$$g(\lambda)g'(\mu) = \lambda g'(\lambda\mu) ,$$

choosing $\mu = 1$ and denoting $g'(1) = P$, we obtain the simple differential equation

$$\lambda g'(\lambda) = g(\lambda)P$$

or

$$\frac{g'(\lambda)}{g(\lambda)} = \frac{P}{\lambda} .$$

The left hand side of this is

$$\frac{\partial}{\partial \lambda} \ln g(\lambda) = \frac{1}{g(\lambda)} \frac{\partial g(\lambda)}{\partial \lambda}$$

which leads to the unique solution

$$g(\lambda) = \lambda^P . \quad (5.4)$$

Using this, Eq.(5.1) can now be written as

$$F(\lambda x) = \lambda^P F(x) , \quad (5.5)$$

we have established that $g(\lambda)$ is power-like. To show that a homogeneous function of one variable must also be power-like, consider the case of $\lambda = x^{-1}$ in Eq.(5.5):

$$F(1) = x^{-P} F(x) ,$$

which gives

$$F(x) = x^P F(1) .$$

If $F(1) = C$, for constant C then

$$F(x) = Cx^P . \quad (5.6)$$

Consider a homogeneous function of two variables, defined as

$$F(\lambda x, \lambda y) = g(\lambda) F(x, y) , \quad (5.7)$$

repeating the method outlined for the function with one variable shows that $g(\lambda) = \lambda^P$. As λ is arbitrary, choosing $\lambda = y^{-1}$ for Eq.(5.7) gives

$$F\left(\frac{x}{y}, 1\right) = g(\lambda) F(x, y) . \quad (5.8)$$

Note that the left function is of one variable only. If a function $f(z)$ is defined as

$$f(z) = F(z, 1) \quad (5.9)$$

then any homogeneous function can be written in the form

$$F(x, y) = y^P f\left(\frac{x}{y}\right) \quad (5.10)$$

or

$$F(x, y) = x^P \tilde{f}\left(\frac{x}{y}\right) , \quad (5.11)$$

where

$$\tilde{f}(z) = F(1, z) \quad . \quad (5.12)$$

We can also have generalized homogeneity for the two-argument function:

$$F(\mu^u x, \mu^v y) = \mu^P F(x, y) \quad (5.13)$$

where u, v are arbitrary. If $\lambda = \mu^P$ then this can be rewritten as

$$F(\lambda^{\frac{u}{P}} x, \lambda^{\frac{v}{P}} y) = \lambda F(x, y) \quad ,$$

or, using $a = \frac{u}{P}$ and $b = \frac{v}{P}$

$$F(\lambda^a x, \lambda^b y) = \lambda F(x, y) \quad . \quad (5.14)$$

So a generalized homogeneous function is characterized by two parameters (a and b). If the arbitrary λ is set to $\lambda = y^{-\frac{1}{b}}$ then by using Eq.(5.9), Eq.(5.14) becomes

$$y^{\frac{1}{b}} f\left(\frac{x}{y^{\frac{a}{b}}}\right) = F(x, y) \quad , \quad (5.15)$$

this satisfies Eq.(5.10) for an ordinary homogeneous function.

5.2 Widom Scaling

We are now in a position to discuss Widom scaling for the free energy, $f(t, h)$. Near the critical point we will assume that this f consists of two parts: the regular f_R element and a singular f_S that describes the physics relevant for a phase transition

$$\begin{aligned} f(t, h)|_{T \rightarrow T_c} &= f_R(t, h)|_{T \rightarrow T_c} + f_S(t, h)|_{T \rightarrow T_c} \\ &= f_R(t, h) + f(t, h) \quad . \end{aligned} \quad (5.16)$$

One then assumes that the singular part $f(t, h)$ is a generalized homogeneous function

$$f(t, h) = \lambda^{-1} f(\lambda^a t, \lambda^b h) \quad (5.17)$$

this is known as static scaling or Widom scaling of the free energy. In order to allow one to derive both the scaling relations and their corresponding universal amplitude ratios simultaneously we alter this equation to include the metric factors K_t and K_h , two non-universal constants

$$f(t, h) = \lambda^{-1} f(K_t \lambda^a t, K_h \lambda^b h) \quad . \quad (5.18)$$

Now one can look to find the critical exponents in terms of the unknowns a and b . Differentiating both sides of Eq.(5.17) with respect to h gives

$$M(t, h) = K_h \lambda^{b-1} M(K_t \lambda^a t, K_h \lambda^b h) . \quad (5.19)$$

By setting $h = 0$, Eq.(5.19) gives the spontaneous magnetization as

$$M(t, 0) = K_h \lambda^{b-1} M(K_t \lambda^a t, 0) . \quad (5.20)$$

by the arbitrary nature of λ , it can be set to $\lambda = K_t^{-\frac{1}{a}} t^{\frac{-1}{a}}$. Using this value of λ in Eq.(5.20) gives the magnetization in terms of temperature

$$M(t, 0) = K_h K_t^{\frac{1-b}{a}} t^{\frac{1-b}{a}} M(1, 0) . \quad (5.21)$$

Comparing this to the notation for the magnetization from Eq.(2.3) reveals the values of both the critical exponent β and the amplitude B in terms of a, b , and the metric factors

$$\beta = \frac{1-b}{a} \quad (5.22)$$

$$B = K_t^\beta K_h M(1, 0) . \quad (5.23)$$

A similar method can be used to derive the exponent δ and amplitude D . Using Eq.(5.19), set $t = 0$ and $\lambda = K_h^{-\frac{1}{b}} h^{\frac{-1}{b}}$. The result is

$$M(0, h) = K_h^{\frac{1}{b}} h^{\frac{1-b}{b}} M(0, 1) . \quad (5.24)$$

By comparing this to the definition of δ and D from Eq.(4.45) reveals δ and D in terms of a, b and the metric factors

$$\delta = \frac{b}{1-b} \quad (5.25)$$

$$D = K_h^{1+\frac{1}{\delta}} M(0, 1) . \quad (5.26)$$

The critical exponent γ and associated amplitude Γ , can also be found via this method. Consider that by Eq.(4.46) the susceptibility can be defined as the derivative of the magnetization with respect to the external field. Applying this to Eq.(5.19) gives

$$\chi(t, h) = K_h^2 \lambda^{2b-1} \chi(K_t \lambda^a t, K_h \lambda^b h) . \quad (5.27)$$

When $T > T_c$ and $H = 0$, setting the arbitrary λ to $\lambda = K_t^{-\frac{1}{a}} (t)^{\frac{-1}{a}}$ turns Eq.(5.27) into

$$\chi(t, 0) = K_h^2 K_t^{\frac{1-2b}{a}} t^{\frac{1-2b}{a}} \chi(1, 0) . \quad (5.28)$$

By comparing this to the definition of the exponent γ_+ from Eq.(4.47) it can be seen that the value of γ_+ in terms of a and b is

$$\gamma = \frac{2b-1}{a} , \quad (5.29)$$

and the amplitude Γ_+ is

$$\Gamma_+ = K_h^2 K_t^{-\gamma} \chi(1, 0) . \quad (5.30)$$

Likewise, the critical exponent γ_- is found to be the same using $T \rightarrow T_c^-$. Therefore

$$\gamma_+ = \gamma_- = \frac{2b-1}{a} , \quad (5.31)$$

and

$$\Gamma_{\pm} = K_h^2 K_t^{-\gamma} \chi(\pm 1, 0) . \quad (5.32)$$

The exponents α_+ and α_- are related to the specific heat of the system around the critical point. The specific heat, C , is defined by Eq.(4.51) as the second derivative of the free energy with respect to t . With this in mind, differentiating both sides of Eq.(5.18) twice with respect to t results in

$$C(t, h) = K_t^2 \lambda^{2a-1} C(K_t \lambda^a t, K_h \lambda^b h) , \quad (5.33)$$

which when under a zero external field $h = 0$ and with the arbitrary λ set to $\lambda = K_t^{-\frac{1}{a}} t^{\frac{-1}{a}}$, becomes

$$C(t, 0) = K_t^{2+\frac{1-2a}{a}} t^{\frac{1-2a}{a}} C_H(1, 0) . \quad (5.34)$$

Comparing this to Eq.(4.52) shows that

$$\begin{aligned} -\alpha &= \frac{1-2a}{a} \\ \alpha &= 2 - \frac{1}{a} \end{aligned} \quad (5.35)$$

and

$$A_{\pm} = K_t^{2-\alpha} C(\pm 1, 0) , \quad (5.36)$$

as was the case with γ_+ and γ_- , here $\alpha_+ = \alpha_-$.

The critical exponents β , δ and γ are now all known in terms of a and b . By rearranging to make a and b the subject, we find for b using Eq.(5.25),

$$b = \frac{\delta}{1+\delta} . \quad (5.37)$$

Then for a , using Eq.(5.37)

$$a = \frac{1}{\beta} \frac{1}{\delta+1} , \quad (5.38)$$

using these values of a and b in Eq.(5.31) will give a scaling relation for γ

$$\gamma_+ = \gamma_- = \gamma = \beta(\delta-1) \quad (5.39)$$

this is known as Griffith's law.

Likewise, rearranging Eq.(5.26) to make K_h the subject gives

$$K_h \propto D^{\frac{\delta}{1+\delta}} \quad (5.40)$$

and combining this with Eq.(5.23) to make K_t the subject gives

$$K_t \propto B^{\frac{1}{\beta}} D^{\frac{-\delta}{\beta(1+\delta)}} \quad , \quad (5.41)$$

where proportions are used instead of equalities to eliminate universal terms which are superfluous to the goals of this section such as $m(1, 0)$. Using these in Eq.(5.32) allows the universal critical amplitude ratio to be derived

$$\Gamma_{\pm} \propto D^{\frac{2\delta}{1+\delta}} B^{\frac{-\gamma}{\beta}} D^{\frac{\delta\gamma}{\beta(1+\delta)}}$$

$$\Gamma_{\pm} \propto B^{\frac{-\gamma}{\beta}} D^{\frac{\delta}{1+\delta}(2+\frac{\gamma}{\beta})} \quad ,$$

then by using Griffith's law $\frac{\gamma}{\beta} = \delta - 1$, leaving the amplitude combination

$$\frac{\Gamma_{\pm} B^{\delta-1}}{D^{\delta}} \quad . \quad (5.42)$$

universal.

Through use of a , Eq.(5.35) can be substituted into Eq.(5.38), and then combined with Eq.(5.39) to find another scaling relation for the critical exponents.

$$\alpha = 2 - \beta(\delta + 1)$$

$$2 = \alpha + 2\beta + \gamma \quad (5.43)$$

this scaling relation is known as Rushbrooke's law.

A second universal critical amplitude ratio can also be found, using Eq.(5.36) and (5.41)

$$A_{\pm} \propto \left(B^{\frac{1}{\beta}} D^{\frac{-\delta}{\beta(1+\delta)}} \right)^{2-\alpha} \quad ,$$

then consider that Eq.(5.42) can be rearranged to $D^{\delta} \propto \frac{\Gamma_{\pm}}{B^{1-\delta}}$, giving

$$A_{\pm} \propto \left(B^{\frac{1}{\beta}} \left(\frac{\Gamma_{\pm}}{B^{1-\delta}} \right)^{\frac{-1}{\beta(1+\delta)}} \right)^{2-\alpha} \quad ,$$

$$A_{\pm} \propto \left(B^{1-\frac{\delta-1}{1+\delta}} \Gamma_{\pm}^{\frac{-1}{1+\delta}} \right)^{\frac{2-\alpha}{\beta}} \quad ,$$

$$A_{\pm} \propto \left(B^{\frac{2}{1+\delta}} \Gamma_{\pm}^{\frac{-1}{1+\delta}} \right)^{\frac{2-\alpha}{\beta}} \quad ,$$

then by using Rushbrooke's law from Eq.(5.43) and Griffith's law from Eq.(5.39) one finds that

$$\frac{2 - \alpha}{(1 + \delta)\beta} = 1 ,$$

so the powers cancel out leaving the amplitude combination

$$\frac{A_{\pm}\Gamma_{\pm}}{B^2} . \quad (5.44)$$

universal.

A further scaling relation can be derived from the ‘‘hyperscaling hypothesis’’. This is the hypothesis that the free energy is universally proportional the inverse correlation volume

$$f(t, 0) \propto \xi^{-d} . \quad (5.45)$$

Recall the exponent relation for ξ from Eq.(4.60). Inserting this gives the hyperscaling hypothesis as

$$f(t, 0) \propto N_{\pm}^{-d}|t|^{\nu d} . \quad (5.46)$$

Consider the second derivative of this hyperscaling hypothesis with respect to t :

$$\frac{\partial^2 f}{\partial t^2} \propto \nu d(\nu d - 1)N_{\pm}^{-d}|t|^{\nu d - 2} , \quad (5.47)$$

recall that the specific heat of the system is defined in Eq.(4.51) as the second derivative of the free energy. Therefore The exponent relation for c from Eq.(4.52) can be compared to Eq.(5.47) to show both a new scaling relation

$$\alpha = 2 - \nu d , \quad (5.48)$$

known as Josephson's law (or the hyperscaling relation), and a critical amplitude relation

$$A_{\pm} \propto N_{\pm}^{-d}$$

thus

$$A_{\pm}N_{\pm}^d \quad (5.49)$$

is universal.

The final scaling relation and amplitude ratio are derived from the correlation function. Consider the sum over all spin pairings of the correlation function defined in Eq.(4.54):

$$\sum_{i,j} G(x) = \sum_{i,j} [\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle] , \quad (5.50)$$

by taking the two sides of the Eq.(5.50) separately, the left hand side is

$$\sum_{ij} G(x) = \sum_i \sum_j G(x_i - x_j) = N \int dx^d G(x) = N \int G(x) x^{d-1} dx \quad (5.51)$$

and using Eq.(3.6) the right hand side is

$$\sum_{i,j} [\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle] = \langle MM \rangle - \langle M \rangle \langle M \rangle = \langle M^2 \rangle - \langle M \rangle^2 = N\chi \quad (5.52)$$

Matching the two sides back up allows the magnetic susceptibility to be given in terms of the correlation function

$$\chi(t, 0) = \int_0^{\xi(t)} G(x) x^{d-1} dx \quad (5.53)$$

Using the definition of $G(x)$ from Eq.(4.57) here, this becomes

$$\chi(t, 0) = \Theta \int_0^{\xi(t)} x^{1-\eta} dx = \Theta \xi^{2-\eta} \quad (5.54)$$

From here, recalling the definitions of the susceptibility and correlation length Eq.(4.49) and (4.60) and inserting them into Eq.(5.54) reveals

$$\Gamma_{\pm} |t|^{-\gamma} = \Theta N_{\pm}^{2-\eta} |t|^{-\nu(2-\eta)}.$$

Matching up the exponents and amplitudes then gives Fisher's law - the fourth scaling relation

$$\gamma = \nu(2 - \eta) \quad (5.55)$$

and the final critical amplitude relation

$$\Gamma_{\pm} \propto \Theta N_{\pm}^{2-\eta}$$

therefore

$$\frac{\Theta N_{\pm}^{2-\eta}}{\Gamma} \quad (5.56)$$

is universal.

