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Linked-cluster Expansions for Lattice Spin Models

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LINKED-CLUSTER EXPANSIONS FOR LATTICE SPIN MODELS

by

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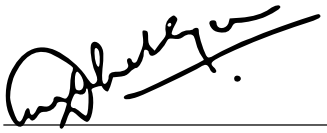
Approved: 

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Contents

Abstract

Similar to various series expansions that are used to approximate mathematical functions, the linked-cluster expansion is an approximation method that allows us to approach the actual values of a very large physical system's different physical quantities by systematically studying smaller systems embedded in this larger system. The main concept in linked-cluster expansion, weight, represents the additional contribution to a certain physical quantity by increasing the system size by one unit. These weights are used to eventually build up the result on a larger system. In our case, we focus on the partition function, a quantity that can be used to calculate several essential thermodynamic aspects of the system such as average energy, specific heat, magnetic susceptibility, etc. We study these weights for the Ising and Potts models on a one dimensional lattice and Bethe lattice, with and without an external magnetic field. Previous studies have shown that in the one dimensional Ising model, adding more than two lattice sites to the system does not create any additional contribution to the partition function (i.e. their weights are all zero), giving us the result for an infinitely large system with just two lattice sites, a remarkable simplification. In our study, we prove that this property holds not only for the Ising model, but also its generalization, the Potts model, and show that it is a result of a spin flip symmetry inherent in the system. In order to test this, we break this symmetry using an externally applied magnetic field and show that in this case, for magnetic dipole energies comparable with the exchange energy between neighboring spins, this special property vanishes.

Chapter 1

Introduction

We are often curious about the world around us as to why rocks are hard and why broken glass can never be fixed. In our life, all solid materials such as crystals and metals consist of particles. The interactions of these particles (atoms and molecules) determine the internal energies and ultimately the physical structures of the materials. For instance, ice melts when it encounters hotter environment and becomes water; diamonds and pencil leads are both carbon while one being impermeable and the other one fragile; and a magnet can lose its magnetization at high temperature.

In fact, the complexity of material structures and their physical properties goes well beyond the cases mentioned above. In order to understand the different material systems, their fundamental properties, and applications, scientists develop models and approximation methods to calculate physical quantities that would otherwise be hard to approach. In our case, we use linked-cluster expansion method to approximate the results of an infinitely large lattice system using a finite one. This method has been shown to provide faster convergence, i.e., smaller errors coming from the finite size, compared to other approximation methods, and potentially improves the results for several physical systems[1].

Modeling is the first step to isolate certain properties of the material and simplify the system for analysis. Models such as the Ising model and the Potts model are significant in representing systems containing particles with simple short-range interactions. These models define a relationship between any two adjacent particles (say

on a line) based on their individual properties. The models apply these properties to particles on a lattice structure e.g., which defines the physical structure of the system. For instance, whether it looks like a ring, a square, or a tree.

There are plenty of ways a system can behave, and there are several methods of studying this behavior experimentally and theoretically. Theoretically, statistical mechanics[2] offers a powerful tool to give us access to physical quantities such as the average energy, magnetization, and partition function of a system starting with a microscopic model as described above. Various mathematical tools such as those used in the field of graph theory are naturally integrated into statistical mechanics, and can provide deep insight into the fundamental properties of the system. The linked-cluster method we use here is based in such graph theoretic techniques and theorems.

With the models applied to different lattice types, graph theory provides an abstract way to analyze the relationship between different sections in the lattice system. If we take a solid crystalline system with 10^{23} particles within, and look at it microscopically, we can see that the particles within are structured in a certain way. The structure then is the the lattice type of the system. Due to the difference in lattice structures, the number of bonds attached to one lattice site is different, thus different physical properties. Surprisingly, such rigid lattice systems can also be used to describe properties of gases and liquids.

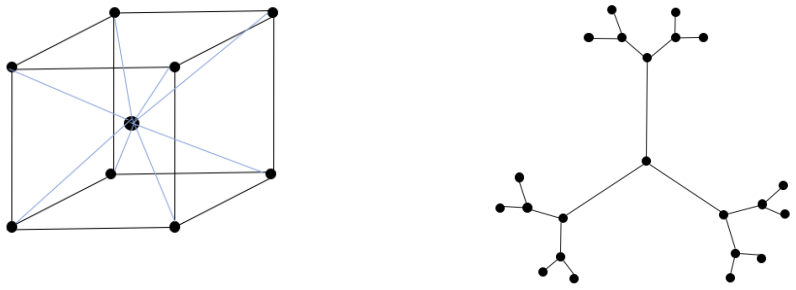

Figure 1.1: Left: Body-centered three-dimensional lattice (9 lattice sites in total) Right: Tree-like Bethe lattice (22 lattice sites in total)

The two lattices in Figure 1.1 represent different material structures and describe

how the crystals with these structure would grow. In fact, there are many lattice types that leads to different calculations of the models applied. In this thesis, the one-dimensional and Bethe lattice are closely studied.

Graph theory provides ideas that can explain the physical relationships between two graphs. As an example, consider the three graphs in Figure 1.2 that can be deemed as parts of the Bethe lattice on the right of Figure 1.1, and can be also called subgraphs.

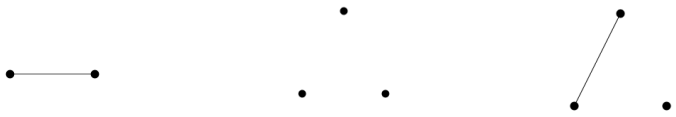

Figure 1.2: Three subgraphs for Bethe lattice

By knowing the relationship between the subgraph and the original graph, we can construct physical quantities on the larger graph using those on the subgraphs In this way, it helps with using a finite system to approximate an infinite lattice system. This is the basis of the linked-cluster expansion.

Linked-cluster expansion method (LCE) [3, 4] considers an infinite system as built from smaller finite size system. It starts with a small subsystem (or subgraph), and "grows" this by adding single units (say a lattice site), and looks at how this changes the properties. This process is carried on iteratively until the desired accuracy is reached. The key point is how quickly the difference between any finite system and the infinite system becomes acceptably small. As mentioned earlier, it has been shown [1] that the linked-cluster method gives a much smaller error than other approximation methods for comparable system sizes, but it is not known whether this is model specific, or more generally what are the conditions under which the LCE outperforms other methods.

In this thesis, we examine precisely this question by studying the one dimensional Ising model, where a particularly dramatic speed-up in convergence is observed. We then study what the underlying properties of this model are that allows this, and generalize the results to a broader class of models, the Potts models.

The thesis is organized as follows: In Chapter 2, I discuss some of the essential concepts in statistical mechanics that we use in our calculations. Chapter 3 and 4 look at the particular spin models we use and discuss the different lattices we set these models on. In chapter 5, we take a quick look at some basic notions in graph theory. Chapter 6 with a summary of the linked-cluster method and leads to a derivation of our main results. In Chapter 7 we study the effect of an externally applied magnetic field to explicitly check that intrinsic symmetries lead to the effect we observe, and I conclude in Chapter 8.

Chapter 2

Statistical Mechanics

Statistical mechanics [2] is a theoretical approach to study the thermodynamics of physical systems, and provides methods to calculate physical quantities such as average energies, magnetic susceptibility, and can provide information about phase transitions (like ice to water) for a given model of inter-particle and environmental interactions. It serves as the basis for our calculations using the linked-cluster expansion method. In this chapter, we will discuss the the concepts of ensembles, multiplicity, and the partition function as a preparation for our calculations in Chapters 6 and 7.

2.1 Ensembles

In statistical mechanics, one calculates an average of properties like energy over many imaginary copies of the system, each copy representing a different configuration of the system. This set of copies is called an *ensemble*, a fundamental notion that serves as the origin of the idea of doing "statistics" on a physical system. Depending on the details of what sort of copies are allowed, there are three ensembles in statistical mechanics: 1) microcanonical ensemble, 2) canonical ensemble, and 3) grand-canonical ensemble. In short, they vary in the interaction between the system and its environment in terms of whether or not exchange of energy and material content is allowed or not.

Microcanonical Ensemble

The microcanonical ensemble represents an isolated system of particles that does not interact with the environment around or any adjacent systems, which we call reservoir. This means that, in a microcanonical ensemble, the volume, pressure, total energy and any physical quantities would not change for any configurations of the system. In other words, the copies in the ensemble only differ in internal configurations of a fixed total energy and number of particles.

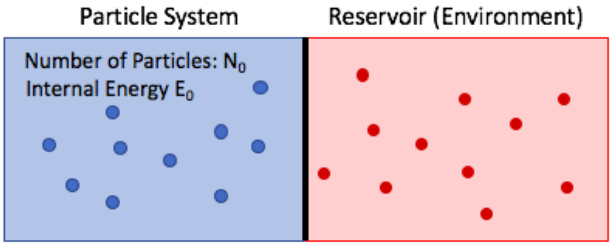

Figure 2.1: Microcanonical ensemble: The blue box on the left represents the microcanonical ensemble that does not exchange particles or energy with the environment(indicated by the red box on the right)

As shown in Figure 2.1, the particle system has consistent number of particle and internal energy . These physical properties are not affected by the reservoir (environment) that it is put into contact. In other words, this system is solely independent and we do not have to account other factors in analyzing a system like the microcanonical ensemble.

Canonical Ensemble

The canonical ensemble is a system that is in thermal equilibrium with a heat bath at some fixed temperature. In this case, the heat transfer would result in the varying total energy of the system. For instance, when a cube of ice is placed outside in

the sun, it will absorb the heat until it melts into water and remains the same temperature as the environment that it is in. When the ice completes its melting and remains its water form with a constant temperature, the process reaches its thermal equilibrium. Systems in the canonical ensemble are, however, not allowed to exchange any material content, i.e., the number of particles is fixed.