Thus, Widom scaling has been used to derive a set of scaling relations for critical exponents and corresponding critical amplitude relations. all of these relations are universal quantities.

6 The One-Dimensional Ising Model

The history of the Ising model was discussed in section 3.2, where Ernst Ising's solution to the one-dimensional model was briefly addressed. Here, Ising's work is restated and proven, with the values of all critical exponents derived.

6.1 Free Energy and Magnetization

Recall the partition function of a thermodynamic system from Eq.(3.12). It can be expressed in its fullest form as

$$Z = \sum_{\{S_i\}} \exp - \left[\left(-J \sum_i^N S_i S_j - H \sum_i^N S_i \right) / kT \right]$$

where $j = i + 1$. This can be simplified by using Eq.(3.11) and

$$K = J\beta \tag{6.1}$$

giving the partition function as

$$Z = \sum_{\{S_i\}} \exp \left(K \sum_{i=1}^N S_i S_j + h \sum_{i=1}^N S_i \right) . \tag{6.2}$$

Consider the $\sum_{i=1}^N S_i S_j$ part of Eq(6.2). By expanding this, observe that for the case of a one-dimensional model this sum can be rewritten

$$\sum_{i=1}^N S_i S_j = S_1 S_2 + S_2 S_3 + \dots + S_N S_1 = \sum_{i=1}^N S_i S_{i+1} \tag{6.3}$$

as by use of periodic boundary conditions the N th particle in the system is directly connected to the 1st particle. For the other sum from Eq(6.2),

$$\sum_{i=1}^N S_i = \sum_{i=1}^N S_{i+1} ,$$

therefore

$$\begin{aligned} 2 \sum_{i=1}^N S_i &= \sum_{i=1}^N S_i + \sum_{i=1}^N S_{i+1} \\ \sum_{i=1}^N S_i &= \frac{\sum_{i=1}^N S_i + \sum_{i=1}^N S_{i+1}}{2} = \frac{1}{2} \sum_{i=1}^N (S_i + S_{i+1}) . \end{aligned} \tag{6.4}$$

Inserting this back into Eq.(6.2) means that the partition function is expressed symmetrically,

$$Z = \sum_{\{S_i\}} \exp \left(K \sum_{i=1}^N S_i S_{i+1} + \frac{h}{2} \sum_{i=1}^N (S_i + S_{i+1}) \right) , \tag{6.5}$$

This partition function can now be expressed explicitly as

$$Z = \sum_{\{S_i\}} e^{KS_1S_2 + \frac{h}{2}(S_1+S_2)} e^{KS_2S_3 + \frac{h}{2}(S_2+S_3)} \times \dots \times e^{KS_N S_1 + \frac{h}{2}(S_N+S_1)} . \quad (6.6)$$

Observe that the exponential part of the partition function has been factored into a series of terms involving just a spin and its neighbour, such that if V is defined as

$$V(S, S') = \exp\left(KSS' + h\frac{S+S'}{2}\right) \quad (6.7)$$

(where S' denotes a neighbouring spin to spin S), this allows the partition function to become

$$Z = \sum_S V(S_1, S_2)V(S_2, S_3)\dots V(S_{N-1}, S_N)V(S_N, S_1) . \quad (6.8)$$

This choice of V is such that the function is symmetric, i.e.

$$V(S, S') = V(S', S) . \quad (6.9)$$

The $V(S, S')$ on the right hand side of Eq.(6.8) can be regarded as elements of a two-by-two matrix

$$\mathbf{V} = \begin{pmatrix} V(+, +) & V(+, -) \\ V(-, +) & V(-, -) \end{pmatrix} = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix} , \quad (6.10)$$

thereby turning the partition function into successive multiplications of two-by-two matrices.

$$Z = \text{Trace } \mathbf{V}^N \quad (6.11)$$

The matrix \mathbf{V} is known as the transfer matrix. If the two eigenvectors of \mathbf{V} are written as $\mathbf{x}_1, \mathbf{x}_2$, with corresponding eigenvalues λ_1, λ_2 , then

$$\mathbf{V}\mathbf{x}_i = \lambda_i\mathbf{x}_i, \quad i = 1, 2 . \quad (6.12)$$

Consider a two-by-two matrix \mathbf{P} , with column vectors $\mathbf{x}_1, \mathbf{x}_2$

$$\mathbf{P} = (\mathbf{x}_1, \mathbf{x}_2) \quad (6.13)$$

then by Eq.(6.11)

$$\mathbf{V}\mathbf{P} = \mathbf{P} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} . \quad (6.14)$$

By Eq.(6.10) observe that \mathbf{V} is symmetric, so by the properties of matrices there must exist values of \mathbf{x}_1 and \mathbf{x}_2 that are orthogonal and linearly independent. Choosing such values of \mathbf{x}_1 and \mathbf{x}_2 results in matrix \mathbf{P} being non-singular, therefore \mathbf{P}^{-1} exists. Then, by multiplying Eq.(6.14) by \mathbf{P}^{-1} we obtain

$$\mathbf{V} = \mathbf{P} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \mathbf{P}^{-1} , \quad (6.15)$$

and by substituting this back into Eq.(6.11) gives the partition function as

$$Z = \text{Trace} \left(\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \right)^N = \lambda_1^N + \lambda_2^N . \quad (6.16)$$

This can be rewritten

$$\frac{\ln Z_N}{N} = \ln \lambda_1 + N^{-1} \ln [1 + (\lambda_2/\lambda_1)^N] \quad (6.17)$$

where we may use the convention

$$\lambda_1 > \lambda_2 . \quad (6.18)$$

Via this property of the eigenvalues the second natural logarithm on the right hand side of Eq.(6.17) tends to zero as $N \rightarrow \infty$.

Consider the free energy per site of the system from Eq.(3.14). Substituting Eq.(6.17) into this yields

$$f(t, h) = -kT \ln \lambda_1 . \quad (6.19)$$

The eigenvalue λ_1 can be evaluated using the characteristic equation for matrices on matrix \mathbf{V} from Eq.(6.10)

$$\begin{aligned} \det(\mathbf{V} - \lambda I) &= 0 \\ \det \begin{pmatrix} e^{K+h} - \lambda & e^{-K} \\ e^{-K} & e^{K-h} - \lambda \end{pmatrix} &= 0 \\ (e^{K+h} - \lambda)(e^{K-h} - \lambda) - e^{-2K} &= 0 \\ \lambda^2 - (e^{K+h} + e^{K-h})\lambda + e^{2K} - e^{-2K} &= 0 . \end{aligned}$$

This quadratic for λ can be solved using the hyperbolic functions for sinh and cosh, yielding

$$\begin{aligned} \lambda &= \frac{(e^{K+h} + e^{K-h}) \pm \sqrt{(e^{K+h} + e^{K-h})^2 - 4(e^{2K} - e^{-2K})}}{2} \\ \lambda &= e^K \cosh h \pm \sqrt{e^{2K} \sinh^2 h + e^{-2K}} . \end{aligned} \quad (6.20)$$

By Eq.(6.18), λ_1 has been defined as the larger of the two eigenvalues so

$$\lambda_1 = e^K \cosh h + \sqrt{e^{2K} \sinh^2 h + e^{-2K}} .$$

Reinserting this into Eq.(6.19) gives

$$f(t, h) = -kT \ln \left(e^K \cosh h + \sqrt{e^{2K} \sinh^2 h + e^{-2K}} \right) , \quad (6.21)$$

which shows that the free energy per site $f(H, T)$ is an analytic function for all real H and $T > 0$. The free energy can now be differentiated to find the magnetization, yielding

$$m(t, h) = \frac{e^K \sinh h}{\sqrt{e^{2K} \sinh^2 h + e^{-2K}}} . \quad (6.22)$$

The magnetization per site of the system $m(t, h)$ is an analytic function of H (where $H = kTh$). This analyticity combined with the analyticity of the free energy indicates there is no phase transition for this system for any positive temperature. Ernst Ising originally obtained this result through his work on the model.

6.2 Correlations

The probability of a thermodynamic system being in any given state s is

$$Z^{-1} \exp(-\beta E(s)) . \quad (6.23)$$

Applying this to the one-dimensional Ising model, by Eq.(6.8) the probability of the system being in state $S = \{S_1, \dots, S_N\}$ is

$$Z^{-1} V(S_1 S_2) V(S_2 S_3) \dots V(S_N S_1) . \quad (6.24)$$

By applying the formula for average thermodynamic values of a system from Eq.(1.22), one can determine that the average thermodynamic value of a pair of spins (for example, $\langle S_1 S_2 \rangle$) is

$$\langle S_1 S_2 \rangle = Z_N^{-1} \sum_S S_1 V(S_1, S_2) S_2 V(S_2, S_3) V(S_3, S_4) \dots V(S_N, S_1) . \quad (6.25)$$

This can be written in matrix format. Take a diagonal matrix \mathbf{S}

$$\mathbf{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (6.26)$$

where \mathbf{S} has elements

$$S(S, S') = S \delta(S, S') , \quad (6.27)$$

by using this and the \mathbf{V} derived in Eq.(6.10), the average thermodynamic value of $\langle S_1 S_2 \rangle$ becomes

$$\langle S_1 S_2 \rangle = Z_N^{-1} \text{Trace} \mathbf{S} \mathbf{V} \mathbf{S} \mathbf{V} \dots \mathbf{V} = Z_N^{-1} \text{Trace} \mathbf{S} \mathbf{V} \mathbf{S} \mathbf{V}^{N-1} . \quad (6.28)$$

For a general case, $\langle S_i S_j \rangle$, where $0 \leq j - i \leq N$, we can similarly write

$$\langle S_i S_j \rangle = Z_N^{-1} \text{Trace} \mathbf{S} \mathbf{V}^{j-i} \mathbf{S} \mathbf{V}^{N+i-j} . \quad (6.29)$$

while for an individual spin, $\langle S_i \rangle$

$$\langle S_i \rangle = Z_N^{-1} \text{Trace} \mathbf{S} \mathbf{V}^N \quad (6.30)$$

The translational invariance of the system is explained in the two preceding equations. Note that $\langle S_i S_j \rangle$ only depends on i and j through the distance between i and j , while $\langle S_i \rangle$ is independent of i .

With the eigenvalues known, the corresponding eigenvectors can be derived. Using Eq.(6.8),

$$\begin{aligned} \mathbf{V} \mathbf{x}_i &= \lambda_i \mathbf{x}_i \\ \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix} \begin{pmatrix} a_i \\ b_i \end{pmatrix} &= \lambda_i \begin{pmatrix} a_i \\ b_i \end{pmatrix} \\ a e^{K+h} + b e^{-K} &= \lambda a \\ \frac{b}{a} &= e^K (\lambda - e^{K+h}) \\ \frac{b}{a} &= e^K \left(-e^K \sinh h \pm \sqrt{e^{2K} \sinh^2 h + e^{-2K}} \right) . \end{aligned} \quad (6.31)$$

Likewise, it turns out that

$$\frac{a}{b} = e^K \left(e^K \sinh h \pm \sqrt{e^{2K} \sinh^2 h + e^{-2K}} \right) . \quad (6.32)$$

If a number ϕ is defined such that

$$\cot 2\phi = e^{2K} \sinh h \quad 0 < \phi < \frac{\pi}{2} , \quad (6.33)$$

then

$$\tan 2\phi = \frac{e^{-2K}}{\sinh h}$$

and by the property of tan

$$\tan 2\phi = \frac{2 \tan \phi}{1 - \tan^2 \phi} ,$$

therefore

$$\begin{aligned} 2 \tan \phi &= \frac{e^{-2K}}{\sinh h} - \frac{e^{-2K}}{\sinh h} \tan^2 \phi \\ 0 &= \frac{e^{-2K}}{\sinh h} \tan^2 \phi + 2 \tan \phi - \frac{e^{-2K}}{\sinh h} . \end{aligned}$$

Solving for $\tan \phi$,

$$\begin{aligned} \tan \phi &= \frac{-2 \pm \sqrt{4 + 4 \left(\frac{e^{-2K}}{\sinh h} \right)^2}}{2 \frac{e^{-2K}}{\sinh h}} \\ &= e^K \left(-e^K \sinh h \pm \sqrt{e^{2K} \sinh^2 h + e^{-2K}} \right) . \end{aligned} \quad (6.34)$$

The right hand side of this is equivalent to that of Eq.(6.31), so we can say

$$\frac{b}{a} = \tan \phi = \frac{\sin \phi}{\cos \phi} .$$

Therefore the eigenvectors are

$$\mathbf{x}_i = \begin{pmatrix} \cos \phi \\ \sin \phi \end{pmatrix} . \quad (6.35)$$

This allows an orthogonal matrix \mathbf{P} to be chosen, where

$$\mathbf{P} = \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} . \quad (6.36)$$

Using Eq.(6.14), \mathbf{V} can be replaced in the average thermodynamic value equations by

$$\mathbf{P}^{-1} \mathbf{V} \mathbf{P} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} , \quad (6.37)$$

and similarly for \mathbf{S} ,

$$\mathbf{P}^{-1} \mathbf{S} \mathbf{P} = \begin{pmatrix} \cos 2\phi & -\sin 2\phi \\ -\sin 2\phi & -\cos 2\phi \end{pmatrix} . \quad (6.38)$$

Substituting these back into Eq.(6.29) and Eq.(6.30) and taking the limit $N \rightarrow \infty$ results in

$$\langle S_i S_j \rangle = Z_N^{-1} \text{Trace} \mathbf{P}^{-1} \mathbf{S} \mathbf{P} (\mathbf{P}^{-1} \mathbf{V} \mathbf{P})^{j-i} \mathbf{P}^{-1} \mathbf{S} \mathbf{P} (\mathbf{P}^{-1} \mathbf{V} \mathbf{P})^{N+i-j} ,$$

one finds

$$\langle S_i S_j \rangle = \cos^2 2\phi + \sin^2 2\phi \frac{\lambda_1^N \left(\left(\frac{\lambda_2}{\lambda_1} \right)^{j-i} + \left(\frac{\lambda_2}{\lambda_1} \right)^N \left(\frac{\lambda_1}{\lambda_2} \right)^{j-i} \right)}{\lambda_1^N \left(1 + \left(\frac{\lambda_2}{\lambda_1} \right)^N \right)} .$$

Given that $\lambda_1 > \lambda_2$; when $N \rightarrow \infty$, $\left(\frac{\lambda_2}{\lambda_1} \right)^N \rightarrow 0$. Which reduces to

$$\langle S_i S_j \rangle = \cos^2 2\phi + \sin^2 2\phi \left(\frac{\lambda_2}{\lambda_1} \right)^{j-i} . \quad (6.39)$$

Similar considerations for $\langle S_i \rangle$ yield

$$\langle S_i \rangle = Z_N^{-1} \text{Trace} \mathbf{P}^{-1} \mathbf{S} \mathbf{P} (\mathbf{P}^{-1} \mathbf{V} \mathbf{P})^N ,$$

which gives

$$\langle S_i \rangle = Z_N^{-1} \text{Trace} \begin{pmatrix} \cos 2\phi & -\sin 2\phi \\ -\sin 2\phi & -\cos 2\phi \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}^N ,$$

and leads to

$$\langle S_i \rangle = \cos 2\phi \frac{1 - \left(\frac{\lambda_2}{\lambda_1}\right)^N}{1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N} .$$

As $N \rightarrow \infty$, $\left(\frac{\lambda_2}{\lambda_1}\right)^N \rightarrow 0$, leaving

$$\langle S_i \rangle = \cos 2\phi . \quad (6.40)$$

Recall the equation for correlation length, $G(i, j)$, from Eq.(4.54)

$$G(i, j) = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle \quad (6.41)$$

using Eq.(6.39) and Eq.(6.40) this can clearly be written as

$$G(i, j) = \sin^2 2\phi \left(\frac{\lambda_2}{\lambda_1}\right)^{|j-i|} . \quad (6.42)$$

It has previously be established that $\lambda_1 > \lambda_2$, so $\lambda_2/\lambda_1 \rightarrow 0$ as $(j - i) \rightarrow \infty$. Therefore $G(i, j)$ will exponentially decay to zero as $|j - i|$ becomes large, so must be compatible with the decay of correlation from Eq.(4.56). For this, consider that Eq.(6.42) can be written

$$G(i, j) \sim \left(\frac{\lambda_2}{\lambda_1}\right)^{|j-i|}$$

$$G(i, j) \sim e^{\ln\left(\frac{\lambda_2}{\lambda_1}\right)^{|j-i|}}$$

$$G(i, j) \sim e^{|j-i| \ln\left(\frac{\lambda_2}{\lambda_1}\right)}$$

$$G(i, j) \sim e^{-r \ln\left(\frac{\lambda_1}{\lambda_2}\right)} \sim e^{-r/\xi}$$

so it can be seen that for the case of the 1-D Ising model the correlation length ξ is

$$\xi = [\ln(\lambda_1/\lambda_2)]^{-1} . \quad (6.43)$$

6.3 Critical behaviour near $T=0$

For positive T and real H , $\lambda_1 > \lambda_2 \rightarrow |\lambda_2/\lambda_1| < 1$. But when under zero external field $H = 0$

$$\frac{\lambda_2}{\lambda_1} = \frac{e^K - \sqrt{e^{-2K}}}{e^K + \sqrt{e^{-2K}}}$$

If $T \rightarrow 0$ then from Eq.(6.2) $K = J\beta \rightarrow \infty$. Then

$$\lim_{t \rightarrow 0^+} \left(\frac{\lambda_2}{\lambda_1} \right) = 1 \quad , \quad (6.44)$$

similarly, using Eq.(6.43)

$$\lim_{t \rightarrow 0^+} (\xi) = \lim_{t \rightarrow 0^+} [\ln(\lambda_1/\lambda_2)]^{-1} = \infty \quad (6.45)$$

The critical point of a phase transition model can be defined as the point at which the correlation length ξ becomes infinite, so for this one-dimensional Ising model the critical point must occur at $H = T = 0$

Consider the value of $\sinh h = \frac{1}{2}(e^h - e^{-h})$. For small values of h one may combine the Taylor expansions

$$\begin{aligned} e^x &= 1 + x + \frac{x^2}{2!} + \dots \\ e^{-x} &= 1 - x + \frac{x^2}{2!} - \dots \quad , \end{aligned}$$

such that

$$e^x - e^{-x} = 2x + \mathcal{O}(x^3)$$

therefore

$$\sinh h = h + \mathcal{O}(h^3) \approx h \quad . \quad (6.46)$$

Also, seen as the critical point being investigated occurs at $H = T = 0$ the later two variables need to be replaced by the reduced external field h and

$$t = e^{-2K} \quad (6.47)$$

Application of Eq.(6.46) to Eq.(6.22) yields a new result for the magnetization

$$\begin{aligned} M &= \frac{e^K(h + \dots)}{e^{-K}\sqrt{e^{4K}h + 1 + \dots}} \\ M &= \frac{e^{2K}(h + \dots)}{\sqrt{1 + e^{4K}h + \dots}} \\ M &= e^{2K}h + \mathcal{O}(h^3) \quad , \end{aligned} \quad (6.48)$$

then, by considering

$$t = e^{-2K} = e^{-2J/kT} \approx e^{-2\beta} , \quad (6.49)$$

the magnetization can be written

$$M = t^{-1}h + \mathcal{O}(h^3) .$$

When $h = 0$ this is clearly constant, so through comparison to Eq.(2.3) one determines that the critical exponent

$$\beta = 0 . \quad (6.50)$$

For the critical exponent δ , consider that for small values of x $\sinh(x) \approx x$. Therefore one may write Eq.(6.22) using (6.49) as

$$M \approx \frac{h}{\sqrt{h^2 + t^2}} , \quad (6.51)$$

so when $t = 0$, one notes that

$$M \approx 1 = h^0 . \quad (6.52)$$

Via comparison to Eq.(4.45), one determines that $\frac{1}{\delta} = 0$, therefore the critical exponent

$$\delta = \infty . \quad (6.53)$$

The exponent γ is found by differentiating both sides of Eq.(6.48) to find the isothermal susceptibility (by Eq.(3.28))

$$\chi = e^{2K} + \dots \sim e^{2K}$$

and using Eq.(6.49),

$$\chi \sim t^{-1} .$$

Comparing this result to Eq.(4.49) yields the value of the exponent

$$\gamma = 1 . \quad (6.54)$$

To find the associated exponent for the specific heat, one begins by considering the reduced free energy by taking Eq.(6.21) when $h = 0$

$$\beta f = -\ln(e^\beta + e^{-\beta})$$

$$\beta f = -\ln e^\beta (1 + e^{-2\beta})$$

$$\beta f = -\ln e^\beta - \ln(1 + e^{-2\beta})$$

$$\beta f = -\beta - \ln(1 + t) .$$

The critical behaviour of f is given by the second term

$$f \sim \ln(1 + t) .$$

due to the small values of t being used here one can apply the Taylor expansion for $\ln(1+x)$ and obtain

$$f \sim t + \dots . \quad (6.55)$$

The specific heat of Eq.(4.52) scales as

$$c \sim t^{-\alpha} ,$$

the general integral of this is

$$e \sim \int c dt \sim t^{1-\alpha} ,$$

and by intergrating a second time

$$f \sim \int e dt \sim t^{2-\alpha} . \quad (6.56)$$

Then by equating Eqs.(6.55) and (6.56) one obtains the value of the critical exponent

$$\alpha = 1 . \quad (6.57)$$

Recall the eigenvalues from Eq.(6.20). If $h = 0$ then

$$\lambda_1 = e^K + \sqrt{e^{-2K}} = e^K + e^{-K} ,$$

this can be rearranged using the properties of the hyperbolic function for cosh to

$$\lambda_1 = 2 \cosh K . \quad (6.58)$$

Likewise, for the second eigenvalue,

$$\begin{aligned} \lambda_2 &= e^K - e^{-K} \\ \lambda_2 &= 2 \sinh K . \end{aligned} \quad (6.59)$$

These results can be used to evaluate the correlation length ξ of the model, through Eq.(6.43). First, consider the fraction λ_1/λ_2

$$\frac{\lambda_1}{\lambda_2} = \frac{2 \cosh K}{2 \sinh K} = \coth K$$

then from the properties of the hyperbolic cotangent coth

$$\coth K = \frac{e^{2K} + 1}{e^{2K} - 1} = \frac{e^{2K} + 1}{e^{2K} - 1} \frac{(e^{-2K})}{(e^{-2K})} = \frac{1 + e^{-2K}}{1 - e^{-2K}} ,$$

using the substitution for t from Eq.(6.49), this becomes

$$\frac{\lambda_1}{\lambda_2} = \frac{1+t}{1-t} , \quad (6.60)$$

and inserting into Eq.(6.43) gives

$$\xi = \left(\ln \frac{1+t}{1-t} \right)^{-1} .$$

Consider the logarithm here. The relevant series expansion is

$$\ln \frac{1+t}{1-t} = \ln(1+t) - \ln(1-t) = 2t + \frac{2t^3}{3} + \frac{2t^5}{5} + \dots$$

but when $t \rightarrow 0$, $(1+t)/(1-t) \approx 1$, so the series converges quickly. Therefore the correlation length is

$$\xi \sim (2t)^{-1} . \quad (6.61)$$

The correlation length is expected to be of the form outlined in Eq.(4.60), so the critical exponent ν for this model is

$$\nu = 1 . \quad (6.62)$$

Consider the behaviour of the correlation function at the critical point from Eq.(4.57), displaying a decay by a power law. As established in Eq.(6.44), at the critical point $\lambda_1 = \lambda_2$. This means that the correlation function for this model $G(i, j)$ as derived in Eq.(6.42), must be constant. To satisfy this, the power to which r is taken must be zero. Therefore

$$0 = -d + 2 - \eta = -1 + 2 - \eta ,$$

so for the critical exponent η ,

$$\eta = 1 . \quad (6.63)$$

By inputting these derived values of the exponents into the four scaling relations of Eqs.(5.41), (5.43),(5.48) and(5.55) one finds that all scaling relations are satisfied by the exponents of the one dimensional Ising model.

Looking back at Eq.(6.49), it can be seen that the definition of $t = e^{-2K}$ is not entirely correct. The e^{-2K} could be replaced by $e^{(-2K)N}$ with no effect on the rest of the model. This would merely convert $2 - \alpha$, γ and ν into $N(2 - \alpha)$, $N\gamma$ and $N\nu$ respectively. Therefore the definitions of these critical exponent are not entirely correct, though their relations hold. Overall it can be said that of the critical exponents for this model

$$\begin{aligned} \beta &= 0, \quad \delta = \infty, \quad \eta = 1 \\ \alpha &= 1, \quad \gamma = 1, \quad \nu = 1 . \end{aligned} \quad (6.64)$$

While these exponents are only valid for a zero-temperature phase transition of a one-dimensional Ising model, they present further value in that they can be compared to those gained from other models, and other dimensions.

7 Mean Field Theory

7.1 Introduction to Mean Field Theory

Mean field theory is a “cell” approximation. Cell approximations are those where the behaviour of a few components from one “cell” within the system is used to extrapolate the behaviour of the whole system. The interaction between the “cell” and the rest of the system is approximated.

In mean field theory the interaction terms between all the cells in the system are replaced by one mean average interaction term.

Mean field theory offers the benefit of correctly predicting the qualitative behaviour that occurs between temperature, magnetism and the magnetic field for a ferromagnet undergoing a phase transition. It is also relatively simple to solve when compared to alternative approximation methods. It has been shown to be very accurate for the behaviour of a real system away from the critical temperature where the phase transition occurs.

The downside to mean field theory is that it can become inaccurate close to the critical temperature. This is due to the highly erratic behaviour of the interaction terms around the critical point.

There are multiple methods of solving the mean field model, of varying complexity. Two such methods are detailed in this section - Weiss and Bragg-Williams mean field theory.

7.2 Weiss Mean Field Theory

Consider the equation for the partition function from Eq.(3.12). by noting the common factor of $\sum_i S_i$ the partition function can be written

$$Z = \sum_{\{S_i\}} e^{\sum_i S_i (K \sum_j S_j + h)} . \quad (7.1)$$

In mean field theory one is not concerned with the interactions between spins but with an effective field representing the interactions between a spin and all other spins. Therefore the effective field h_m replaces everything within the bracket of the above equation in order to create independence of spins. So the partition function from Eq.(7.1) is now

$$Z = \sum_{\{S_i\}} e^{h_m \sum_i S_i} , \quad (7.2)$$

which can be expanded to

$$Z = \sum_{\{S_i\}} e^{h_m (S_1 + S_2 + \dots)}$$

$$Z = \sum_{\{S_i\}} e^{h_m S_1} e^{h_m S_2} e^{h_m S_3} \dots .$$

Therefore the partition function can be expressed as a product over all sites

$$Z = (e^{h_m(+1)} + e^{h_m(-1)})(e^{h_m(+1)} + e^{h_m(-1)}) \dots (e^{h_m} + e^{-h_m})$$

each site has the identical energy $(e^{h_m} + e^{-h_m})$, giving

$$Z = \prod_{i=1}^N (e^{h_m} + e^{-h_m}) \quad (7.3)$$

so through use of the hyperbolic function for cosh, the partition function for Weiss mean field theory is

$$Z = \prod_{i=1}^N (2 \cosh h_m) = (2 \cosh h_m)^N . \quad (7.4)$$

Consider that the free energy per site of this system by Eq.(3.14) is

$$f = -\frac{1}{\beta} \ln(2 \cosh h_m) , \quad (7.5)$$

then by using Eq.(3.16) the magnetization per site is

$$m = \frac{-\beta}{-\beta} \frac{\partial}{\partial h} \ln(2 \cosh h_m)$$

and by using the chain rule for differentiation

$$m = \frac{2 \sinh h_m}{2 \cosh h_m} .$$

This simplifies to the Weiss mean field equation for magnetization per site

$$m = \tanh(h_m) , \quad (7.6)$$

so for the magnetization of a configuration one has

$$M = N \tanh(h_m) . \quad (7.7)$$

The mean field is assumed to be proportional to the magnetization, so the total reduced field acting on a spin will be the sum of the reduced external field h and a reduced product of M and some unknown constant, λ

$$h_m = \lambda \beta M + h . \quad (7.8)$$

This means that Eq.(7.7) becomes

$$M = N \tanh(h + \lambda \beta M) . \quad (7.9)$$

Consider that in the absence of an external field $h = 0$, so Eq.(7.9) will take the form

$$M = N \tanh(\lambda\beta M) \quad (7.10)$$

There are non-zero solutions for this when operating under the zero external field that can be found by plotting both sides of the equation against each other. The critical point occurs when the plots meet as shown by Fig.11