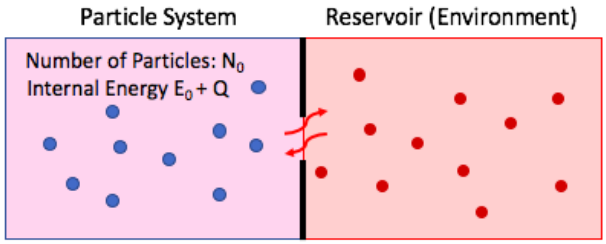

Figure 2.2: Canonical ensemble: The blue box on the left represents the canonical ensemble that interacts only with a heat reservoir without changing the number of particles, or volume of the system

The heat bath is also considered as a heat reservoir that has a difference in energy with the original particle system. As shown on figure 2.2, the particle system represents a typical canonical ensemble and the reservoir is either inputting or outputting energy into the ensemble until they reach a thermal equilibrium. The reservoir is also assumed to be infinitely large so that it can maintain a constant temperature T independent of exchanging heat with the system. The temperature can be considered as a parameter that fixes the equilibrium average energy in the system.

Grand Canonical Ensemble

The grand canonical ensemble describes a system in thermal and chemical equilibrium with the reservoir. Whereas thermal equilibrium represents the consistency of temperature, chemical equilibrium represents an equilibrium of particle movement. For instance, when we pour milk into our coffee, the milk would first stay together in the cup and then gradually spread out. As we stir the coffee and milk in the cup, the milk and coffee will eventually nicely mixed and stay as coffee latte. This

stable form is considered as in chemical equilibrium. The chemical equilibrium is parametrized by the *chemical potential*, that can be thought of as a parameter that fixes the average equilibrium number of particles in the system.

Therefore, the difference between a grand-canonical ensemble and a canonical ensemble is that, there is particle exchange in addition to the energy exchange.

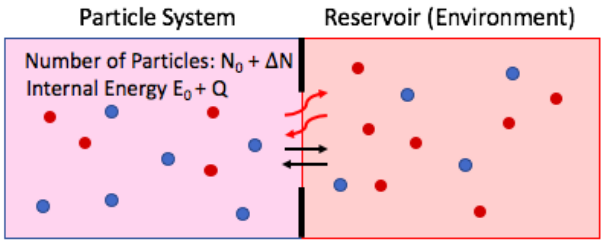

Figure 2.3: Grand Canonical ensemble: The blue box on the left represents the grand canonical ensemble that exchange both energy and particles with another system(environment or reservoir).

As shown on figure 2.2, the total number of particles and total energy all change as the particle system is put in contact with the reservoir. The grand canonical ensemble resembles systems that have very active particle movements such as liquid and gas. Compared to the grand canonical ensemble, the canonical ensemble simulates systems that have less active particle movements but heat conductive, such as a solid chuck of iron or silver.

The three ensembles correspond to physically different system-environment interactions, and the grand-canonical ensemble is the most general of these. It corresponds to not fixing the energy and particle number, but the temperature and chemical potential, a more realistic model of a physical system and its environment. However, all three ensembles have their advantages and value. The technicalities of the linked-cluster method also restrict us to the grand canonical ensemble, and all our calculations will be based on this.

In the following section, we will describe the notion of multiplicity, that will lead us to how we can calculate averages in the three different ensembles.

2.2 Multiplicity

Multiplicity is the simplest concept in the study of statistical mechanics. It explains the basic ideas similar as what we know as probability. For all the particles in the material system, the number of ways they can be arranged can be indicated by multiplicity.

Since the multiplicity of the system is really big due to the large number of particles within, let's start with a simple example. When rolling a die, we know that there are 6 numbers we can get, and each one has the same probability of occurrence (assuming an unweighted die). In statistical mechanics, we call all of these numbers different microstates, and there are 6 microstates in this system in total. However, if the manufacturer produces a faulty die with two sixes on the surface and no fives, which means it has 1,2,3,4,6,6, then there are still 6 microstates in the system but two microstates are actually the same. In this case, we say there are five macrostates, 1,2,3,4,6, and macrostate 6 has most microstates which means it has a higher probability of occurrence.

The problem of rolling one die a few times actually get us closer to our main idea of multiplicity. For instance, if someone is asked to roll a dice three times, the possibility of getting all sixes would be $\frac{1}{6} \times \frac{1}{6} \times \frac{1}{6} = \frac{1}{36}$, but the possibility of getting two fives and a six would be $3 \times (\frac{1}{6} \times \frac{1}{6} \times \frac{1}{6}) = \frac{3}{36}$. In other words, there are thrice as many microstates with two fives and a six (556, 565, 655) than only sixes (666), which means the macrostate with two fives and a six is more likely to occur. In this example, we are considering the states *with* ordering as microstates, the macrostates being described the number of occurrences of each digit. The number of different ways of arrangements is called multiplicity, and in this case, the total multiplicity is $6 \times 6 \times 6 = 36$.

We represent multiplicity with Ω. When rolling a dice three times, the total multiplicity Ω is 36. Whereas Ω in this case is pretty small, it could get very large for macroscopic systems. For instance, if there are 10^{23} molecules in a small box and each molecule could have 10^{23} ways to stay in the box, then there are 10^{529} configurations, i.e., $\Omega = 10^{529}$.

It is clear that enumerating each configuration of the system is tedious. In the microcanonical ensemble, averaging requires choosing all configurations that lead

to the same macrostate (energy) and this is a highly constrained process. This is possible to do for simple systems, but as we'll see below, it is often easier to use the canonical ensemble, which allows a slightly less constrained process of choosing microstates since it allows configurations of different energies in the average.

2.3 Partition Function

The partition function is a physical quantity in statistical mechanics, which helps calculate the average energy, probability and other statistical quantities. Based on what we know about the multiplicity of the system, we realize there are different configurations resulting in different states. In the microcanonical ensemble, we directly count microstates to find the multiplicity of a particular macrostate to calculate probabilities of occurrence of a given microstate.

In the canonical ensemble, since we are also allow energy fluctuations, we need a way to average over all the different microstates including with different energy. In order to do this, a microstate with energy E is given a weight $e^{-\beta E}$ where $\beta = \frac{1}{k_B T}$, k_B is the Boltzmann constant and T is temperature of reservoir (for a derivation, see Ref. [2]). The Boltzmann constant serves to convert temperature to an equivalent energy. This weight, called the Boltzmann factor indicates the relative occurrence of a state with energy E occurring in the ensemble. There are many states for a system depending on the configurations of the particles inside the system and their internal energy. The E in the partition function is then the total internal energy of one configuration.

The formula for the partition function of a certain system is then,

$$Z = \sum_{\{\text{All Configurations}\}} e^{-\beta E} \tag{2.1}$$

which sums up all the Boltzmann factors of different energy states.

A simple example for the partition function is: if we have a system with only four configurations and the total energies are 1, 1, 0, -1 for each of the four configurations,

the partition function Z for this is,

$$\begin{aligned} Z &= e^{-(1)\beta} + e^{-(1)\beta} + e^{-(0)\beta} + e^{-(-1)\beta} \\ &= 2e^{\beta} + 1 + e^{-\beta} \end{aligned} \tag{2.2}$$

In this case, the Boltzmann factors for all the configurations(energy states) are listed out respectively according to the energy E the configuration has. For configuration with energy 1, the Boltzmann factor is $e^{-(1)\beta}$; for that with energy 0, the Boltzmann factor is $e^{-(0)\beta} = 0$; and for that with energy -1, the Boltzmann factor is $e^{-(-1)\beta} = e^{\beta}$. Since there are two configurations with energy 1, and one configuration each for energy 0 and -1, the partition function is the sum of all the Boltzmann factors $2e^{\beta} + 1 + e^{-\beta}$. This is a very simple system with only four configurations. For a more generalized explanation, if the system has 10 configurations with one of energy A, two of energy B, three of energy C, and four of energy D. Then the partition function for the system is,

$$Z = e^{-A\beta} + 2e^{-B\beta} + 3e^{-C\beta} + 4e^{-D\beta} \tag{2.3}$$

where $e^{-A\beta}, e^{-B\beta}, e^{-C\beta}$ and $e^{-D\beta}$ are the Boltzmann factor for energy A, B, C and D respectively. However, imagine a real molecular system with 10^{50} ways of arranging the particles, the partition function can get quite complicated to calculate exactly. This clarifies why we need effective approximation methods.

The partition function is therefore similar to the total multiplicity Ω defined earlier. Below, we will show how we can use it to calculate averages.

The calculation of the partition function shown above will be heavily used later in chapter 6 and 7, due to its significance in this study of research.

Probability

By knowing the concepts of the Boltzmann factors and the partition function , we can write out the probability of each microstates in the system. As mentioned above,

the Boltzmann factor is the relative weight configuration with energy E. Therefore, the probability P of the state with energy E occurring is

$$P = \frac{e^{-\beta E}}{\sum e^{-\beta E}} = \frac{e^{-\beta E}}{Z} \tag{2.4}$$

The numerator is the Boltzmann factor of an arbitrary configuration(state) that has energy E, and the denominator is the partition function including all the configurations. Since P is only the probability for one configuration, all the configurations in a system should have probabilities summed up to 1. In this case, if we add up all the probabilities, it should write out as,

$$\begin{aligned} \sum P &= \sum \frac{e^{-\beta E}}{\sum e^{-\beta E}} \\ &= \frac{\sum e^{-\beta E}}{Z} \\ &= \frac{1}{Z} \sum e^{-\beta E} \\ &= \frac{1}{Z} \times Z \\ &= 1 \end{aligned} \tag{2.5}$$

Mean Values

The mean value of energy, that is, the average energy of a specific state is simply a weighed average over all energies, weighted by the Boltzmann factors:

$$\bar{E} \equiv \frac{E e^{-\beta E}}{\sum e^{-\beta E}} = \frac{E e^{-\beta E}}{Z} \tag{2.6}$$

Note that we can also obtain this average as a derivative of the partition function:

$$\bar{E} \equiv \frac{E e^{-\beta E}}{Z} = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\partial \log Z}{\partial \beta}. \tag{2.7}$$

This the partition function serves as a powerful quantity that captures a significant amount of information about the system.

Continuing, the formula for standard deviation is,

$$\Delta E = \sqrt{\bar{E^2} - \bar{E^2}} \tag{2.8}$$

and with the same reasoning we know that,

$$\bar{E^2} = \frac{E^2 e^{-\beta E}}{\sum e^{-\beta E}} = \frac{E^2 e^{-\beta E}}{Z}. \tag{2.9}$$

We can again represent this quantity in terms of a second derivative of the partition function. Standard deviation gives us a sense of the fluctuations in the energy.

2.3.1 Grand Canonical Partition Function

Since the grand canonical ensemble allows fluctuations in particle number, the sum in Eq. (2.1) is over configurations of different particle number, that removes one more constraint on the canonical partition function sum. Unusually, allowing for a more physically accurate picture has made our calculations simpler in some ways. We still need approximations since it is still not possible to carry out these sums for any sizable system.

The partition function is thus particularly important in every aspect of analyzing a material system, since it allows us access to many physical properties. Therefore, in applying the linked-cluster expansion method on different lattices and models, we use the partition function for the first step of for each specific model to provide more physical understanding of the system behaviors. We will derive it for specific models later.

In the next chapter, we describe the models that we use as a basis for our study.

Chapter 3

Spin Models

Now that we've covered the relevant concepts of partition function and ensembles in statistical mechanics, let's look at spin models that are studied in this work.

Spin models attempt to capture the physics of interactions between the magnetic properties of electrons in materials, rather than the electric properties. A striking example is ferromagnetism, where a macroscopic piece of material can get magnetized because of alignment of the tiny atomic and electronic magnets in the material.

Interestingly the physics of spin models has many parallels with other seemingly disparate systems. Generally, a spin model assigns a *spin* to each lattice site (we'll consider only lattice models), which can take some set of values, and a relationship between the two spins on adjacent lattice sites, i.e., an internal energy. This then allow us to calculate how these properties can contribute to the collective system behaviors.

We will discuss lattices in a little more detail in the next chapter. For now, imagine a crystal with atoms and bonds in between some of the atoms. We can describe this using a geometric lattice, with sites (or nodes) representing the atoms, and edges representing the bonds holding them together with a corresponding internal energy. The spin models that we discuss in this thesis are Ising model and Potts model that are very commonly used in physics and other fields[5].

3.1 Ising Model

The Ising model[2] plays a significant role in this thesis because it can be used to simulate many physical systems. We will talk about the basic formula and definition in this section and their applications in the thesis will be presented later. Ising model is important in the history of statistical mechanics as it explains the most typical and simplest idea of spins and system energy. The basic method of Ising model is to look at each node or site on a graph as representing two possible configurations. We often call them up spin and down spin. In this case, we can physically portray them as actual spins, but in fact in physics, they only represent certain properties that can be modeled using two states – they are often not electron spins. This model was originally developed to study the properties of systems with interacting magnetic dipoles where two spins simulate two orientations of the dipole.

Between each two nodes there is always a bond similar to that between two atoms. The magnitude and meaning of these bonds are dependent on the relationship between two nodes and what the nodes themselves represent. We consider the simple case where the spins can take values ± 1. Considering the value of the up spin to be $s_i = +1$, down spin to be $s_i = -1$. If two adjacent spins, call them s_1 and s_2, have the same direction spins, the bond takes the value $s_1 s_2 = +1$; if they have opposite spins, the bond has the value $s_1 s_2 = -1$. The total energy in a Ising model system is the sum of all these values of bonds. If we consider the different spins as the only contributing factor of the internal energy, we can get energy of each bond,

$$E_{ij} = -J s_i s_j \tag{3.1}$$

where J is a quantity with the units of energy and sets the energy scale for the model. For $J > 0$, the net negative sign indicates that the low energy configuration corresponds to aligned spins. Thermodynamically therefore, such a system will prefer all spins aligned in what is called a *ferromagnetic* configuration. If $J < 0$, we get negative energies when neighboring spins are anti-aligned, an *anti-ferromagnetic* configuration.

The total energy of the system is given by

$$E = -J \sum_{\langle ij \rangle} s_i s_j \tag{3.2}$$

where $\langle ij \rangle$ indicates that the sum is only over adjacent (or nearest) neighbors.

In this case, magnitude of the spin at each lattice site is not included in the total energy, which makes the model simpler. s_i and s_j represent the adjacent spin in the system. Setting J to -1, we show two examples of how a 4×4 Ising model system looks like with different spins.

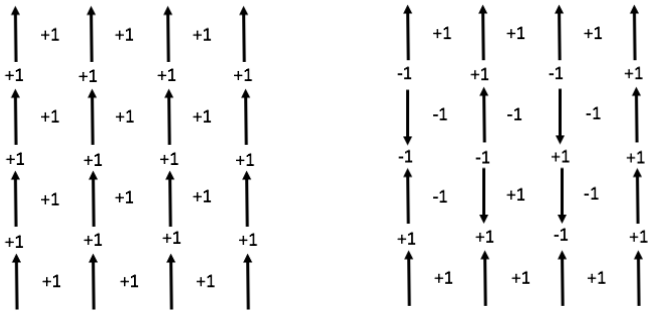

Figure 3.1: Ising model on a 4×4 square with internal energy of each bond included. Left: All the spins are pointing up, resulting in the value of +1 for all the bond energy. Right: 4 spins are pointing down in the system. The bond between spins with different direction has energy -1, whereas the spin with the same direction has bond energy +1

As shown in Figure 3.1 on the right, the third row has two adjacent down spins. The internal energy between is still the same as the internal energy of two adjacent up spins, with value +1.

If we add an external magnetic field, then the spin at each site appears in the energy. In this situation, we simply need to add up the magnetic energy carried by each spin to the original energy. Therefore, we obtain formula,

$$E = -J \sum_{\langle ij \rangle} s_i s_j + H \sum_i s_i \tag{3.3}$$

where H is the magnitude of the energy of each spin in the external magnetic field. When magnetic field is applied, the system is no longer simple. The external field acts to increase or decrease the total energy depending whether the spins are aligned or anti-aligned with it. This creates a competition between the two terms above, especially if J is negative. Adding one more factor increases the complexity and affects the system behaviors as a whole. In our research, we study the Ising model

under both conditions and they appear to be very different in lots of cases, and by comparing these two gives us insights to how symmetry plays a role in the linked-cluster expansion.

3.2 Potts Model

When Ising model simulates systems with specifically two possible values for each "spin", Potts model[6] generalizes this so the spins can take many values. Potts Model can therefore be deemed as the generalized version of Ising model and they implement very similar ideas.

In Potts Model, instead of having +1 and -1 as value of the bonds, each bond has value +1 or 0 depending on whether the adjacent spins have the same direction or not. In Potts Model, there can be more than two directions for a spin and the number of spins is called q. In this case, Potts model can also be called the q-state Potts model. When $q = 2$, the model is similar to Ising model with only two directions of spins, but with different values for the internal energy,

$$E = -J \sum_{\langle ij \rangle} \delta_{s_i s_j} \tag{3.4}$$

where,

$$\delta_{s_i s_j} = \begin{cases} 1, & \text{if } s_i = s_j, \\ 0, & \text{if } s_i \neq s_j. \end{cases} \tag{3.5}$$

In this case s_i can take values from $1 \dots q$. For $q = 2$, $s_i = \{1, 2\}$. Superficially, this doesn't look like the Ising model, but can be brought into the standard form by a simple change of variables. As we can see from Equation 3.4, up to a constant, the values of the bonds between adjacent spins s_i and s_j are the same as those of the Ising model for all q. By assigning more directions of spins, there are more possible configurations of the system, and this influences its properties. A major result of this work involves showing that the Potts model also has the unique property found for the Ising model under the linked-cluster expansion. We show this for arbitrary q.

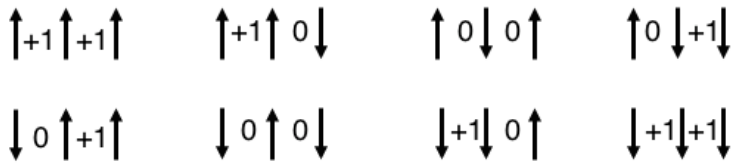

Figure 3.2: All possible configurations for q=2 Potts model with three total spins. The numbers in between spins represent the internal energy between the two adjacent spins with J = -1

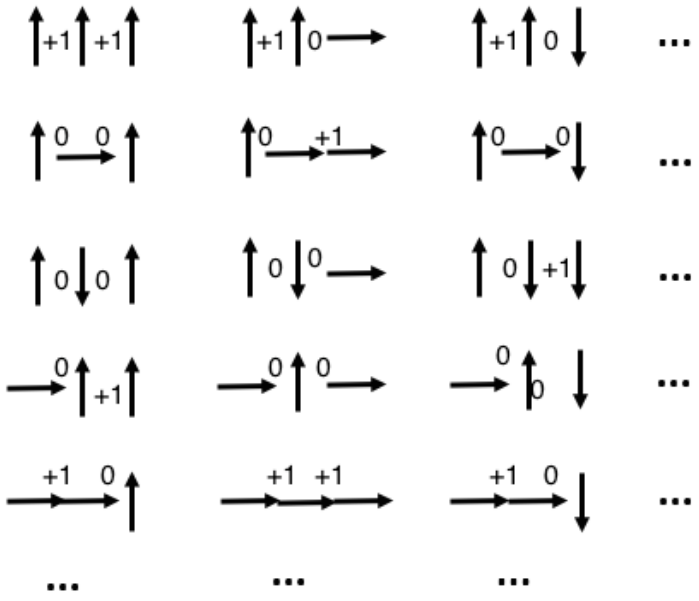

Figure 3.3: Some possible configurations for q=3 Potts model with three total spins. The numbers in between spins represent the internal energy between the two adjacent spins with J = -1.

As shown in Figure 3.2, this is only a simple system with three lattice sites. When $q = 2$, the spins point either up or down. However, for figure 3.3, when $q = 3$, the spins point up, right, or down with three directions in total.

Potts model assigns more properties to each individual lattice site therefore simulates more complicated systems compared to the Ising model.