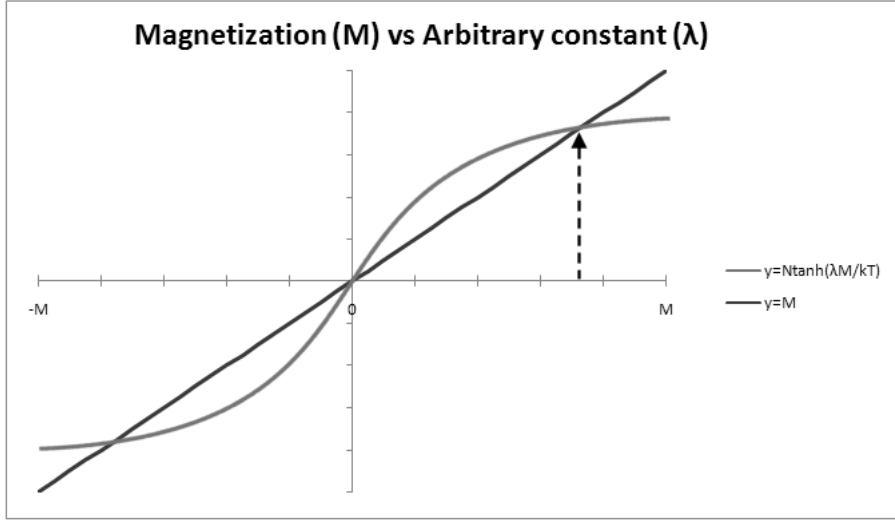


Figure 11: Graphical solution to Eq.(7.10)

When operating close to the critical point, $\lambda\beta_c M$ will be small. This allows the Maclaurin series expansion for \tanh to be used

$$\tanh x = x - \frac{1}{3}x^3 + \dots \quad (7.11)$$

This series will converge quickly so that all but the first term can be ignored, giving the temperature at the critical point

$$M = N\lambda\beta_c M$$

$$T_c = \frac{N\lambda}{k} \quad (7.12)$$

Recall the magnetization per site, m , from eq.(7.6). Through use of Eqs.(7.8) and (7.12) observe that it can be written

$$m = \tanh(h + mx) \quad (7.13)$$

where

$$x = \frac{T_c}{T} \quad (7.14)$$

By using one of the properties of \tanh ,

$$\tanh(a+b) = \frac{\tanh(a) + \tanh(b)}{1 + \tanh(a)\tanh(b)}$$

Eq.(7.13) can be written

$$m = \frac{\tanh h + \tanh mx}{1 + \tanh h \tanh mx} ,$$

which can be rearranged to

$$\tanh h = \frac{m - \tanh mx}{1 - m \tanh mx} . \quad (7.15)$$

Both m and h are small around the critical point, so the Maclaurin series expansion for \tanh from Eq.(7.11) can be used resulting in

$$\begin{aligned} h &= (m - \tanh mx)(1 + m \tanh mx) \times \dots \\ &= m - \tanh mx + m^2 \tanh mx - m \tanh^2 mx + \dots \\ h &= m(1 - x) + m^3(x - x^2 + \frac{1}{3}x^3) + \dots . \end{aligned} \quad (7.16)$$

In the zero magnetic field this becomes

$$0 = m(1 - x) + m^3(x - x^2 + \frac{1}{3}x^3)$$

so that

$$m^2 = \frac{1(1-x)}{(x - x^2 + \frac{1}{3}x^3)} = 3 \left(\frac{T_c - T}{T} \right) = 3(-t) .$$

Rearranging this to make m the subject gives

$$m = \sqrt{3(-t)} = \sqrt{3}(-t)^{\frac{1}{2}} , \quad (7.17)$$

then via comparison to Eq.(2.3) one can deduce the value of the critical exponent β

$$\beta = \frac{1}{2} . \quad (7.18)$$

As $T \rightarrow T_c$, $x \rightarrow 1$. Substituting this into Eq.(7.16) gives

$$h = m(0) + m^3(1 - 1 + \frac{1}{3}) ,$$

therefore

$$H \sim m^3$$

or

$$m \sim H^{\frac{1}{3}} . \quad (7.19)$$

Through comparison of this result with the exponent relation for δ from Eq.(4.45), one notes that the critical exponent

$$\delta = 3 \quad (7.20)$$

for the Weiss mean field model.

To find the exponent γ , differentiate both sides of Eq.(7.16) with respect to H where $T = \text{constant}$ (therefore β is also constant)

$$\begin{aligned} \left(\frac{\partial}{\partial H}\right)_T (h) &= \left(\frac{\partial}{\partial H}\right)_T (m(1-x)) + \left(\frac{\partial}{\partial H}\right)_T \left(m^3(x-x^2 + \frac{1}{3}x^3)\right) \\ \beta &= \left(\frac{\partial m}{\partial H}\right)_T (1-x) + 3m^2 \left(x-x^2 + \frac{1}{3}x^3\right) + m^3 \left(\frac{\partial}{\partial H}\right)_T \left(x-x^2 + \frac{1}{3}x^3\right) . \end{aligned} \quad (7.21)$$

When $T > T_c$, the magnetization per site m is zero. Then Eq.(7.21) becomes

$$\left(\frac{\partial m}{\partial H}\right)_{T \rightarrow T_c^+} = \beta(1-x)^{-1} \sim (T - T_c)^{-1} . \quad (7.22)$$

Comparing the equation for isothermal susceptibility χ for $T \rightarrow T_c^+$ from Eq.(4.47) to the derived result reveals that the critical exponent

$$\gamma = 1 . \quad (7.23)$$

One may obtain the values of the critical exponents α_+ and α_- via differentiation of the free energy per site. Consider first that without an external field $h = 0$ and by Eq.(7.8) $h_m = \lambda\beta M$. By definition of a temperature-driven ferromagnetic phase transition when $T > T_c$, $M = 0$. Therefore Eq.(7.5) becomes

$$f = \ln(2 \cosh 0) = \ln 2$$

therefore by Eq.(3.42),

$$\frac{\partial^2 f}{\partial T^2} = c = 0$$

Via comparison to Eq.(4.52), one determines that the critical exponent

$$\alpha_+ = 0 . \quad (7.24)$$

When approaching the critical point from below, $T < T_c$, the free energy per site is

$$f = \ln(2 \cosh \lambda\beta M) ,$$

and by using the substitution from Eq.(7.18) one may write

$$f \sim \ln(\cosh t^{\frac{1}{2}}) .$$

It follows that the derivative of this with respect to T is

$$e = \frac{\partial f}{\partial t} = \frac{1}{\cosh t^{\frac{1}{2}}} \sinh t^{\frac{1}{2}} \frac{1}{2} t^{-\frac{1}{2}}$$

$$e = \frac{1}{2} \left(\tanh t^{\frac{1}{2}} \right) \frac{1}{2} t^{-\frac{1}{2}}$$

And by the expansion for \tanh from Eq.(7.11),

$$e = \frac{1}{2} t^{\frac{1}{2}} \frac{1}{2} t^{-\frac{1}{2}} = \frac{1}{2}$$

therefore the specific heat is of the form

$$c = \frac{\partial e}{\partial t} = \text{constant}$$

and the exponent α_- must be

$$\alpha_- = \alpha_+ = 0 . \quad (7.25)$$

Thus, the values of all critical exponents for Weiss mean field theory have been derived. An alternative method of mean field theory will now be consider to allow for comparison of results.

7.3 Bragg-Williams Mean Field Theory

Consider the energy of the system from Eq.(3.10). Under the conditions of Bragg-Williams mean field theory this is altered to

$$E(S) = -\frac{qJ}{N-1} \sum_{(i,j)} S_i S_j - H \sum_{i=1}^N S_i . \quad (7.26)$$

Where q represents the number of neighbours of each spin. The first sum in Eq.(7.26) refers to all the distinct pairs (i, j) within the system, of which there are $\frac{1}{2}N(N-1)$.

Consider also the equation for the magnetization of any configuration of spins from Eq.(3.6). By squaring this one obtains

$$\begin{aligned} M^2 &= (S_1 + S_2 + \dots + S_N)(S_1 + S_2 + \dots + S_N) \\ &= S_1^2 + S_1 S_2 + S_1 S_3 + \dots \\ &\quad + S_2 S_1 + S_2^2 + S_2 S_3 + \dots \\ &\quad \vdots \\ &= S_1^2 + S_2^2 + \dots + S_N^2 + 2(S_1 S_2 + S_1 S_3 + \dots + S_{N-1} S_N) \end{aligned}$$

$$\begin{aligned}
&= \sum_i^N S_i^2 + 2 \sum_{i,j} S_i S_j \\
&= \sum_i^N S_i^2 + \left(M^2 - \sum_i^N S_i^2 \right) \\
&= \sum_i^N S_i^2 + M^2 - \sum_i^N 1 \\
M^2 - N &= 2 \sum_{i,j} S_i S_j \quad . \tag{7.27}
\end{aligned}$$

This can be used to eliminate the sums over spins from Eq.(7.26) to

$$E(S) = \frac{-qJ(M^2 - N)}{2(N - 1)} - HM \quad . \tag{7.28}$$

Therefore the only relation between the energy of Bragg-Williams mean field to S_1, S_2, \dots, S_N is through the total magnetization for a spin combination, M . Inserting the energy from Eq.(7.28) into the partition function of Eq.(3.12) gives the partition function of the Bragg-Williams mean field:

$$Z = \sum_{\{S_i\}} e^{\frac{\beta q J (M^2 - N)}{2(N-1)}} + hM \quad . \tag{7.29}$$

By the definition of the Ising model, all spins within this system must point either up or down with values ± 1 . If r spins face down (-1) and $N - r$ spins face up (+1), then by Eq.(3.6)

$$M = N - 2r \tag{7.30}$$

with cNr possible combinations of spins. Applying Eq.(7.30) to Eq.(7.29) gives the equation for the partition function as

$$Z = \sum_{r=0}^N \frac{N!}{r!(N-r)!} e^{\left(\frac{\beta q J (N-2r)^2 - N}{2(N-1)} + h(N-2r) \right)} = \sum_{r=0}^N c_r \quad , \tag{7.31}$$

where c_r is used henceforth to represent everything within the sum $\sum_{r=0}^N$.

Consider that by Eq.(3.30)-(3.31) and Eq.(7.30), the average magnetization per site for Bragg-Williams MFT is

$$m = \frac{\langle M \rangle}{N} = \left\langle \frac{N - 2r}{N} \right\rangle = \left\langle 1 - \frac{2r}{N} \right\rangle = Z^{-1} \sum_{r=0}^N (1 - 2r/N) c_r \quad . \tag{7.32}$$

If d_r is defined such that $c_{r+1} = d_r c_r$, then

$$d_r = \frac{c_{r+1}}{c_r} = \frac{N - r}{r + 1} e^{-2\beta q J \frac{N-2r-1}{N-1} - 2h} \quad . \tag{7.33}$$

As discussed in section 1, for realistic systems N will be a massive number (of an order of at least 10^{24}) representing the number of particles in the system. Therefore the quantity of particles is effectively infinite, $N \rightarrow \infty$. Consider the effect this has on Eq.(7.33) as r increases from $r = 0$ to $r = N - 1$

$$\begin{aligned} d_0 &= \frac{N}{1} e^{-2\beta q J - 2h} \\ &\vdots \\ d_{N-1} &= \frac{1}{N} e^{2\beta q J - 2h} . \end{aligned}$$

As $r \rightarrow N - 1$, d_r decreases monotonically from very large values to very small ones (provided $\beta q J$ is not too large). During this decrease there must exist a value of r such that $d_r = 1$. This value of r is denoted r_0

$$d_{r_0} = 1 . \quad (7.34)$$

Recalling that $c_{r+1} = d_r c_r$, it can be seen that for $d_r > 1$, $c_{r+1} > c_r$. Similarly, when $d_r < 1$, $c_{r+1} < c_r$. Therefore c_{r_0} must be the largest possible value for c_r . By dividing Eq.(7.33) by N it can be rewritten

$$d_r = \frac{c_{r+1}}{c_r} = \frac{1 - \frac{r}{N}}{\frac{r}{N} + \frac{1}{N}} e^{-2\beta q J \frac{1 - \frac{2r}{N} - \frac{1}{N}}{1 - \frac{1}{N}} - 2h} .$$

Consider also that as $N \rightarrow \infty$, $\frac{1}{N} \rightarrow 0$. So for large N

$$d_r = \frac{1 - \frac{r}{N}}{\frac{r}{N}} e^{-2\beta q J (1 - \frac{2r}{N}) - 2h} .$$

Let $x = 1 - \frac{2r}{N}$. Then

$$\frac{2r}{N} = 1 - x \rightarrow \frac{r}{N} = \frac{1 - x}{2}$$

and

$$d_r = \frac{1 + x}{1 - x} e^{-2\beta q J x - 2h}$$

if we define the right hand side of the above equation by $\phi(x)$, then

$$d_r = \phi\left(1 - \frac{2r}{N}\right) = \phi(x) = \frac{1 + x}{1 - x} e^{-2\beta q J x - 2h} \quad (7.35)$$

where $d_{r_0} = 1 = \phi(x_0)$ i.e. x_0 is the solution to $\phi(x) = 1$. For large N , r_0 can be found through

$$1 - 2r_0/N = x_0 . \quad (7.36)$$

Given that c_{r_0} is the largest c_r , an assumption can be made that c_{r_0} dominates over all the other c_r , to the extent that the other c_r have a negligible effect. Thus, these c_r can be replaced by c_{r_0} in the sums of c_r in Eq.(7.31) and Eq.(7.32). Therefore

$$Z = c_{r_0}$$

and

$$m = 1 - \frac{2r_0}{N} = x_0 \quad . \quad (7.37)$$

Using Eq.(7.35), $\phi(x_0) = 1$. Therefore $\phi(m) = 1$. So m is given by

$$1 = \frac{1+m}{1-m} e^{-2\beta Jm-2h} \quad .$$

which can be rearranged using to make m the subject

$$\begin{aligned} (1-m) &= (1+m)e^{-2\beta Jm-2h} \\ (1-m) &= e^{-2\beta Jm-2h} + me^{-2\beta Jm-2h} \\ (1 - e^{-2\beta Jm-2h}) &= m + me^{-2\beta Jm-2h} = m(1 + e^{-2\beta Jm-2h}) \\ m &= \frac{1 - e^{-2\beta Jm-2h}}{1 + e^{-2\beta Jm-2h}} \end{aligned}$$

observe that this can be converted into a format equivalent to the hyperbolic function for tanh

$$\begin{aligned} m &= \frac{1 - e^{-2\beta Jm-2h} e^{-\beta qJm-h}}{1 + e^{-2\beta Jm-2h} e^{-\beta qJm-h}} \\ m &= \frac{e^{-\beta qJm-h} - e^{\beta qJm+h}}{e^{-\beta qJm-h} + e^{\beta qJm+h}} \\ m &= \tanh(\beta qJm + h) \quad . \end{aligned} \quad (7.38)$$

This is the equation for the magnetization that Bragg and Williams derived in 1934. From here the free energy could be found via intergration, but an easier method is to consider that for large values of N , the sum from Eq.(7.31) is dominated by values of r close to r_0 to the extent that it can be stated that $Z = c_{r_0}$. Therefore the free energy per site of the system from Eq.(3.14) becomes

$$\frac{-f}{kT} = \lim_{N \rightarrow \infty} \frac{1}{N} \ln c_{r_0} \quad . \quad (7.39)$$

Stirling's approximation for large factorials is

$$n! \sim \sqrt{2\pi n} \left(\frac{n}{e}\right)^n \quad (7.40)$$

Using this, combined with Eqs.(7.31) and (7.37) allows the free energy to be given as

$$\frac{-f}{kT} = \frac{1}{2} \ln \left(\frac{4}{1-M^2} \right) - \frac{qJM^2}{2kT} \quad (7.41)$$

Here the free energy is expressed as a function of the magnetization and the temperature of the system.