3.3 Ising Model and Potts Model Application

Other than modeling physical systems, Ising model and Potts model are also applicable in other fields of study such as socio-economic systems, business decision making, language change and urban segregation [7]. All the applications of Ising and Potts model on social science introduced can be found in Refs. [7, 8, 9].

For business managers in analyzing the world economy, their opinions could impact each other's just like the ferromagnetic system. In this case, the Ising model in two-dimensional can simulate how the average opinion is more leaning towards positive, negative, or neutral by setting up a certain number of lattice sites and the relationship between each two lattice sites. In a Ising ferromagnetic system, there is a tendency for all the spins to align, and contribute to magnetization, which is similar to how the overall opinions would tend to go one way. However, if there are too many positive and negative professional opinions spreading out, then the crowd would not be able to lean towards one opinion. This is also similar to the Ising ferromagnetic system that, if there is too much noise within the system (high temperature), there could be little magnetization.

For urban segregation, the Nobel economist Thomas Schelling proposed the similarity between Ising model and segregation. If people are allowed to choose where to live in one area by their own preference but no other factors, the segregation is similar to Ising model with $T = 0$. However, when there are more and more factors included in urban segregation such as racial pressure and bad living environment in certain areas, the segregation is similar to when T starts to get higher. In this case, Potts model could also be utilized in simulating this system, due to the more factors contained in the situation.

Language change is a good example as well. Nettle uses Ising model to simulate

how one language that is spoken by everyone can be replaced by another (or one language feature being replaced by another language feature). This mostly depend on population size, as how the rate of language switch would be affected by the population. This is then similar to the rate of magnetization due to the lattice size. Setting temperatures higher and increase the number of factors in the system (Such as using Potts model instead), the system starts to magnetized slower and slower. Similar to language switch, the larger the population, the slower the language change happens. There are more papers related to language switch simulation, see Ref. [10, 11].

Chapter 4

Lattices

Spin models merely simulates the relationship between two adjacent particles in a system. However, the number of particles, and how the particles are arranged also affect the internal energy. For instance, if the system only has a single line of particles, then one particle is only attached with two bonds. However, if the system is a cube of particles, then one particle is attached with six bonds, which results in different physics of the model. Therefore, it is necessary to provide generalizations for these different structures of the particle systems, and analyze the same model under different conditions. In this chapter, we will introduce spin models on specific lattices and introduce the partition functions of these.

Lattices are geometric representations of how we look at a system [3, 2] and they could be in different dimensions such as a ring, a cube, a two-dimensional triangle, or even a sphere. The lattice sites within the system represent the spins, and as the number of spins increases, the number of lattice sites increases. The different dimensions contain different physics for us to observe, and allow us to systematically interpret how each of them affects the physics. However, there are also lattices that don't necessarily have a well-defined dimensionality. The idea of lattices is significant in the study of materials because it has very practical applications in any model study or even industrial manufacture. For instance, nanotechnology deals with very thin layers of materials that can be represented by the two-dimensional lattice, and artificial diamonds are made from changing the carbons from one lattice type to another.

4.1 One-Dimensional Lattice

One-dimensional lattice is the most simple lattice among all. It is basically a line of lattice sites. Even though it is relatively simple, the physics behind gives us intuitions to the very essential behaviors of the lattice models. In addition, by knowing the one-dimensional phenomenon, we could apply it to more complex system which could be dissected analogously to one-dimensional cases.

Figure 4.1: One-Dimensional Lattice: n=2, n=3, n=4

Here is the graphic example as how one-dimensional system looks like (Fig. 4.1, and n represents the number of lattice sites in the system. The lines between the lattice sites are the internal bonds that have certain energies.

When $n = 1$, there is only one lattice site with no bond in between, the energy is 0 for all configuration, unless there is an external magnetic field as discussed earlier.

1D Ising Model Partition Function

For the Ising model, when $n = 1$, there are two configurations with the particle having up spin or down spin. However, for each two of the spin, there is no internal bond, thus the energy $E = 0$. Using the formula for partition function: $Z = \sum e^{-E\beta}$ (it is customary to write the log of the partition function as it scales linearly with system size, unlike the partition function, which scales exponentially),

$$\log Z_1 = \log(e^0 + e^0) = \log(2) \tag{4.1}$$

When $n = 2$, there are two lattice sites on a line and each lattice sites have two configurations. The total number of configurations is then $2 \times 2 = 4$, two of which have aligned spins, and the other two with anti-aligned spins. We also know that

$E = -1$ for different spin, and $E = 1$ for same spin (we set $J = -1$). Therefore, the partition function becomes

$$\begin{aligned} \log Z_2 &= \log(e^{-\beta} + e^{-\beta} + e^{\beta} + e^{\beta}) \\ &= \log(2e^{-\beta} + 2e^{\beta}) \\ &= \log(2 \times (e^{-\beta} + e^{\beta})) \\ &= \log(2) + \log(e^{-\beta} + e^{\beta}) \end{aligned} \tag{4.2}$$

When $n = 3$, with each lattice site having two spins, the number of configurations become $2^3 = 8$. The partition function becomes

$$\begin{aligned} \log Z_3 &= \log(2 \times e^{-2\beta}) + 4 \times (e^{0\beta} + 2 \times e^{2\beta}) \\ &= \log(2 \times (e^{-2\beta} + 2e^{0\beta} + e^{2\beta})) \\ &= \log(2) + 2\log(e^{-\beta} + e^{\beta}) \end{aligned} \tag{4.3}$$

As we can see, the partition function gets more complicated as number of particles in the system goes higher.

Boundary conditions

In the 1D lattice, each site has two bonds emerging from it, except the ones on the ends. There are two possible ways to treat these. We can leave it as it is, and such a setup is said to have *open* boundary conditions. Alternatively, we could attach a bond between the first and the last site creating *closed* or *periodic* boundary conditions. For a sufficiently large system size, the choice doesn't affect the results for physical quantities, but for small sizes it does. In the linked-cluster expansion, due to the nature of the construction, we always use open boundary conditions.

4.2 Square Lattice

When one-dimensional lattice represents the most simple cases, two-dimensional lattices brings more physics. Square lattice is a typical 2-D system that vertices are all

on the corner of a square, whereas the lines are the sides of the squares. In open boundary conditions, each lattice sites at one end of the graph has no connection with lattice sites other than the adjacent ones. On the other hand, for periodic boundary conditions, the vertices on the end of one side are connected to the other end as if there is an extra line. It converts the 2D square lattice into a torus (donut) geometry.

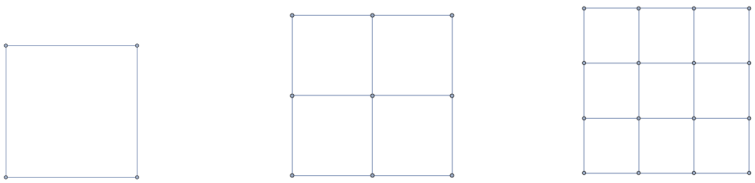

Figure 4.2: Two-Dimensional Square Lattice: n=4, n=9, n=16

Here are the examples of how two-dimensional lattices look like. Same as the one-dimensional lattice, when $n = 1$, there would be only a single lattice site in the system. Therefore, the physics of $n = 1$ is the same for every lattice. When the square is taken into consideration, we can see that one particle could have more than two bonds attached to it (such as the middle one in $n = 3$, and the middle four lattice sites in $n = 4$). The loops of the small squares in a big square are what bring interesting new physics in the system. Through the calculation of partition function, we are able to see the differences.

2D Partition Function

When $n = 1$, we have the exact same graph as 1D system. Therefore, the partition function is simply $\log Z_1 = \log(2)$.

In a square lattice, the next possible value is $n = 2 \times 2$. There are four particles in the system, and each has two possibilities. Therefore, there are $2^4 = 16$ configurations. Out of the 16 configurations, 12 of them have total energy of 0, with two +1, and two -1. Beside, there are two configurations that they all have the same spin relating to their neighbors and two configurations that have all different spin

relating to their neighbors. Accordingly, we can derive that

$$\begin{aligned} \log Z_{2\times 2} &= \log(12 \times e^{0} + 2 \times e^{-4\beta} + 2 \times e^{4\beta}) \\ &= \log(12 + 2e^{-4\beta} + 2e^{4\beta}) \end{aligned} \tag{4.4}$$

The next possible lattice has $n = 3 \times 3$, the complexity compounds. There are 9 particles in the system which leads to $2^9 = 512$ configurations. Under this circumstance, it is hard to calculate the partition function by hand. Using computer calculation, we obtain

$$\begin{aligned} \log Z_{3\times 3} = &\log(144 + 2e^{-12\beta} + 8e^{-8\beta} + 32e^{-6\beta} + 46e^{-4\beta} \\ &+ 96e^{-2\beta} + 96e^{2\beta} + 46e^{4\beta} + 32e^{6\beta} + 8e^{8\beta} + 2e^{12\beta}) \end{aligned} \tag{4.5}$$

The partition function appears to be particularly long due to many different configurations. However, we can still obtain information from the equation we got. We can tell that there are 144 configurations that have internal energy zero, 2 configurations with internal energy -12, and 8 configurations with energy -8, etc.

For $n = 16$, we can imagine how complex the system could be. With 16 particles in the system, there are $2^{16} = 65,536$ configurations to be considered.

The partition function obtained from the computer is,

$$\begin{aligned} \log Z_{4\times 4} = &\log[11472 + 2e^{-24\beta} + 8e^{-20\beta} + 32e^{-18\beta} + 72e^{-16\beta} + 224e^{-14\beta} + 584e^{-12\beta} + 1216e^{-10\beta} \\ &+ 2638e^{-8\beta} + 4928e^{-6\beta} + 7344e^{-4\beta} + 9984e^{-2\beta} + 9984e^{2\beta} + 7344e^{4\beta} + 4928e^{6\beta} + \\ &2638e^{8\beta} + 1216e^{10\beta} + 584e^{12\beta} + 224e^{14\beta} + 72e^{16\beta} + 32e^{18\beta} + 8e^{20\beta} + 2e^{24\beta}] \end{aligned} \tag{4.6}$$

whereas it is possible to compute the partition function for larger systems, the task takes increasingly longer as the number of configurations grows faster than exponentially. For instance, for $n = 25$, we have a total of $2^{25} \approx 33.5$million. To put this in context, a macroscopic chunk of metal contains over 10^{23} particles leading to almost $10^{10^{23}}$ configurations.