7.3.1 Phase Transition

Rearrange Eq.(7.38) to make h the subject

$$\begin{aligned}
 m &= \tanh(\beta q J m + h) \\
 \operatorname{artanh} m &= \beta q J m + h \\
 h &= \operatorname{artanh}(m) - \beta q J m \quad , \tag{7.42}
 \end{aligned}$$

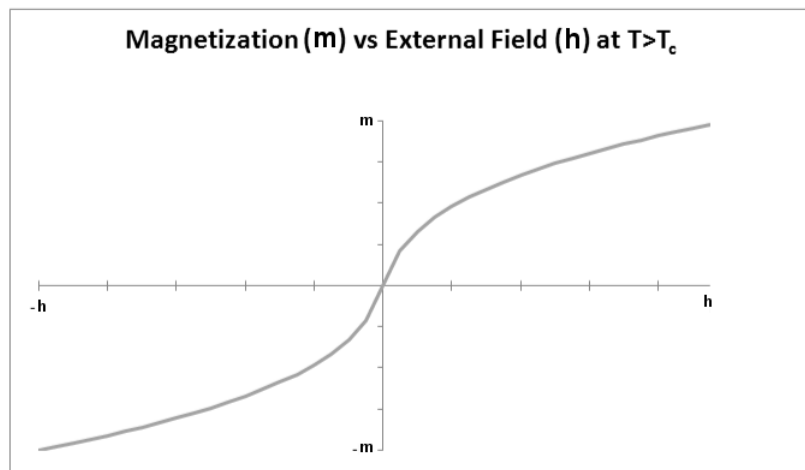


Figure 12: A typical high-temperature graph

Eq.(7.42) can be used to plot h as a function of m over the magnetic range $-1 < m < 1$. Likewise, it can be reversed to plot m as a function of h . If $\beta q J < 1$, this graph Fig(12) of m against h resembles that for one without a phase transition, $T > T_c$. This displays typical analytic behaviour, with no spontaneous magnetization present.

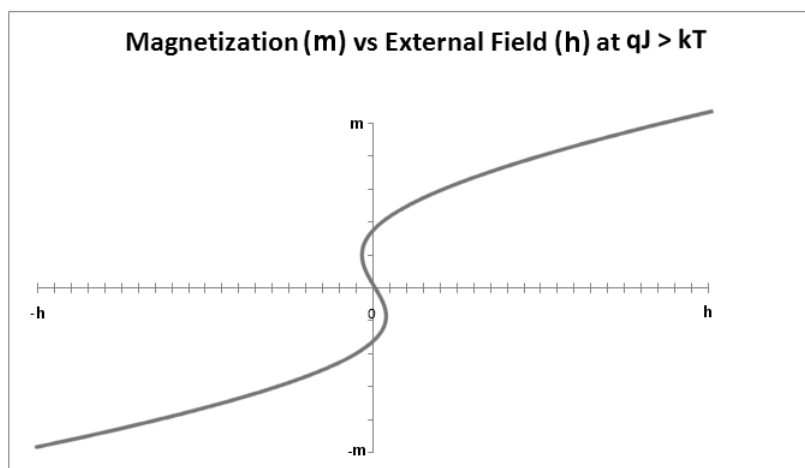


Figure 13: m as a function of h when $\beta q J > 1$

If $\beta qJ > 1$, the graph resembles Fig(13). This graph is contradictory to information already gathered on the subject, as it displays three values of m for $h \approx 0$ whereas the function should be analytic for all values of h .

The multi-valued result occurs because if $\beta qJ > 1$, the RHS of Eq.(7.33) is not a monotonic decreasing function of r but instead provides three values of r when $d_r \approx 1$ Fig(14).

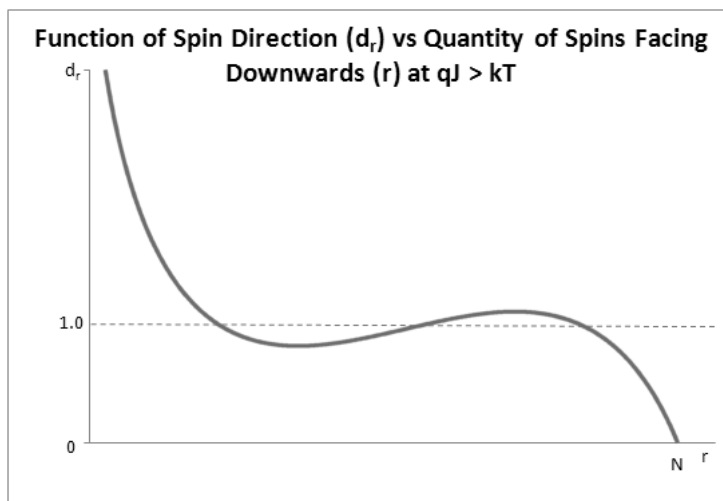


Figure 14: d_r as a function of r when $\beta qJ > 1$

If $d_r = 1$ has three solutions, then c_r contains three turning points - two maxima and a minimum in between the two Fig(15)

These turning points correspond to the solutions to m for Eq.(7.38). For $h > 0$ the left maximum value is higher, and if $h < 0$ the right maximum is higher.

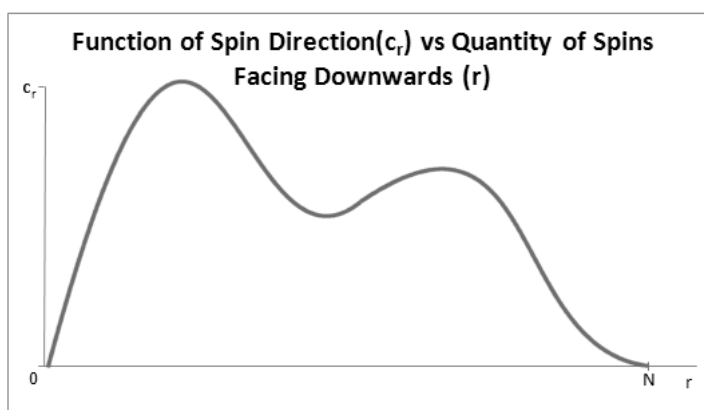


Figure 15: c_r as a function of r when $\beta qJ > 1$

The assumptions of Bragg-Williams mean field theory are maintained, so the sum in Eq.(7.31) is still dominated by values of r around r_0 , and r_0 is the value of r that maximizes

c_r . So if Eq.(7.38) gives three solutions for m and $h > 0$ then choose the solution where r_0 is the smallest (therefore m is largest). If $h < 0$ choose the solution where r_0 is the largest (therefore choosing the smallest solution for m). This effectively turns Fig(13) into Fig(16) whereby the multi-valued graph has been converted into a single-valued one.

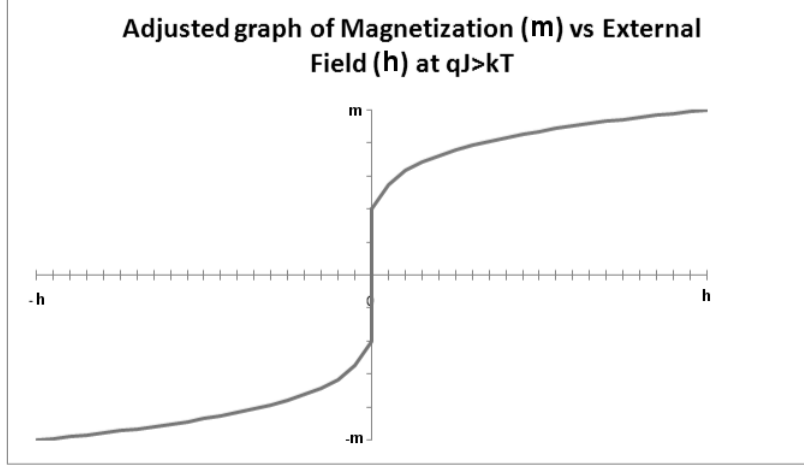


Figure 16: Graph of m against h at $\beta qJ > 1$ where spurious solutions have been eliminated

Note that this graph resembles the graph of m against h for $T < T_c$. in particular it has m_0 values (two values of m when $h = 0$) known as the spontaneous magnetization, given by

$$m_0 = \tanh(\beta qJ m_0) , \quad m_0 > 0 \quad (7.43)$$

provided that $\beta qJ > 1$. So the mean field model has a ferromagnetic phase transition for $T < T_c$, where T_c is the Curie temperature

$$T_c = \frac{qJ}{k} . \quad (7.44)$$

7.3.2 Zero Field Properties And Critical Exponents

Using $t = (T - T_c)/T_c$ and Eq.(7.44), the equation for spontaneous magnetization Eq.(7.43) can be rearranged

$$\begin{aligned} \operatorname{artanh}(m_0) &= \beta qJ m_0 \\ \operatorname{artanh}(m_0) &= \frac{T_c m_0}{T} \\ m_0 &= (1 + t) \operatorname{artanh}(m_0) . \end{aligned} \quad (7.45)$$

For $T > T_c$, m_0 is small but non-zero. Thus the $\operatorname{artanh}(m_0)$ part in Eq.(7.45) becomes $m_0 + m_0^3/3$. solving this for m_0 gives

$$m_0 = \sqrt{-3t}(1 + \mathcal{O}(t)) , \quad (7.46)$$

where $\mathcal{O}(t)$ is the order of (t) . It turns out that the order of t in fact has a minimal effect on the model to the extent where it can be ignored, leaving $m_0 \propto -t^{\frac{1}{2}}$. Comparison of this result to Eq.(2.3) allows one to determine the value of the critical exponent β for this model,

$$\beta = \frac{1}{2} . \quad (7.47)$$

To find the values of exponents α_{\pm} , consider that if $h \rightarrow 0$ for $T > T_c$, then $m \rightarrow 0$. Inserting these values onto Eq.(7.41) allows the free energy for the system to be simplified to

$$\frac{-f}{kT} = \ln 2 , \quad (7.48)$$

whereas if $T < T_c$ then $m \rightarrow m_0$. For small values of m_0 Eq.(7.41) becomes

$$\begin{aligned} \frac{-f}{kT} &= \frac{1}{2} \ln \left(\frac{4}{1 - m_0^2} \right) - \frac{qJm_0^2}{2kT} \\ \frac{-f}{kT} &= \frac{1}{2} \ln 4 - \frac{1}{2} \ln(1 - m_0^2) - \frac{qJm_0^2}{2kT} . \end{aligned} \quad (7.49)$$

Using the Taylor expansion for small x ,

$$\ln(1 + x) = \ln 1 + x + \frac{x^2}{2} + \dots = x + \frac{x^2}{2} + \mathcal{O}x^3 ,$$

the second logarithm can be changed to

$$\ln(1 - m_0^2) = m_0^2 - \frac{m_0^4}{2} + \mathcal{O}m_0^6 .$$

Inserting this into Eq.(7.49) yields

$$\frac{-f}{kT} = \ln 2 - \frac{1}{2} \left(m_0^2 - \frac{m_0^4}{2} + \mathcal{O}m_0^6 \right) - \frac{qJm_0^2}{2kT} ,$$

which can be rearranged to

$$\frac{-f}{kT} = \ln 2 - \frac{1}{2} m_0^2 \left(1 - \frac{qJ}{kT} \right) + \frac{m_0^4}{4} + \mathcal{O}(m_0^6) . \quad (7.50)$$

Consider the Taylor expansion of $(1 + x)^n$ for small x is

$$(1 + x)^n = 1 + nx + \frac{n(n-1)}{2!} x^2 + \dots = 1 + \mathcal{O}x ,$$

using this one notes that squaring Eq.(7.46) results in

$$m_0^2 = -3t(1 + \mathcal{O}(t))^2$$

$$m_0^2 = -3t(1 + \mathcal{O}(t)) ,$$

and

$$\mathcal{O}(M_0^2) = \mathcal{O}(t) .$$

By utilizing these results along with Eq.(7.44) and Eq.(7.46) for small t , Eq.(7.50) can be written

$$\frac{-f}{kT} = \ln 2 - \frac{1}{2}(-3t(1 + \mathcal{O}(t))) \left(1 - \frac{T_c}{T}\right) + \frac{9t^2(1 + \mathcal{O}(t))}{4} + \mathcal{O}(t^3) . \quad (7.51)$$

Consider that

$$t = \frac{T - T_c}{T_c} \rightarrow T_c t = T - T_c \rightarrow T = T_c(t + 1) , \quad (7.52)$$

then

$$1 - \frac{T_c}{T} = 1 - \frac{T_c}{T_c(t + 1)} = 1 - \frac{1}{t + 1} .$$

For small values of t the Maclaurin series expansion can be used

$$f(x) = f(0) + x f'(0) + \frac{x^2}{2!} f''(0) + \dots ,$$

application of the expansion here yields

$$\begin{aligned} f(x) &= (1 + x)^{-1} \rightarrow f'(x) = -(1 + x)^{-2} \rightarrow f''(x) = 2(1 + x)^{-3} \dots \\ f(x) &= 1 - x + x^2 - \dots , \end{aligned}$$

therefore

$$1 - \frac{1}{t + 1} = 1 - (1 - t + t^2 + \dots) = t - t^2 + \dots .$$

Then by applying this to the free energy from Eq.(7.51),

$$\begin{aligned} \frac{-f}{kT} &= \ln 2 - \frac{-3t}{2} t(1 - t)(1 + \mathcal{O}(t)) + \frac{9t^2(1 + \mathcal{O}(t))}{4} + \mathcal{O}(t^3) \\ \frac{-f}{kT} &= \ln 2 - \frac{-3}{2} t^2(1 + \mathcal{O}(t)) + \frac{9}{4} t^2(1 + \mathcal{O}(t)) + \mathcal{O}(t^3) \\ \frac{-f}{kT} &= \ln 2 + \frac{3t^2}{4} + \mathcal{O}(t^3) . \end{aligned} \quad (7.53)$$