4.3 Bethe Lattice

Bethe lattice is a type of lattice that could be both two-dimensional or three-dimensional, although the dimensionality of this lattice isn't easy to define [12] [13].

Bethe lattice can be considered as a tree graph with only two growing branches. Each of the new branch would grow two new branches so on and so forth. This can simulate some growing process of crystals that occurs in nature. For Bethe lattice, when $n = 1$, there is only one lattice site, and $n = 2$ with two lattice sites and a line. Up to $n = 3$, Bethe lattice has the same structure as one-dimensional lattice.

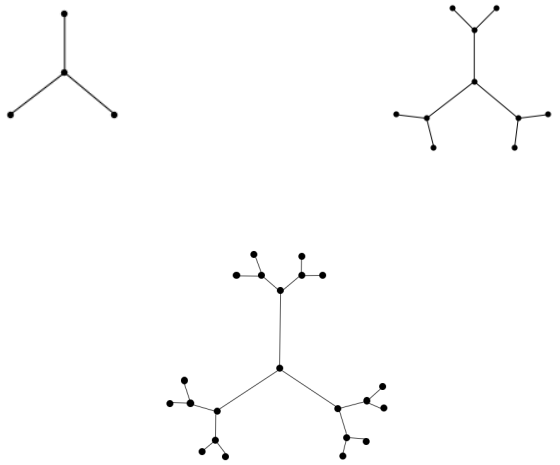

Figure 4.3: Bethe Lattice: $n = 4$, $n = 10$, $n = 22$

Bethe Lattice Partition Function

As we can see from the graphic examples in Fig. 4.3, the first three lattices are the same with one dimensional lattice. Starting from $n = 4$, the number of edges are still the same as one-dimensional lattice, but with different degrees (the degree of a vertex is the number of edges connected to it) for the vertices.

$$\begin{aligned} \log Z_1 &= \log(e^0 + e^0) = \log(2) \\ \log Z_2 &= \log(2) + \log(e^\beta + e^\beta) \\ \log Z_3 &= \log(2) + 2\log(e^{-\beta} + e^\beta) \end{aligned} \tag{4.7}$$

Equation 4.7 is derived from equation 4.1, equation 4.2 and equation 4.3, which represent the partition functions for the first three lattice sites of the particle system.

Chapter 5

Graph Theory

The models and lattices that we study are all simplifications of how physical systems can look like and behave. Normally, we use vertices and edges to represent the particles and internal bonds within a physical model. The most typical lattice models are: one-dimensional lattice that is basically a line, two-dimensional lattice with square-like appearance and three-dimensional lattice that could either being simply a cube, or a cube with a vertex at the center. There are also more lattice models as Bethe lattice that grows like trees. In this chapter, I will be focusing on talking about one-dimensional, two dimensional and Bethe lattice. Based on the graphic representations we have (vertices and edges), physicists and mathematicians developed new ways of implicating geometry into physics model study.

Graph theory is a mathematical method in studying various properties of abstract lattices, which are only defined by the number of nodes or vertices and the set of edges between these vertices. It also assists us to better understand the physics of a system and studying the linked-cluster expansion. In order to represent all geometric situations in model studies, graph theory provides names and meanings for different types of relationships between graphs, such as isomorphic graphs, subgraphs, and section graphs that will be explained later in the chapter. Along with these definitions, there are also theorems that directly lead to the linked-cluster expansion and its application to physics.

Most important to this work, graph theory helps us learn how to identify the

relationships between a smaller section of a graph and the graph itself. Thus, we can apply this to the study of a smaller section of the system in relation to the system as a whole.

5.1 Basic Notions

There are several ways to find the relationship between two graphs, but there are a few definitions that and central to our study. This section will be focusing on the very basic ideas of what graph theory includes, and some general concepts that explain how we can apply graph theory to our study of physics.

The graphing style that we use here are all dots (lattice sites) and lines, imitating particles and bonds in a physical system. We name all the dots in a graph *vertices* and lines of a graph *edges*. One edge has to have vertices at both end, but one vertex can be hanging by itself. Therefore, we developed a specific way of numbering to represent graphs that have different numbers of vertices and edges. We start with only one vertex to be the first graph g_1. By adding one more vertex to the system, it comes g_2. Each time after adding one more vertex, there should be an edge added before another vertex is added. Therefore, g_3 has two vertices and one edge connecting them. With the same reasoning, we can obtain g_4, g_5, g_6, and g_7 as the following,

Figure 5.1: g_1

Figure 5.2: g_2

Figure 5.3: g_3

Figure 5.4: g_4

Figure 5.5: g_5

Figure 5.6: g_6

Figure 5.7: g_7

As we can see from the above examples, the rule for numbering is to first add one vertex and then connect it with an edge. g_4 has one additional vertex compared to g_3 and g_5 has one additional edge compared to g_4, because we need to fill in the gap between two unconnected vertices before we go to the next level of g. However, g_4 has zero edges compared to g_3. When we are able to number all the lattice graphs, we can do calculations with the graphic representations later on in the theorem section.

However, after the first six graphs, the shapes start to become different as the ways of growing become different as well. For instance,

Figure 5.8: g_6

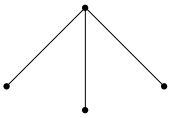

Figure 5.9: g_7

Embeddings

For a specific graph G, the subtraction of some vertices and edges would result in a smaller graph G' that can be embedded in G. There are two types of embeddings: *strong embeddings* and *weak embeddings*. For a strong embedding, G has to have an exact section that contains all the vertices and edges that G' has without having or missing one edge, and are connected similarly. Whereas for a weak embedding, G only has to have the same number of vertices as G' but not necessarily the same number or set of edges. The graph numbers introduced actually helps us better explain this situation.

As shown in Fig. 5.2 g_2 has two only two vertices and zero edge. If we want to weakly embed g_2 onto g_6, there are three ways of embeddings. However, if we want

to strongly embed g_2 onto g_6, there is only one way, as only one pair of the vertices in g_6 have no edge connected.

Graph Types

When two graphs have the exact same numbers of vertices and edges and they are all connected in the same way without being oriented at a specific angle, they are called *isomorphic graphs*, where iso means "the same" and morph means "shape" in Greek. A set of isomorphic graphs is shown in Fig. 5.10.

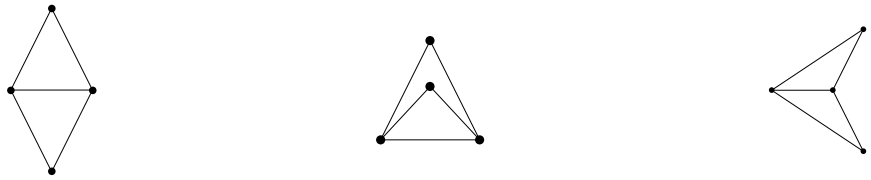

Figure 5.10: Isomorphic Graphs

These three graphs in Fig. 5.10 appear to have very different shapes. However, they all have four vertices and five edges in one graph. Out of the four vertices, two vertices are connected to each other and the other two vertices at the same time with three total edges. As well, the other two vertices individually are not connected to each other but have edges of two connected to the initial two vertices.

Another type of graphic relation that we want to talk about in this thesis is *homeomorphic* graphs. Before we talk about homeomorphs, it is necessary to first learn the concepts of *insertion* and *suppression*. Suppression is taking out a vertex A of degree 2 from a graph G along with the two edges connected to it, and joining the two vertices that were originally connected to the other sides of the edges with one edge. The reverse of this process is then insertion.

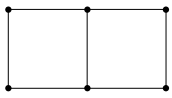

Figure 5.11: Before Suppression

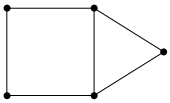

Figure 5.12: After Suppression

For any graph G, the insertion or suppression would result in a new graph G' that is defined as the homeomorphic graph of G. Therefore, Fig. 5.11 on the left is the homeomorph of Fig. 5.12.

In addition, based on what we discussed about strong and weak embeddings, we have graph types as *section graphs* and *subgraphs*. Section graphs of a graph G are basically graphs that can be embedded strongly onto the graph, and subgraphs are graphs that can be embedded weakly onto it. Of course, section graphs can also be embedded weakly onto the graph G, but subgraphs cannot be embedded strongly onto the graph. Therefore, sections graphs can also be considered as the subgraphs, but not vice versa.

Figure 5.13: Section Graph: g_7 on the left is the section graph of the graph on the right

For the graph g_7 in Figure 5.13, it can be strongly embedded on the right graph in two ways, upper triangle and lower triangle. In addition, g_7 can also be weakly embedded on the right graph in the same two ways. However, subgraphs can only be embedded weakly into the system.

Figure 5.14: Subgraph: g_4 on the left is the subgraph of the graph on the right

As we can see from Figure 5.14, the graph on the left can be weakly embedded

on the right graph in 6 ways, with three for the upper triangle and three for the lower triangle. A subgraph cannot be strongly embedded on the original graph but contains the same number of vertices as part of the original graph. Compared to section graphs the concept of subgraphs is what we use more often in the study of this research thesis.

For instance, we would be interested in looking at the properties of a two-dimensional lattice. If we take a two-by-two square lattice as an example, we can find out its subgraphs as shown in Fig. 5.15 and 5.16.

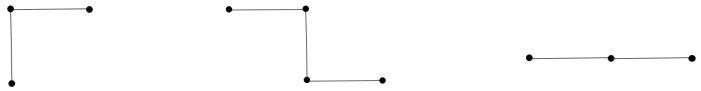

Figure 5.15: Subgraphs

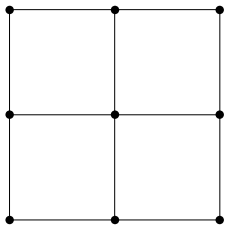

Figure 5.16: 2D Square

Therefore, we can also see that there are many different section graphs and subgraphs this two-by-two square lattice can have and this significantly helps with further analyzing a system using linked-cluster expansion method.