The specific heat per site of the system is defined as the second derivative of the free energy with respect to temperature. Considering the critical exponents α_+ and α_- defined by Eq.(4.52), there must be a discontinuity present for the specific heat at the critical point, so these α_+ , α_- can be discarded. Alternatively, consider the free energy around the singularity at the critical point to be

$$f_s(t, 0) = f_+(t, 0) - f_-(t, 0)$$

which has the relation

$$f_s(t, 0) \sim t^{2-\alpha} , \quad \alpha = \alpha_{\pm} ,$$

applying this to the free energies evaluated when approaching the critical point from above and below by Eq.(7.48) and (7.53),

$$f_s(t, 0) = \ln 2 - \left(\ln 2 + \frac{3t^2}{4} + \mathcal{O}t \right)$$

$$f_s(t, 0) = -\frac{3t^2}{4} .$$

So we can say that the critical exponent

$$\alpha = \alpha_{\pm} = 0 . \tag{7.54}$$

Now consider the magnetic susceptibility of the system, defined by Eq.(3.28). The susceptibility for the Bragg-Williams mean field model can be found by differentiating both sides of Eq.(7.42) with respect to H .

$$\frac{\partial}{\partial H} H = \frac{\partial}{\partial H} (kT \operatorname{artanh}(m) - qJm)$$

$$1 = kT \frac{1}{1-m^2} \underbrace{\frac{\partial m}{\partial H}}_{\chi} - qJ \underbrace{\frac{\partial m}{\partial H}}_{\chi} ,$$

then by using Eqs.(2.2) and (7.44), one obtains $T = \frac{qJ}{k}(t+1)$, so

$$1 = \frac{qJ\chi(t+1)}{1-m^2} - qJ\chi$$

$$1 = \chi qJ \left(\frac{t+1}{1-m^2} - 1 \right)$$

$$\chi = \frac{1}{\frac{qJ(t+m^2)}{1-m^2}}$$

$$\chi = \frac{1-m^2}{qJ(t+m^2)} \tag{7.55}$$

Let $H \rightarrow 0$. If $T > T_c$ then $m \rightarrow 0$. This means the susceptibility is

$$\chi = \frac{1}{qJt} \quad T > T_c . \tag{7.56}$$

If $T < T_c$ then $m \rightarrow m_0$. The susceptibility is then

$$\begin{aligned}\chi &= \frac{1 - m_0^2}{qJ(t + m_0^2)} \\ \chi &= \frac{1 + 3t + \mathcal{O}(t^2)}{qJt(-2 + \mathcal{O}(t))} \\ \chi &= \frac{1 + \mathcal{O}(t)}{-2qJt} \times \frac{1}{(1 + \mathcal{O}(t))} .\end{aligned}$$

By using the Taylor expansion of $(1 + x)^n$ for small x

$$\frac{1}{1 + x} = 1 - x + \dots = 1 - \mathcal{O}x ,$$

the susceptibility becomes

$$\begin{aligned}\chi &= \frac{(1 + \mathcal{O}(t))(1 - \mathcal{O}(t))}{-2qJt} \\ \chi &\cong \frac{1}{-2qJt} \quad T < T_c .\end{aligned}\tag{7.57}$$

Observe the critical exponent equation concerning the susceptibility χ from Eq.(4.48) and (4.49). By comparing these to Eq.(7.56) and Eq.(7.57) one can see that for this model the critical exponents

$$\gamma_+ = \gamma_- = \gamma = 1 .\tag{7.58}$$

Referring back to Eq.(7.42), via Eq.(7.52) and Eq.(7.44), at the critical point the external field can be rewritten such that

$$\begin{aligned}h &= \text{artanh}(m) - \beta k T_c m , \\ h &= \text{artanh}(m) - m\end{aligned}\tag{7.59}$$

Using the Taylor expansion for $\text{artanh}(x)$

$$\text{artanh}(x) = x + \frac{x^3}{3} + \frac{x^5}{5} + \dots ,$$

the equation of state when m is small (around the critical point) is then

$$h = \left(m + \frac{m^3}{3} + \dots \right) - m$$

the negligible effect of the higher terms means that they can be ignored, leaving

$$h \approx \frac{1}{3}m^3 ,\tag{7.60}$$

Via comparison of this to the original equation for the exponent delta from Eq.(4.45), it is clear that the value of δ in Bragg-Williams mean field theory is

$$\delta = 3 . \tag{7.61}$$

Thus, all critical exponents for Bragg-Williams mean field theory have been evaluated. These exponents values are in fact the same as those derived from Weiss mean field theory, so although different methods were used the same conclusion has been reached. Mean field theory has yielded the set of exponents:

$$\begin{aligned} \beta &= \frac{1}{2}, \quad \delta = 3, \\ \alpha &= 0, \quad \gamma = 1, \end{aligned} \tag{7.62}$$

with η and ν unable to be evaluated.

8 Fisher Renormalization

When the values of the critical exponents of real, constrained systems are experimentally measured, it can be found that they will deviate significantly from the values offered by the ideal models of said system (such as the Ising model) due to the effects of the constraints on the real system.

For example, the specific heat of an ideal system will display a power-law divergence, but experimental measurements of the real system show it to instead reach a finite cusp.

Trinidad-born physicist Michael Ellis Fisher (1931-) proposed that this difference in values was a result of hidden variables, and found exponent relations that link the ideal and constrained systems.

Fisher's renormalization of critical exponents has been shown to produce more accurate results than their unnormalized counterparts.

8.1 The Renormalization Process

The free energy of the ideal system is typically denoted as $f(t, h)$ where the reduced temperature t is given by Eq.(2.2) and the reduced external field is h is given by Eq.(3.11). The Fisher renormalization process requires certain assumptions on the relationship between the real and ideal systems to be made. First, it is assumed that the free energy of the real constrained system f_x can be written in terms of the free energy of the ideal system f such that

$$f_x(t, h, u) = f(t^*, h^*) \quad (8.1)$$

where t^* and h^* are analytic functions, defined as

$$t^* = t^*(t, h, u) \quad (8.2)$$

$$h^* = h^*(t, h, u) \quad (8.3)$$

An assumption must also be made to prevent hidden degrees of freedom from biasing non-zero values of h at the critical point

$$h^* = h^*(t, h, u) = h\mathcal{J}(t, h, u) \quad (8.4)$$

where \mathcal{J} is an analytic function of (t, h, u) . By using this assumption, if $h_c = 0$ then $h_c^* = 0$. So the critical magnetic field in both the constrained and ideal systems equates to zero.

Recall the definition of the critical reduced temperature for the constrained system from Eq.(2.2). Clearly, a counterpart must exist for the ideal system

$$t^* = \frac{T^* - T_c^*}{T_c^*} . \quad (8.5)$$

We wish to allow for the real system to be critical at $t^* = 0$ ($T^* = T_c^*$) and the ideal system to be critical at $t = 0$ ($T = T_c$). However, the critical points of the two systems are not identical

$$T_c \neq T_c^* .$$

Consider that the magnetization of the ideal system is defined by Eq.(3.43), the discontinuity found for m when $h = 0$, $t \leq 0$ in the ideal system is

$$\Delta m(t) = \lim_{h \rightarrow 0} (m(t, h) - m(t, -h)) . \quad (8.6)$$

The discontinuity Δm visualized in Fig.17 vanishes at $t = 0$, so it can be seen as a defining quality of the ideal system's critical point.

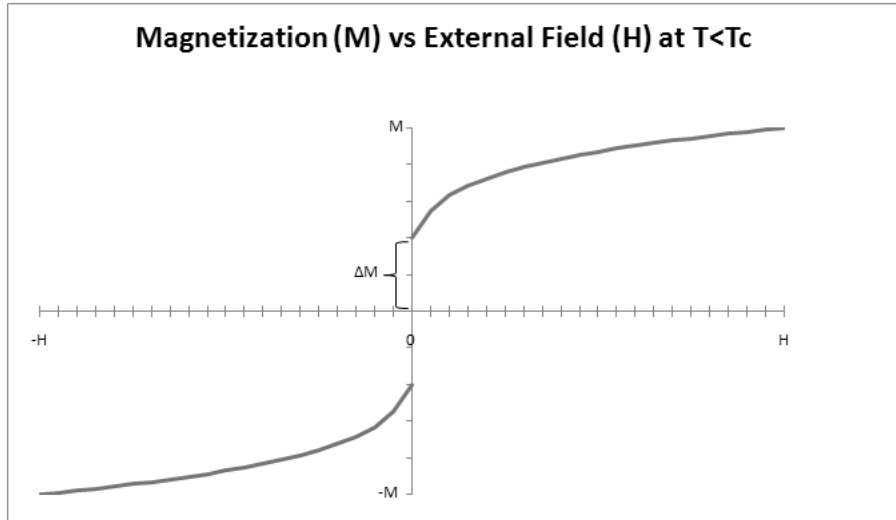


Figure 17: Graphical representation of Δm

Now consider the magnetization of the real system. By Eq.(8.1) the discontinuity in the magnetization of the real system can be stated

$$\Delta m_x(t, 0, u) = \frac{\partial f_x}{\partial h} = \frac{\partial f}{\partial h^*} \frac{\partial h^*}{\partial h} + \frac{\partial f}{\partial t^*} \frac{\partial t^*}{\partial h} \quad (8.7)$$

$$= \lim_{h^* \rightarrow 0} [m(t^*, h^*) - m(t^*, -h^*)] \mathcal{J}(t, 0, u) \quad (8.8)$$

$$\Delta m^*(t^*, 0) = \Delta m(t^*, 0) \mathcal{J}(t, 0, u) , \quad (8.9)$$

one assumes that $\mathcal{J} \neq 0$, so that the critical point of the real constrained system must be given by the value of t that makes $t^*(t, 0, u) = 0$

$$m_x(t, h, u) = e(t^*, h^*) \frac{\partial t^*}{\partial h} + m(t^*, h^*) \left(\mathcal{J}(t, h, u) + h \frac{\partial \mathcal{J}}{\partial h}(t, h, u) \right)$$

$$\Delta m_x(t, 0, u) = \Delta m(t^*, 0) \mathcal{J}(t, 0, u)$$

$$t^*(t, 0, u) = 0 .$$

A further assumption is made with regards to the free energy of the ideal system. Assume that when $h = 0$ and for small values of t the ideal free energy behaves as a Taylor expansion

$$f(t, 0) = a_{\pm} |t|^{2-\alpha} + \dots , \quad (8.10)$$

therefore by Eq.(3.41) the internal energy of the system must be the derivative of Eq.(8.10) with respect to t

$$e(t, 0) = \frac{\partial f}{\partial t} = \frac{\partial f}{\partial |t|} \frac{\partial |t|}{\partial t} = a_{\pm} (2 - \alpha) |t|^{1-\alpha} \frac{\partial |t|}{\partial t} . \quad (8.11)$$

Consider the properties of $|t|$ here,

$$\text{if } t > 0, \quad |t| = t \quad \frac{\partial |t|}{\partial t} = \frac{\partial t}{\partial t} = 1$$

$$\text{if } t < 0, \quad |t| = -t \quad \frac{\partial |t|}{\partial t} = \frac{\partial(-t)}{\partial t} = -1$$

therefore

$$\frac{\partial |t|}{\partial t} = \pm 1 . \quad (8.12)$$

Inserting this back into Eq.(8.11) gives

$$e(t, 0) = a_{\pm} (2 - \alpha) |t|^{1-\alpha} (\pm 1) . \quad (8.13)$$

The specific heat can now be found through differentiating the internal energy of Eq.(8.13) with respect to the reduced temperature

$$c(t, 0) = \frac{\partial e}{\partial t} = a_{\pm} (2 - \alpha) (1 - \alpha) |t|^{-\alpha} . \quad (8.14)$$

This is actually the singular part of the equation for the specific heat. The full equation also includes a regular part $+C_{\pm}$ too, but as C_{\pm} is unaffected by the renormalization process this work will focus solely on the singular element.

By considering the singular element of the equation for the specific heat from Eq.(4.52), it is clear that the coefficient of $|t|$ in Eq.(8.14) must equate to this, giving the critical amplitude A_{\pm} in terms of α

$$A_{\pm} = a_{\pm}(2 - \alpha)(1 - \alpha) . \quad (8.15)$$

Thermodynamic variables are often linked in conjugate pairs, whereby one is the derivative of the internal energy of the system with respect to the other (for example pressure and volume, or temperature and entropy). In this case, consider that the hidden variable x effecting the relationship between the ideal and constrained critical exponents is conjugate to a force u such that

$$x(t, h, u) = \frac{\partial f_x(t, h, u)}{\partial u} . \quad (8.16)$$

where

$$\frac{\partial f_x(t, h, u)}{\partial u} = \frac{\partial f}{\partial t^*} \frac{\partial t^*}{\partial u} + \frac{\partial f}{\partial h^*} \frac{\partial h^*}{\partial u} . \quad (8.17)$$

The constraint imposed upon the real system is

$$x(t, h, u) = X(t, h, u) \quad (8.18)$$

and is assumed to be an analytic function.