5.2 Theorems

With all the different types of graph relations, we are mostly interested in looking at the graphs produced by strong and weak embeddings. Therefore, there are a

few theorems in graph theory that can help us better understand the mathematical part of the study, which are described in more details in paper [3]. As mentioned previously, graph g_2 has the same number of vertices but not edges as a part of the graph g_6, then it can be weakly embedded on the graph. When a graph g_3 has same number of edges and vertices as g_6, and they are connected in the same way as a part of G, then it can be strongly embedded. Therefore, we can also obtain the number of embeddings,$(g_2 : g_6) = 3$

Figure 5.17: g_1

Figure 5.18: g_2

Figure 5.19: g_3

Figure 5.20: g_4

Figure 5.21: g_5

Figure 5.22: g_6

Figure 5.23: g_7

where parenthesis $(g : G)$represent the number of weak embeddings and square brackets $[g : G]$ represent the number of strong embeddings.

Therefore, we can calculate a list of strong and weak embeddings,

$$\begin{aligned}
(g_1 : g_7) &= 3, \qquad [g_1 : g_7] = 3, \\
(g_2 : g_7) &= 3, \qquad [g_2 : g_7] = 0, \\
(g_3 : g_7) &= 3, \qquad [g_3 : g_7] = 3, \\
(g_4 : g_7) &= 1, \qquad [g_4 : g_7] = 0, \\
(g_5 : g_7) &= 3, \qquad [g_5 : g_7] = 0, \\
(g_6 : g_7) &= 3, \qquad [g_6 : g_7] = 0, \\
(g_7 : g_7) &= 1, \qquad [g_7 : g_7] = 1,
\end{aligned} \tag{5.1}$$

Therefore, it is not hard to understand this theorem,

$$(g_i : G) = \sum_i (g_i : g_j)[g_j : G] \tag{5.2}$$

The number of weak embeddings of graph g_i on graph G, is the sum of the products of number of weak embeddings of graph g_i on all other graphs represented by g_j and the number of strong embeddings of graph g_j on graph G. Here, both g_i and g_j are both subgraphs of graph G.

For instance, if select g_3 as g_i and g_7 as G, all the other subgraphs that have the same or more vertices as g_3 are: g_3, g_4, g_5, and g_6. Calculating the left side of Equation (5.2) we get $(g_3 : g_7) = 3$. The right side then is

$$\begin{aligned}
&(g_3 : g_3) \times [g_3 : g_7] + (g_3 : g_4) \times [g_4 : g_7] + (g_3 : g_5) \times [g_5 : g_7] + (g_2 : g_6) \times [g_6 : g_7] \\
&= 1 \times 3 + 0 \times 0 + 1 \times 0 + 2 \times 0 = 3.
\end{aligned} \tag{5.3}$$

This can also be represented by matrix. If we rewrite the elements,

$$(g_i; G) = p_i, [g_j; G] = P_i, (g_i; g_j) = a_{ij}, \tag{5.4}$$

then Equation (5.2) becomes,

$$p_i = \sum_i a_{ij} P_j, v_i = v_j \tag{5.5}$$

which we could also obtain,

$$p(r) = A(r)P(r) \tag{5.6}$$

For more detailed explanations see paper [3] [14] [15]. This theorem forms the basis of the linked-cluster expansion, described in the next chapter.

Chapter 6

Linked-Cluster Expansion

The linked-cluster expansion is an approximation method that calculates the physical observable of a model system. Before we talk about the linked-cluster expansion, it is interesting for us to look at other types of expansions to obtain a better idea of what expansion methods are like. There are different types of expansions as high-temperature expansions [16], low-temperature expansions [17] and the linked-cluster expansions. In calculating physical properties of different systems, it is often difficult to calculate those for exact finite-temperature systems. Therefore, using the method of expansions could let us obtain results faster. Similar to Taylor expansion series, these expansion methods provide formula that allows us to approximate a function by adding up terms of increasing order. In this chapter, I will briefly explain high-temperature and low-temperature expansions with detailed focus on the linked-cluster expansion, which is the concentration of the research. We will then present the main results of this work.

6.1 High-Temperature Expansions

A high-temperature expansion is essentially a Taylor series expansion of the partition function around $T = \infty$. We describe this with the help of the Ising model. As

described in chapter 3, we saw that the energy for Ising model is

$$E = -J \sum_{\langle i,j \rangle} s_i s_j \tag{6.1}$$

and partition function is defined as,

$$Z = \sum_{\{E\}} e^{-\beta E} \tag{6.2}$$

where $\{E\}$ is shorthand for sum over all configurations of energy E as well as all energies. The Boltzmann factor β is the inverse of temperature $\beta = \frac{1}{k_B T}$ where k_B is the Boltzmann constant. The high-temperature expansion is therefore an expansion around $\beta = 0$. Therefore, the partition function can be written as

$$Z = \sum_{\{E\}} e^{\beta J \sum_{\langle i,j \rangle} s_i s_j} \tag{6.3}$$

If we define $K = \beta J$, we can obtain expansion

$$Z = \sum_{\{s\}} \prod_{\langle i,j \rangle} e^{K s_i s_j} = \sum_{\langle s \rangle} \prod_{\langle i,j \rangle} \sum_{l=0}^{\infty} \frac{K^l}{l!} (s_i s_j)^l \tag{6.4}$$

For Ising model, s_i and s_j have values of +1 or -1. The term $\langle (s_i s_j)^l \rangle$ can be considered as the l-fold bonds within the system. Since $K = \beta J$ and $\beta = (k_B T)^{-1}$, we can infer that $K = (k_B T)^{-1} J$. If so, when T is very high, K would have a very low value based on their inverse relationship. As the term $e^{K s_i s_j}$ can be expanded to series $\sum_{l=0}^{\infty} \frac{K^l}{l!} (s_i s_j)^l$, the individual value of $\frac{K^l}{l!} (s_i s_j)^l$ would get smaller and smaller as l gets higher. Therefore, the series $\sum_{l=0}^{\infty} \frac{K^l}{l!} (s_i s_j)^l$ would end up adding a smaller and smaller value until $\frac{K^l}{l!} (s_i s_j)^l$ is finally zero. This means the series would eventually converge to a certain value as there is no more numbers to add to the series. Therefore, Equation 6.4 shows that the partition function converges at high temperatures (for more explanations see Ref. [16]). On the other hand, if the temperature is low, the series gets larger as l gets larger, thus it never converges.

Other than Ising model, this high-temperature expansion is also applied other models as quantum Heisenberg model that is not described in this thesis and be generally applied to any model. (see ref [18])

6.2 Low-Temperature Expansion

For low-temperature case, T $\to$ 0 and $\beta \to \infty$. At very large β, only very small E contributes to the partition function. For large E, the factor $e^{-\beta E}$ becomes very small. In order to do this quantitatively, we write the energy $E_n = E_0 + E_n - E_0$, where n is an index that enumerates the different configurations, chosen so that larger n corresponds to larger E_n. The partition function obtained from expansion is then

$$Z = e^{-\beta E_0}[1 + \sum e^{-\beta(E_n - E_0)}]. \tag{6.5}$$

E_0 is the "ground state" energy, i.e., it corresponds to the configuration that gives the lowest energy and E_n is the n^{th} excited state energy. If the gap between these two energy level is ϵ_n, then the Boltzmann factor can be written as $e^{-\beta\epsilon}$. Now, since β is very large, the major contributions to the sum comes from those configurations for which ϵ_n is small. We can write a formal expansion using this.

The high-temperature and low-temperature expansions give us a very good sense of the physics of a system at two extremes, and as we add terms to these expansions we are able to access other temperatures. However, these expansions tend to converge very slowly and are not optimal for finite temperature calculations.

6.3 Linked-Cluster Expansion

We now look at the linked-cluster expansion method (LCE) [3, 4, 17] that serves as another approximation method. Based on the background we have introduced and explanations of how lattices and models work, as well as the idea of partition function in statistical mechanics, we are prepared to understand this new method of studying different systems. Just as other types of expansions, the linked-cluster expansion is simply a way to approximate different properties of a system. The idea of the linked-cluster expansion is that, for any extensive (i.e., that scales with system size) physical property O of a system (such as log of the partition function), its value per lattice sites could be calculated by the contribution of each embeddings:

$$\frac{O(L)}{N} = \sum_c M(c) \times W_o(c) \tag{6.6}$$

where N represents the number of lattice sites (particles) in a system, $M(c)$ represents the multiplicity of each particular embedding of a larger system (number of strong embeddings, introduced in Chapter 5), and $W_o(c)$ represents the weight of different clusters, obtained from the Boltzmann weight for that particular subgraph. As other factors are already introduced in the previous chapters, the idea of weight is new to us and is crucial in the study of the linked-cluster expansion (for more references on LCE including some recent applications, see [19, 20, 21]).

Weight

The LCE builds a larger system by systematically adding units, i.e., vertices. The increasing number of lattice sites would result in different physical properties of the system. Therefore, we are interested in how adding an additional site change the behaviors of the system. In other words, we want to know how adding one more particle/site in the system can contribute to the change in any physical quantity such as partition function. Therefore, the idea of weight was introduced to represent the additional contribution of having an extra particle in a model. In order to calculate weights, we simulate this process by adding an extra vertex to a graph and calculate the change in geometry of the graphs using the idea of embeddings in graph theory.

The definition of weight is,

$$W_O(c) = O(c) - \sum_{s<c} W_O(s). \tag{6.7}$$

In this case $O(c)$ is the partition function $\log Z$ for Ising model. The term $\sum_{s<c} W_O(s)$ represents the sum of the weights of all the subgraphs.

Physically speaking, W_1 is simply the contribution of having one particle in the system compared to zero particles. W_2 starts to provide us with an additional contribution, meaning, in the two particle system, the extra one comparing to W_1 system, has contribution of W_2. Meanwhile, with the same reasoning, W_3 is then the contribution of the extra one particle in the three-particle system, comparing to two-particle system. This is also what we considered as inclusion-exclusion principle due to the cancellations of all previous terms in an equation. Therefore, what we obtained from this calculation represents the additional contribution of one particle under different numbers of particle system. Based on this knowledge, we can start applying this idea onto different models and lattices.