For the case where $h = 0$, observe that

$$h^* = h\mathcal{J} = \frac{\partial h^*}{\partial u} = h \frac{\partial \mathcal{J}}{\partial u} = 0 \quad (8.19)$$

then via Eq.(8.17) and (8.19) one may write Eq.(8.16) when operating under in the absence of an external field as

$$x(t, 0, u) = e(t^*, 0) \frac{\partial t^*}{\partial u} . \quad (8.20)$$

A further assumption is made regarding the function t^* . Observe that around the critical point $T = T_c$, $u = u_c$ at $h = 0$, t^* may be written as a Taylor expansion

$$t^*(t, 0, u) = a_1\mu + a_2\tau + \dots , \quad (8.21)$$

where

$$\mu = u - u_c \quad (8.22)$$

$$\tau = t - t_c \quad (8.23)$$

therefore

$$\frac{\partial t^*}{\partial u} = a_1 . \quad (8.24)$$

This assumption allows the hidden variable x of Eq.(8.20) to be written as

$$x(t, 0, u) = a_1 e(t^*, 0) , \quad (8.25)$$

and when Eq.(8.13) is considered, it can be seen that

$$e(t^*, 0) = a_{\pm}(2 - \alpha)|t^*|^{1-\alpha} , \quad (8.26)$$

so one may state

$$x(t, 0, u) = a_1(\pm 1)a_{\pm}(2 - \alpha)|t^*|^{1-\alpha} . \quad (8.27)$$

One then assumes that the behaviour of the magnetic field close to the critical value h_c in Eq.(8.21) is approximately

$$t^* \approx a_1\mu + \dots ,$$

and by rearranging t make μ the subject

$$\mu = \frac{1}{a_1}t^* + \dots . \quad (8.28)$$

This can then be used in the Taylor expansion equation for the constraint X

$$X(t, 0, u) = X(0, 0, u_c) + d_1\mu t + d_2t + \dots , \quad (8.29)$$

then by Eq.(8.18) one may equate Eq(8.27) and Eq.(8.29) to give the constraint as

$$\pm a_1(2 - \alpha)a_{\pm}|t^*|^{1-\alpha} = X(0, 0, u_c) + d_1\mu + d_2t + \dots . \quad (8.30)$$

Given that $X(0, 0, u_c) = 0$, multiplying both sides of the equation by a_1 gives

$$\pm a_1^2(2 - \alpha)a_{\pm}|t^*|^{1-\alpha} = d_1t^* + d_2a_1t + \dots ,$$

from here it can be seen that there are two possible outcomes depending on the value of α (one disregards the case where $\alpha = 0$, as this would mean there is no relationship between the specific heat and temperature):

- If $\alpha < 0$, then $|t^*|^{-\alpha}$ must be smaller than t^* . So the regular term dominates, and one may state that

$$0 = d_1t^* + d_2a_1t + \dots$$

$$t^* = t .$$

Therefore the real and ideal temperatures are equal, deeming the renormalization process unnecessary. In support of this statement, consider the effect this would have on the value for the specific heat. When $\alpha < 0$, c must scale to a positive power of the reduced temperature. This prevents one from obtaining a discontinuity for the specific heat (as would be obtained in a second-order phase transition), one must make the assumption that Fisher renormalization is only valid for cases where $\alpha > 0$

- If $\alpha > 0$, then

$$\pm a_1(2 - \alpha)a_{\pm}|t^*|^{1-\alpha} = d_2t + \dots$$

$$|t^*| = \left(\frac{d_2}{a_1(2 - \alpha)}\right)^{\frac{1}{1-\alpha}} \left(\frac{1}{a_{\pm}}\right)^{\frac{1}{1-\alpha}} (\pm t)^{\frac{1}{1-\alpha}}$$

then by using the substitution

$$a = \left(\frac{d_2}{a_1(2 - \alpha)}\right)^{\frac{1}{1-\alpha}} \quad (8.31)$$

one obtains

$$|t^*| = a \left(\frac{|t|}{a_{\pm}}\right)^{\frac{1}{1-\alpha}} . \quad (8.32)$$

This equation for $|t^*|$ turns out to be vital for determining the renormalized exponents and amplitudes, as will be shown later in this section.

Differentiating Eq.(8.32) with respect to the reduced temperature yields

$$\frac{\partial t^*}{\partial t} = \frac{a}{1 - \alpha} a_{\pm}^{-\frac{1}{1-\alpha}} |t|^{\frac{\alpha}{1-\alpha}} , \quad (8.33)$$

using this enables one to deduce the real internal energy. Consider that

$$e_x(t, 0, u) = \frac{\partial f_x}{\partial t} = \frac{\partial f}{\partial t^*} \frac{\partial t^*}{\partial t} + \frac{\partial f}{\partial h^*} \frac{\partial h^*}{\partial t} , \quad (8.34)$$

which can clearly be simplified via $\frac{\partial h^*}{\partial t} = 0$ at $h = 0$ to

$$e_x(t, 0, u) = e(t^*, 0) \frac{\partial t^*}{\partial t} . \quad (8.35)$$

Here, the internal energy has been expressed as a product of Eq.(8.26) and eq.(8.33). Writing this explicitly yields

$$e_x(t, 0, u) = a_{\pm}(2 - \alpha)|t^*|^{1-\alpha} \frac{a}{(1 - \alpha)} a_{\pm}^{-\frac{1}{1-\alpha}} |t|^{\frac{\alpha}{1-\alpha}}$$

then using Eq.(8.32) and the substitution $\frac{\alpha}{1-\alpha} + 1 = \frac{1}{1-\alpha}$ one obtains

$$e_x(t, 0, u) = \frac{2 - \alpha}{1 - \alpha} a^{2-\alpha} a_{\pm}^{-\frac{1}{1-\alpha}} |t|^{\frac{1}{1-\alpha}} . \quad (8.36)$$

Differentiation of Eq.(8.36) with respect to t then gives the renormalized specific heat of the system, c_x

$$c_x(t) = \frac{2 - \alpha}{(1 - \alpha)^2} a^{2-\alpha} a_{\pm}^{-\frac{1}{1-\alpha}} |t|^{\frac{\alpha}{1-\alpha}} . \quad (8.37)$$

Consider now the singular part of Eq.(4.52) for the specific heat

$$c_x(t) = A_{x\pm}|t|^{\alpha_x} \quad (8.38)$$

By comparing the two equations, it becomes apparent that the exponents equate to

$$\alpha_x = \frac{-\alpha}{1-\alpha} \quad (8.39)$$

and the amplitudes correspond to

$$A_{x\pm} = \frac{2-\alpha}{(1-\alpha)^2} a^{2-\alpha} a_{\pm}^{\frac{-1}{1-\alpha}} . \quad (8.40)$$

Now consider that Eq.(8.16) can be rearranged to make a_{\pm} the subject such that

$$a_{\pm} = \frac{A_{\pm}}{(2-\alpha)(1-\alpha)} \quad (8.41)$$

by inserting this into Eq.(8.40) one observes that

$$A_{x\pm} = \frac{2-\alpha}{(1-\alpha)^2} a^{2-\alpha} \left(\frac{A_{\pm}}{(2-\alpha)(1-\alpha)} \right)^{\frac{-1}{1-\alpha}}$$

$$A_{x\pm} = \frac{(2-\alpha)^{1+\frac{1}{1-\alpha}}}{(1-\alpha)^{2-\frac{1}{1-\alpha}}} a^{2-\alpha} A_{\pm}^{\frac{-1}{1-\alpha}} ,$$

then by using

$$1 + \frac{1}{1-\alpha} = \frac{1-\alpha+1}{1-\alpha} = \frac{2-\alpha}{1-\alpha}$$

and

$$2 - \frac{1}{1-\alpha} = \frac{2-2\alpha-1}{1-\alpha} = \frac{1-2\alpha}{1-\alpha}$$

one obtains the renormalized critical amplitude $A_{x\pm}$

$$A_{x\pm} = a^{2-\alpha} \frac{(2-\alpha)^{\frac{2-\alpha}{1-\alpha}}}{(1-\alpha)^{\frac{1-2\alpha}{1-\alpha}}} A_{\pm}^{\frac{-1}{1-\alpha}} . \quad (8.42)$$

8.2 Exponents and Amplitudes

The remaining critical exponents and amplitudes can be derived via insertion of Eq.(8.32) into the equations of their associated thermodynamic functions. First, for the magnetization of eq.(2.3)

$$M_x(t) = M(t^*) = B \left(a \left(\frac{|t|}{a_-} \right)^{\frac{1}{1-\alpha}} \right)^{\beta} \quad t \rightarrow 0^-$$

$$M_x(t) = B a^{\beta} |t|^{\frac{\beta}{1-\alpha}} a_-^{\frac{-\beta}{1-\alpha}}$$

then via Eq.(8.41),

$$M_x(t) = Ba^\beta A_-^{\frac{-\beta}{1-\alpha}} (2-\alpha)^{\frac{\beta}{1-\alpha}} (1-\alpha)^{\frac{\beta}{1-\alpha}} |t|^{\frac{\beta}{1-\alpha}} . \quad (8.43)$$

Therefore the renormalization process for the magnetization yields the critical exponent

$$\beta_x = \frac{\beta}{1-\alpha} , \quad (8.44)$$

and the critical amplitude

$$B_x = Ba^\beta A_-^{\frac{-\beta}{1-\alpha}} (2-\alpha)^{\frac{\beta}{1-\alpha}} (1-\alpha)^{\frac{\beta}{1-\alpha}} . \quad (8.45)$$

By the same method, using the magnetic susceptibility from Eq.(4.49)

$$\chi_x(t) = \chi(t^*) = \Gamma_\pm \left(a \left(\frac{|t|}{a_\pm} \right)^{\frac{1}{1-\alpha}} \right)^{-\gamma}$$

$$\chi_x(t) = \Gamma_\pm a^{-\gamma} |t|^{\frac{-\gamma}{1-\alpha}} a_\pm^{\frac{\gamma}{1-\alpha}}$$

again using Eq.(8.41),

$$\chi_x(t) = \Gamma_\pm a^{-\gamma} A_\pm^{\frac{\gamma}{1-\alpha}} (2-\alpha)^{\frac{-\gamma}{1-\alpha}} (1-\alpha)^{\frac{-\gamma}{1-\alpha}} |t|^{\frac{-\gamma}{1-\alpha}} . \quad (8.46)$$

So the renormalization of the isothermal susceptibility gives the the critical exponent

$$\gamma_x = \frac{-\gamma}{1-\alpha} , \quad (8.47)$$

and the critical amplitude

$$\Gamma_{x\pm} = \Gamma_\pm a^{-\gamma} A_\pm^{\frac{\gamma}{1-\alpha}} (2-\alpha)^{\frac{-\gamma}{1-\alpha}} (1-\alpha)^{\frac{-\gamma}{1-\alpha}} . \quad (8.48)$$

And for the correlation length, from Eq.(4.60)

$$\xi_x(t) = \xi(t^*) = N_\pm \left(a \left(\frac{|t|}{a_\pm} \right)^{\frac{1}{1-\alpha}} \right)^{-\nu}$$

$$\xi_x(t) = N_\pm a^{-\nu} |t|^{\frac{-\nu}{1-\alpha}} a_\pm^{\frac{\nu}{1-\alpha}}$$

$$\xi_x(t) = N_\pm a^{-\nu} A_\pm^{\frac{\nu}{1-\alpha}} (2-\alpha)^{\frac{-\nu}{1-\alpha}} (1-\alpha)^{\frac{-\nu}{1-\alpha}} |t|^{\frac{-\nu}{1-\alpha}} . \quad (8.49)$$

Therefore the renormalized correlation length yields the critical exponent

$$\nu_x = \frac{-\nu}{1-\alpha} , \quad (8.50)$$

and critical amplitude

$$N_{x\pm} = N_\pm a^{-\nu} A_\pm^{\frac{\nu}{1-\alpha}} (2-\alpha)^{\frac{-\nu}{1-\alpha}} (1-\alpha)^{\frac{-\nu}{1-\alpha}} . \quad (8.51)$$

Renormalization of the other exponents and amplitudes does not change their values, therefore one can state

$$\delta_x = \delta \quad (8.52)$$

$$D_x = D \quad (8.53)$$

$$\eta_x = \eta \quad (8.54)$$

$$\Theta_x = \Theta . \quad (8.55)$$

All critical exponents and amplitudes have been Fisher renormalized.

8.3 Involution of Critical quantities

Define S as the set of all critical exponents of the ideal system

$$S = \{\alpha, \beta, \gamma, \delta, \nu, \eta\} , \quad (8.56)$$

and S_x as the set of all renormalized exponents of the real system

$$S_x = \{\alpha_x, \beta_x, \gamma_x, \delta_x, \nu_x, \eta_x\} \quad (8.57)$$

These exponents S_x share some interesting properties in that the transformation between sets of exponents is involutory in nature, such that the transformation is self-invertible and repeating the process will transform the exponent back to the identify. i.e.

$$S_{xx} = \mathcal{F}(\mathcal{F}(S)) \quad (8.58)$$

For example, consider the exponent α_x . By repeating the renormalization process given by Eq.(8.39), one obtains

$$\begin{aligned} \alpha_{xx} &= \frac{-\alpha_x}{1 - \alpha_x} \\ \alpha_{xx} &= \frac{-\left(\frac{-\alpha}{1-\alpha}\right)}{1 - \left(\frac{-\alpha}{1-\alpha}\right)} \\ \alpha_{xx} &= \frac{\frac{\alpha}{1-\alpha}}{1 + \frac{\alpha}{1-\alpha}} \\ \alpha_{xx} &= \frac{\alpha}{(1 - \alpha) + \frac{\alpha(1-\alpha)}{1-\alpha}} \\ \alpha_{xx} &= \frac{\alpha}{1 - \alpha + \alpha} = \alpha . \end{aligned} \quad (8.59)$$

So the renormalization of α can be seen to be involutory in nature. Indeed, one finds that the renormalization of all critical exponents is indeed involutory.

Likewise, it can be shown that if the ideal exponents S_0 obey the standard scaling relations derived in section 5 then the constrained scaling relations S_x do so too. Also, the involution of these standard scaling relations can be shown via algebraic manipulation.

Given the involution of the Fisher renormalized critical exponents, one may assume that the critical amplitudes are also involutory. However, by testing this theory on the critical amplitude A_{\pm} one obtains

$$A_{xx\pm} = a^{2-\alpha_x} \frac{(2-\alpha_x)^{\frac{2-\alpha_x}{1-\alpha_x}}}{(1-\alpha_x)^{\frac{1-2\alpha_x}{1-\alpha_x}}} A_{x\pm}^{-\frac{1}{1-\alpha_x}} .$$

$$A_{xx\pm} = a^{2-\alpha_x} \frac{(2-\alpha_x)^{\frac{2-\alpha_x}{1-\alpha_x}}}{(1-\alpha_x)^{\frac{1-2\alpha_x}{1-\alpha_x}}} \left(a^{2-\alpha} \frac{(2-\alpha)^{\frac{2-\alpha}{1-\alpha}}}{(1-\alpha)^{\frac{1-2\alpha}{1-\alpha}}} A_{\pm}^{-\frac{1}{1-\alpha}} \right)^{\frac{-1}{1-\alpha_x}}$$

$$A_{xx\pm} = a^{2-\alpha_x + \frac{\alpha-2}{1-\alpha_x}} (2-\alpha_x)^{\frac{2-\alpha_x}{1-\alpha_x}} (2-\alpha)^{\alpha-2} (1-\alpha_x)^{\frac{2\alpha_x-1}{1-\alpha_x}} (1-\alpha)^{1-2\alpha} A_{\pm}$$

from here, it can clearly be observed that while there is room for manipulation of the powers of the terms, they will not reduce to the extent that all terms aside from A_{\pm} vanish, therefore one can state with confidence that

$$A_{xx+} \neq A_+ \tag{8.60}$$

the individual critical amplitudes are not involutory.

This setback with the critical amplitudes is explainable. Consider that while the critical exponents and scaling relations share the property of universality, the critical amplitudes are not universal. Perhaps it is universality that causes involution amongst Fisher renormalized quantities?