As we can imagine, for different lattices and models, there are different ways to increase each additional particle resulting in different development of the expansion. The models and lattices we included in this work are: one dimensional Ising model (with and without magnetic field), Potts model, and the Ising model on the Bethe lattice. The idea of weight has already been applied on one-dimensional and two-dimensional Ising model without magnetic field (see Ref. [1]). There, it was shown that the weights vanish for all system sizes larger than $n = 2$, giving us the result of an infinitely large system using one with just two sites. Such a dramatic simplification does not occur in any other approximation scheme. However, the question as to why this happens and if any other model showed this property was left open.

In this thesis, we show new results that addresses the above open question by studying the Ising model with a magnetic field, the Potts model, and the Ising model on the Bethe lattice. First, we review the known results.

6.4 1D-Ising Model Periodic Boundary Condition

One-dimensional Ising model is the simplest model of all. Take partition function as the physical observable we want to look at, which for Ising model is $Z = \sum e^{-E\beta}$. As described in Chapter 4, we know that one-dimensional lattice with one, two and three particles look like the graphs shown in Figure 6.1,

Figure 6.1: One-Dimensional Lattice: $n = 1$, $n = 2$, $n = 3$ (n_1, n_2, n_3)

For n_1, there is no other graphs with less vertices can be embedded on n_1, thus there is no weights for subgraphs. Using the definition of weight (equation 6.7), weight for n_1 is simply its own partition function without subtracting any other terms. For n_2, it has graph n_1 as its only subgraph and the number of embeddings is $(n_1;\, n_2) = 2$. Therefore, the weight for n_2 is the partition function of graph n_2 subtracting all the other weights of n_1. Since there are 2 ways of embeddings, the partition function should subtract the number of embeddings of n_1 times the weight

of n_1, $(n_1; n_2) \times W_1$. It becomes, $\log Z$ - 3 $\times W_1$. For n_3, it has subgraphs n_1 and n_2, with embeddings of $(n_1; n_3) = 3$ and $(n_2; n_3) = 2$. Therefore, the weight for n_3 is its partition function subtracting all the weights of the subgraphs multiplied by the number of embeddings, $\log Z$ - (2 $\times W_2$ + 3 $\times W_1$ From the explanation above, we can write down the set of weight equations as,

$$\begin{aligned} W_1 &= \log Z_1(\beta) = \log(2) \\ W_2 &= \log Z_2(\beta) - 2W_1 = \log(e^{\beta} + e^{-\beta}) - \log(2) \\ W_3 &= \log Z_3(\beta) - 2W_2 - 3W_1 = \log(2) + \log(2 + e^{-2\beta} + e^{2\beta}) \\ &\quad - (\log(e^{\beta} + e^{\beta}) - \log(2)) = 0 \end{aligned} \tag{6.8}$$

where W_1, W_2, and W_3 are the weights for n_1, n_2 and n_3 respectively. W_2 represents the contribution of adding that one extra particle in graph n_2 compared to n_1, and W_3 represents the additional contribution of the particle compared to graph n_2. We can see that $W_3 = 0$, which means there is no additional contribution to the system by adding more particle when there are already two particles in a 1-D Ising model system. Therefore, we wonder if this represents the rest of the weights would go to zero as well. This potentially means, no matter how many particles are added to the two existing particles, there would be no additional effect on the physics of the system.

We then use the same method to calculate W_4, W_5, W_6. For W_4, there are two ways of embeddings for three particles, $(n_3; n_4) = 3$; three ways for two particles, $(n_2; n_4) = 3$; and four ways for one particle, $(n_1; n_4)$. Therefore, the weights are,

$$\begin{aligned} W_4 &= \log Z_4 - 2W_3 - 3W_2 - 4W_1 \\ W_5 &= \log Z_5 - 2W_4 - 3W_3 - 4W_2 - 5W_1 \\ W_6 &= \log Z_6 - 2W_5 - 3W_4 - 4W_3 - 5W_2 - 6W_1. \end{aligned} \tag{6.9}$$

Based on the previous calculations, we know that $W_3 = 0$, thus we can calculate that

$$\begin{aligned} W_4 =& \log Z_4 - 2W_3 - 3W_2 - 4W_1 \\ =& \log Z_4 - 0 - 3W_2 - 4W_1 \\ =& \log(2) + \log(e^{-3\beta} + 3^{3\beta} + 3e^{-\beta} + 3e^{\beta}) - 3 \times (\log(e^{\beta} + e^{-\beta}) \\ & - \log(2)) - 4 \times \log(2) \\ =& \log(e^{-3\beta} + 3^{3\beta} + 3e^{-\beta} + 3e^{\beta}) - 3 \times \log(e^{\beta} + e^{-\beta}) \\ =& 0. \end{aligned} \tag{6.10}$$

Therefore, calculating $\log Z_5$ and $\log Z_6$ using computers, we can plug into these equations,

$$\begin{aligned} W_5 =& \log Z_5 - 2W_4 - 3W_3 - 4W_2 - 5W_1 \\ =& \log Z_5 - 0 - 0 - 4W_2 - 5W_1 \\ =& \log(2) + \log(6e^{-\beta} + e^{-4\beta} + 4e^{-2\beta} + 4e^{2\beta} + e^{4\beta}) - 4 \times (\log(e^{\beta} + e^{-\beta}) \\ & - \log(2)) - 5 \times \log(2) \\ =& \log(6e^{-\beta} + e^{-4\beta} + 4e^{-2\beta} + 4e^{2\beta} + e^{4\beta}) - 4 \times (\log(e^{\beta} + e^{-\beta}) \\ =& 0, \end{aligned} \tag{6.11}$$

$$\begin{aligned} W_6 =& \log Z_6 - 2W_5 - 3W_4 - 4W_3 - 5W_2 - 6W_1 \\ =& \log Z_6 - 0 - 0 - 5W_2 - 4W_1 \\ =& \log(2) + \log(e^{-5\beta} + 5e^{-3\beta} + 10e^{-\beta} + 10e^{\beta} + 5e^{3\beta} + e^{5\beta}) \\ & - 5 \times (\log(e^{\beta} + e^{-\beta}) - \log(2)) - 6 \times \log(2) \\ =& \log(e^{-5\beta} + 5e^{-3\beta} + 10e^{-\beta} + 10e^{\beta} + 5e^{3\beta} + e^{5\beta}) \\ & - 5 \times (\log(e^{\beta} + e^{-\beta}) - \log(2)) \\ =& 0. \end{aligned} \tag{6.12}$$

Simplify these equations we obtain,

$$\begin{aligned} & W_4 = \log Z_4 - 0 - 3W_2 - 4W_1 = 0 \\ \rightarrow\ & W_5 = \log Z_5 - 0 - 0 - 4W_2 - 5W_1 = 0 (W_4 = 0) \\ \rightarrow\ & W_6 = \log Z_6 - 0 - 0 - 0 - 5W_2 - 6W_1 = 0 (W_4, W_5 = 0). \end{aligned} \tag{6.13}$$

In earlier work, it was only established that $W_3 = 0$ and it was assumed that all weights above that also vanish. Here, we conclusively prove this result. Based on the equations shown here, we can easily infer that the rest of the calculations will follow the same reasoning, with all $W_7, W_8, W_9, \ldots$ goes to zero. Therefore, for one-dimensional Ising model periodic boundary condition, if W_3 is zero, rest of the weights go to zero. We can see from the calculations that, the ways of how one and two particles are embedded in a system decides whether W_4, W_5, W_6, ... goes to zero, since all the other terms in the equations are zeros. If W_3 and the rest goes to zero, it represents for a model that having an additional particle when the system has more than two particles, would not change the physics in the system. In addition, new results are obtained for the q-state Potts model on one-dimensional lattice.

6.5 1D q-state Potts model

While one-dimensional Ising model is shown to have very interesting results in the linked-cluster expansion study, Potts model has also been newly explored in this work. Ising model is similar to Potts model with $q = 2$ except for the values of bond that represent the internal energy (See Chapter 3). For $E = \sum_{\langle ij \rangle} \delta_{s_i s_j}$ on Potts model, the same adjacent spins result in E = +1, whereas different spins result in $E = 0$. By not assigning a specific number to q, there is no certain number of spin directions for each particle. In this case, we are able make a strong claim for a family of models that describes a wide variety of behavior.

As described earlier in this chapter, one-dimensional Ising model has consistent physical behavior after three particles (W_3 goes to zero). Therefore, it is interesting to see whether one-dimensional Potts model would provide us with the same phenomenon, given that Potts model is similar to Ising model.

We know from chapter 3 that, q-state Potts model can produce different configurations depending on q.

For $q = 2$, we can consider the particles have up and down spin. Therefore, the graphs for configurations for different n is,

When $n = 1$, there is no internal bonds for any configurations, therefore, the internal energy is zero for each two of the configurations. The partition function

Figure 6.2: All possible configurations for $q = 2$ Potts model when $n = 1$

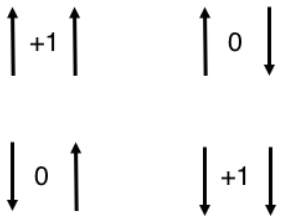

Figure 6.3: All possible configurations for $q = 2$ Potts model when $n = 2$

becomes $Z = e^{0\times\beta} + e^{0\times\beta} = 2 = q$. When n gets higher, we can see that each of the configurations has one internal bond with different energies.

For $q = 3$, we consider the particles to have three spins, up, right, and down spin.

Therefore, when $n = 1$, the partition function is then again $Z = e^{0\times\beta} + e^{0\times\beta} + e^{0\times\beta} = 3 = q$. The rest of the configurations have two internal bonds with total energies $+2$, $+1$, and 0, resulting in $e^{-2\beta}, e^{-\beta}$and $e^{0\beta} = 1$, which is the constant term.