8.4 Involution of Universal Critical Amplitude Ratios

In this section, the substitution

$$\kappa(\alpha) = a^{2-\alpha} \frac{(2-\alpha)^{\frac{2-\alpha}{1-\alpha}}}{(1-\alpha)^{\frac{1-2\alpha}{1-\alpha}}} \tag{8.61}$$

is used in order to simplify the working. This allows the amplitude $A_{x\pm}$ from Eq.(8.42) to be written

$$A_{x\pm} = \kappa(\alpha) A_{\pm}^{-\frac{1}{1-\alpha}} . \tag{8.62}$$

Consider the amplitude ratio associated with these renormalized amplitudes from Eq.(4.53),

$$\frac{A_{x+}}{A_{x-}} = \frac{\kappa(\alpha)A_+^{\frac{-1}{1-\alpha}}}{\kappa(\alpha)A_-^{\frac{-1}{1-\alpha}}} = \left(\frac{A_+}{A_-}\right)^{\frac{-1}{1-\alpha}} . \quad (8.63)$$

To test this to see if it is involutory, define the arbitrary U_0 such that

$$U_0 = \frac{A_+}{A_-}$$

then by Eq.(8.63), the renormalized ratio U_{x0} is

$$U_{x0} = U_0^{\frac{-1}{1-\alpha}} \quad (8.64)$$

Therefore, if the process were to be repeated then

$$U_{xx} = (U_{x0})^{\frac{-1}{1-\alpha_x}} = \left((U_0)^{\frac{-1}{1-\alpha}}\right)^{\frac{-1}{1-\alpha_x}}$$

$$U_{xx} = U_0^{\frac{1}{(1-\alpha)(1-\alpha_x)}} .$$

Then by considering the substitution

$$\frac{1}{(1-\alpha)(1-\alpha_x)} = \frac{1}{(1-\alpha)\left(\frac{1-\alpha}{1-\alpha} - \frac{-\alpha}{1-\alpha}\right)} = \frac{1}{(1-\alpha)(1-\alpha)^{-1}} = 1 \quad (8.65)$$

it is clear that the powers of U_0 reduce leaving

$$U_{xx} = U_0 , \quad (8.66)$$

therefore the renormalized amplitude ratio associated with A_{\pm} must be involutory.

For the second amplitude relation concerning Γ from Eq.(4.50) use of Eq.(8.48) yields the renormalized amplitude ratio

$$\frac{\Gamma_{x+}}{\Gamma_{x-}} = \frac{\Gamma_+ a^{-\gamma} A_+^{\frac{\gamma}{1-\alpha}} (2-\alpha)^{\frac{-\gamma}{1-\alpha}} (1-\alpha)^{\frac{-\gamma}{1-\alpha}}}{\Gamma_- a^{-\gamma} A_-^{\frac{\gamma}{1-\alpha}} (2-\alpha)^{\frac{-\gamma}{1-\alpha}} (1-\alpha)^{\frac{-\gamma}{1-\alpha}}}$$

$$\frac{\Gamma_{x+}}{\Gamma_{x-}} = \frac{\Gamma_+}{\Gamma_-} \left(\frac{A_+}{A_-}\right)^{\frac{\gamma}{1-\alpha}} . \quad (8.67)$$

Then by repeating this process we obtain the twice-renormalized amplitude ratio

$$\frac{\Gamma_{xx+}}{\Gamma_{xx-}} = \frac{\Gamma_{x+}}{\Gamma_{x-}} \left(\frac{A_{x+}}{A_{x-}}\right)^{\frac{\gamma_x}{1-\alpha_x}} . \quad (8.68)$$

This is simply a combination of Eq(8.63) and Eq(8.67). by inserting these one obtains

$$\frac{\Gamma_{xx+}}{\Gamma_{xx-}} = \frac{\Gamma_+}{\Gamma_-} \left(\frac{A_+}{A_-} \right)^{\frac{\gamma}{1-\alpha}} \left(\left(\frac{A_+}{A_-} \right)^{\frac{-1}{1-\alpha}} \right)^{\frac{\gamma_x}{1-\alpha_x}}$$

$$\frac{\Gamma_{xx+}}{\Gamma_{xx-}} = \frac{\Gamma_+}{\Gamma_-} \left(\frac{A_+}{A_-} \right)^{\frac{\gamma}{1-\alpha} - \frac{\gamma_x}{(1-\alpha)(1-\alpha_x)}}$$

By examining the powers of $\frac{A_+}{A_-}$ it can be seen that

$$\frac{\gamma}{1-\alpha} - \frac{\gamma_x}{(1-\alpha)(1-\alpha_x)} = \frac{\gamma}{1-\alpha} - \gamma_x = \gamma_x - \gamma_x = 0$$

therefore

$$\frac{\Gamma_{xx+}}{\Gamma_{xx-}} = \frac{\Gamma_+}{\Gamma_-} \quad (8.69)$$

the universal amplitude ratio for Γ_{\pm} is involutory.

The same process can be used to display the involutory nature of the amplitude ratio from Eq.(4.61). Consider the full equation for the behaviour of the correlation length ξ . By using Eq.(8.51),

$$\frac{N_{x+}}{N_{x-}} = \frac{N_+ a^{-\nu} A_+^{\frac{\nu}{1-\alpha}} (2-\alpha)^{\frac{-\nu}{1-\alpha}} (1-\alpha)^{\frac{-\nu}{1-\alpha}}}{N_- a^{-\nu} A_-^{\frac{\nu}{1-\alpha}} (2-\alpha)^{\frac{-\nu}{1-\alpha}} (1-\alpha)^{\frac{-\nu}{1-\alpha}}}$$

$$\frac{N_{x+}}{N_{x-}} = \frac{N_+}{N_-} \left(\frac{A_+}{A_-} \right)^{\frac{\nu}{1-\alpha}} \quad (8.70)$$

therefore

$$\frac{N_{xx+}}{N_{xx-}} = \frac{N_{x+}}{N_{x-}} \left(\frac{A_{x+}}{A_{x-}} \right)^{\frac{\nu_x}{1-\alpha_x}} \quad (8.71)$$

This can be solved through use of Eq(8.70) and Eq(8.63)

$$\frac{N_{xx+}}{N_{xx-}} = \frac{N_+}{N_-} \left(\frac{A_+}{A_-} \right)^{\frac{\nu}{1-\alpha}} \left(\left(\frac{A_+}{A_-} \right)^{\frac{-1}{1-\alpha}} \right)^{\frac{\nu_x}{1-\alpha_x}}$$

$$\frac{N_{xx+}}{N_{xx-}} = \frac{N_+}{N_-} \left(\frac{A_+}{A_-} \right)^{\underbrace{\frac{\nu}{1-\alpha} - \frac{\nu_x}{(1-\alpha)(1-\alpha_x)}}_{=0}}$$

$$\frac{N_{xx+}}{N_{xx-}} = \frac{N_+}{N_-} \quad (8.72)$$

Thus, the critical amplitude ratio associated with N_{\pm} is involutory.

8.5 Fisher Renormalization of Amplitude Combinations

This thesis has shown the involutory nature of the Fisher renormalized critical exponents and critical amplitude ratios - universal quantities in the field of phase transitions. The four amplitude combinations derived from the scaling relations discussed in section 5 are also universal quantities, so will be tested to see if they also obey involution.

The first combination from Eq.(5.49) can be renormalized by using Eqs.(8.42) and (8.51), with the dimensionality d of the system unaffected by renormalization. this leads to

$$A_{x\pm} N_{x\pm}^d = a^{2-\alpha-\nu d} (2-\alpha)^{\frac{2-\alpha-\nu d}{1-\alpha}} (1-\alpha)^{\frac{2\alpha-1-\nu d}{1-\alpha}} A_{\pm}^{\frac{\nu d-1}{1-\alpha}} N_{\pm}^d$$

which is then simplified using the scaling relation for Josephson's law from Eq.(5.48), resulting in

$$A_{x\pm} N_{x\pm}^d = (1-\alpha)^{-3} A_{\pm} N_{\pm}^d . \quad (8.73)$$

With this result know, repeating the renormalization process yields

$$A_{xx\pm} N_{xx\pm}^d = (1-\alpha_x)^{-3} A_{x\pm} N_{x\pm}^d = (1-\alpha_x)^{-3} (1-\alpha)^{-3} A_{\pm} N_{\pm}^d$$

then through use of the substitution from Eq.(8.65) one obtains

$$A_{xx\pm} N_{xx\pm}^d = A_{\pm} N_{\pm}^d . \quad (8.74)$$

Therefore the renormalized amplitude combination is involutory.

For the second amplitude relation from Eq.(5.56), using the renormalized amplitudes from Eqs.(8.48), (8.51) and Eq.(8.55) gives

$$\frac{\Theta N_{x\pm}^{2-\eta_x}}{\Gamma_{x\pm}} = \frac{\Theta N_{\pm}^{2-\eta}}{\Gamma_{\pm}} a^{\gamma-\nu(2-\eta)} A_{\pm}^{\frac{\nu(2-\eta)-\gamma}{1-\alpha}} (2-\alpha)^{\frac{\gamma-\nu(2-\eta)}{1-\alpha}} (1-\alpha)^{\frac{\gamma-\nu(2-\eta)}{1-\alpha}} .$$

This is simplified using Fisher's law Eq.(5.55) to

$$\frac{\Theta N_{x\pm}^{2-\eta_x}}{\Gamma_{x\pm}} = \frac{\Theta N_{\pm}^{2-\eta}}{\Gamma_{\pm}} . \quad (8.75)$$

Clearly the Fisher renormalization process does not alter the amplitude ration, so by repeating the process the Fisher renormalization of this critical amplitude ratio can be shown to be involutory

$$\frac{\Theta N_{xx\pm}^{2-\eta_{xx}}}{\Gamma_{xx\pm}} = \frac{\Theta N_{\pm}^{2-\eta}}{\Gamma_{\pm}} . \quad (8.76)$$

For the third combination from Eq.(5.42), consider the renormalized values of the individual critical amplitudes used given by Eqs(8.45),(8.48) and (8.53). For the purposes

of this derivation Γ_- is used instead of Γ_{\pm} , the reasoning for which will become clear through the results. By amalgamating the renormalized exponents, the renormalized amplitude combination is

$$\frac{\Gamma_{x-} B_x^{\delta_x-1}}{D_x^{\delta_x}} = \frac{\Gamma_- B^{\delta-1} a^{\beta(\delta-1)-\gamma} A_-^{\frac{\gamma-\beta(\delta-1)}{1-\alpha}} (2-\alpha)^{\frac{\gamma-\beta(\delta-1)}{1-\alpha}} (1-\alpha)^{\frac{\gamma-\beta(\delta-1)}{1-\alpha}}}{D^{\delta}}$$

and through use of Griffith's law from Eq.(5.39) the powers of the additional terms cancel out, leaving

$$\frac{\Gamma_{x-} B_x^{\delta_x-1}}{D_x^{\delta_x}} = \frac{\Gamma_- B^{\delta-1}}{D^{\delta}} . \quad (8.77)$$

Clearly, repeating the renormalization process will not instigate a change in the result, so

$$\frac{\Gamma_{xx-} B_{xx}^{\delta_{xx}-1}}{D_{xx}^{\delta_{xx}}} = \frac{\Gamma_- B^{\delta-1}}{D^{\delta}} , \quad (8.78)$$

Now consider that by universality of the amplitude ratio from Eq.(4.50) one may write

$$\Gamma_- = k\Gamma_+ , k = \text{constant}$$

then the amplitude relation of Eq.(8.78) is equivalent to

$$\frac{\Gamma_{xx-} B_{xx}^{\delta_{xx}-1}}{D_{xx}^{\delta_{xx}}} = k \frac{\Gamma_+ B^{\delta-1}}{D^{\delta}} ,$$

but under the terms of universality one ignores the interference of the factor k , thus

$$\frac{\Gamma_{xx\pm} B_{xx}^{\delta_{xx}-1}}{D_{xx}^{\delta_{xx}}} = \frac{\Gamma_{\pm} B^{\delta-1}}{D^{\delta}} , \quad (8.79)$$

this critical amplitude combination is involutory.

For the final amplitude ratio from Eq.(5.44), the renormalized amplitudes of Eqs.(8.42), (8.45) and (8.48) are required. As with the previous relation only A_- and Γ_- are used at this point in order to accommodate the fact that B is only concerned with temperatures $T \leq T_c$

$$\frac{A_{x-} \Gamma_{x-}}{B_x^2} = \frac{A_-^{\frac{\gamma-1+2\beta}{1-\alpha}} \Gamma_-}{B^2} a^{\frac{2-\alpha-\gamma-2\beta}{1-\alpha}} (2-\alpha)^{\frac{2-\alpha-\gamma-2\beta}{1-\alpha}} (1-\alpha)^{\frac{2\alpha-1-\gamma-2\beta}{1-\alpha}}$$

this can be simplified using Rushbrooke's law from Eq.(5.43) to

$$\frac{A_{x-} \Gamma_{x-}}{B_x^2} = (1-\alpha)^{-3} \frac{A_- \Gamma_-}{B^2} . \quad (8.80)$$

By repeating the renormalization process, one obtains

$$\frac{A_{xx-}\Gamma_{xx-}}{B_{xx}^2} = (1 - \alpha_x)^{-3} \frac{A_{x-}\Gamma_{x-}}{B_x^2} = (1 - \alpha_x)^{-3} (1 - \alpha)^{-3} \frac{A_{-}\Gamma_{-}}{B^2} ,$$

$$\frac{A_{xx-}\Gamma_{xx-}}{B_{xx}^2} = \frac{A_{-}\Gamma_{-}}{B^2} .$$

then, by considering the universality of the amplitude ratios Eqs.(4.53) and (4.50), A_{-} and G_{-} must be interchangeable with A_{+} and G_{+} without affecting the universality

$$\frac{A_{xx\pm}\Gamma_{xx\pm}}{B_{xx}^2} = \frac{A_{\pm}\Gamma_{\pm}}{B^2} . \tag{8.81}$$

so the Fisher renormalization of this amplitude combination is also involutory.

9 Conclusions

Following an introduction to the generalities of statistical mechanics (including to microstates, macrostates and the Boltzmann probability distribution), phase transitions are discussed, with attention focussing on their applications to ferromagnetism. The famous Ising model is outlined and some discussion of its historical context is given. In this framework, the partition function and related thermodynamic functions are introduced: the internal energy, specific heat, the magnetization and the magnetic susceptibility. The associated correlation function and the correlation length are also introduced.

Once the classification system for phase transitions has been outlined, the universal critical exponents and the critical amplitudes - which characterize second order transitions - are introduced. Scaling relations between these exponents are then derived via the Widom method and certain combinations of amplitude ratios are demonstrated to be universal. Explicit solutions of the one-dimensional and mean-field models (the latter effectively an infinite-dimensional model) are given and demonstrate the validity of the scaling relations.

Finally, Fisher renormalization is introduced. This is necessary when the system is subject to certain types of constraint and leads to the renormalization of both the critical exponents and the critical amplitudes. The Fisher renormalized critical exponents also obey the standard scaling relations. Furthermore Fisher renormalization of the critical exponents is shown to be involutory, i.e., to successive applications of it yield the original exponents. Similarly it is shown that, while individual critical amplitudes are not involutory, their universal ratios are. This is the main conclusion of this thesis.

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