As we saw from the above graphic representations of all the configurations, it is not hard to infer that for any q, when $n = 1$, the partition function is

$$\log Z_1 = \log(q) \tag{6.14}$$

When $n = 2$, there will be q^2 configurations with internal energies $+1$, or 0, depending on if the two spins are the same. In fact, there are q number of configurations with energy $+1$ (since spins have to be the same), and $q(q-1)$ number

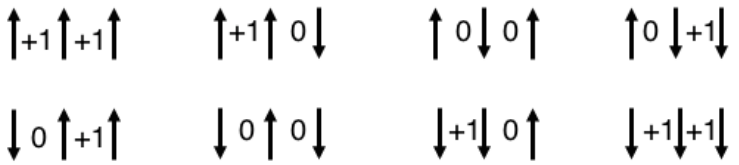

Figure 6.4: All possible configurations for $q = 2$ Potts model when $n = 3$

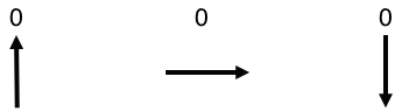

Figure 6.5: All possible configurations for $q = 3$ Potts model when $n = 1$

of configurations with energy 0 (since spins have to be different). Therefore, the partition function for $n = 2$ is,

$$\begin{aligned}\log Z_2 &= \log(qe^{-\beta} + q(q-1)e^{0\beta}) \\ &= \log(q(e^{\beta} + (q-1)) = \log q + \log(e^{-\beta} + q - 1) \\ &= \log(q) + \log(e^{-\beta} + q - 1)\end{aligned} \tag{6.15}$$

Proceeding, when $n = 3$, the internal total energies could be $+2$, $+1$ and 0. Among all the configurations, there are q number of $+2$, $q(q-1)$ number of $+1$ and $q(q-1)(q-1)$ number of 0. Therefore, the partition function for $n = 3$ is,

$$\begin{aligned}\log Z_3 &= \log(qe^{-2\beta} + q(q-1)e^{-\beta} + q(q-1)(q-1)) \\ &= \log(q) + \log(e^{-2\beta} + q - 1 + e^{-\beta} + (q-1)(q-1)) \\ &= \log(q) + \log(e^{-\beta} + q - 1)^2 \\ &= \log(q) + 2\log(e^{-\beta} + q - 1).\end{aligned} \tag{6.16}$$

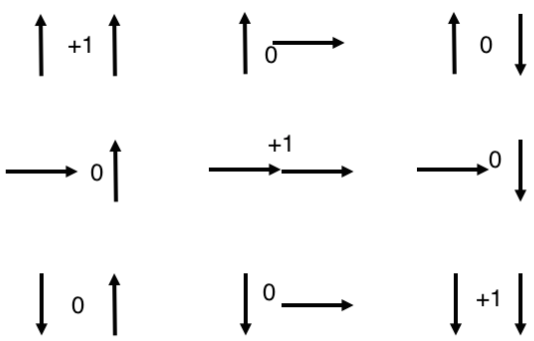

Figure 6.6: All possible configurations for $q = 3$ Potts model when $n = 2$

Rewriting all the partition functions of Potts model with q spins, we obtain the following equations,

$$\begin{aligned} \log Z_1(\beta) &= \log q \\ \log Z_2(\beta) &= \log q + \log(e^{-\beta} + q - 1) \\ \log Z_3(\beta) &= \log q + 2\log(e^{-\beta} + q - 1) \end{aligned} \tag{6.17}$$

Plugging in partition functions for weight calculations, we obtain W_1, W_2 and W_3,

$$\begin{aligned} W_1 &= \log Z_1(\beta) = \log q \\ W_2 &= \log Z_2(\beta) - 2W_1 = \log q + \log(e^{-\beta} + q - 1) - \log q \\ W_3 &= \log Z_3(\beta) - 2W_2 - 3W_1 = \log q + 2\log(e^{-\beta} + q - 1) \\ &\quad - 2(\log q + \log(e^{-\beta} + q - 1) - \log q) - 3\log q = 0. \end{aligned} \tag{6.18}$$

As shown above, the one-dimensional Potts model has W_3 goes to zero, the same as one-dimensional Ising model. Meanwhile, the embeddings of two-particle and three-particle subgraphs are the same as one-dimensional Ising model.

We are also interested in if the rest of the weights W_4, W_5, W_6... would go to zero.

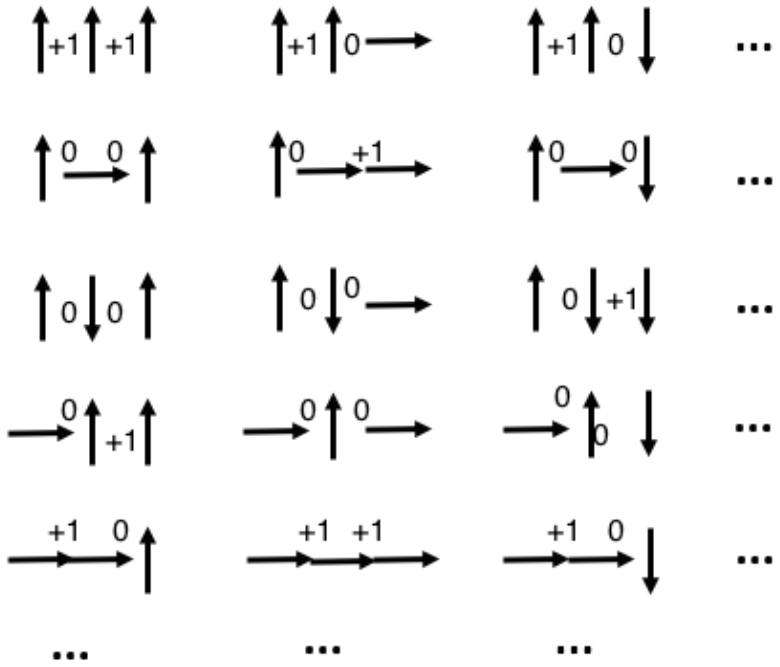

Figure 6.7: All possible configurations for $q = 3$ Potts model when $n = 3$

By calculating the partition functions we obtain

$$\begin{aligned} \log Z_4 &= \log(q) + 3\log(e^{-\beta} + q - 1) \\ \log Z_5 &= \log(q) + 4\log(e^{-\beta} + q - 1) \\ \log Z_6 &= \log(q) + 5\log(e^{-\beta} + q - 1) \\ &\dots \end{aligned} \tag{6.19}$$

Therefore, with the same reasoning as before,

$$\begin{aligned} W_4 &= \log Z_4 - 2W_3 - 3W_2 - 4W_1 \\ &\rightarrow = \log Z_4 - 0 - 3W_2 - 4W_1 \\ &\rightarrow = \log(q) + 3\log(e^{-\beta} + q - 1) - 3(\log(e^{-\beta} + q - 1) - \log(q)) - 4(log(q)) \\ &\rightarrow = 3\log(e^{-\beta} + q - 1) - 3\log(e^{-\beta} + q - 1) \\ &= 0 \end{aligned} \tag{6.20}$$

$$
\begin{aligned}
W_5 =& \log Z_5 - 2W_4 - 3W_3 - 4W_2 - 5W_1 \\
\rightarrow=& \log Z_5 - 0 - 0 - 4W_2 - 5W_1 \\
\rightarrow=& \log(q) + 4\log(e^{-\beta} + q - 1) - 4(\log(e^{-\beta} + q - 1) - \log(q)) - 5(log(q)) \\
\rightarrow=& 4\log(e^{-\beta} + q - 1) - 4\log(e^{-\beta} + q - 1) \\
=& 0
\end{aligned} \tag{6.21}
$$

$$
\begin{aligned}
W_6 =& \log Z_6 - 2W_5 - 3W_4 - 4W_3 - 5W_2 - 6W_1 \\
\rightarrow=& \log Z_6 - 0 - 0 - 0 - 5W_2 - 6W_1 \\
\rightarrow=& \log(q) + 5\log(e^{-\beta} + q - 1) - 5(\log(e^{-\beta} + q - 1) - \log(q)) - 6(log(q)) \\
\rightarrow=& 5\log(e^{-\beta} + q - 1) - 5\log(e^{-\beta} + q - 1) \\
=& 0.
\end{aligned} \tag{6.22}
$$

This new generalization shows that, for any number of n, the partition function $\log Z_n = \log(q) + (n-1)\log(e^{-\beta} + q - 1)$. Since W_2 is $\log(e^{\beta} + q - 1)$ and W_1 is $\log(q)$, we can get,

$$
\begin{aligned}
W_n =& \log Z_n - (n-1)W_2 - nW_1 \\
\rightarrow=& \log(q) + (n-1)\log(e^{-\beta} + q - 1) - (n-1)\log(e^{\beta} + q - 1) - n\log(q) \\
\rightarrow=& 0
\end{aligned} \tag{6.23}
$$

This is telling us that, for the spin models with one dimensional lattice, all the weights after $n = 2$, W_3, W_4, W_5... always goes to zero. Whereas for both these spin models it is possible to obtain the infinite system result exactly (as we have shown above, we have the partition function for any n), it is still a unique feature that W_3 onwards are zero, and we want to understand this feature – we address this in the next chapter.

6.6 Models on Bethe lattice

Ising model on Bethe lattice is no longer a one-dimensional linear system, and the embeddings of each subgraphs are more complex and intricate. In Bethe lattices,

since each graph may grow in different ways with different directions, the subgraphs of three or more lattice sites are not limited to one graph. The embeddings of subgraphs with less lattice sites to subgraphs with more sites would therefore have multiple outcomes.

Most importantly, the isomorphic graphs under Bethe lattice Ising model have the same partition functions, which leads to results of weights simpler than expected. The easy way to understand this is that– in Ising model, the only factor that decides its total energy is the relationship between two lattice sites, which is what we call bonds. Regardless of the way these sites are connected on Bethe lattices, the number of bonds in a graph is always the same with the same number of lattice sites. Therefore, the spin flips happen with the same regularity as one-dimensional lattice.

In 1D-Ising system, it is derived that,

$$\begin{aligned} W_3 &= \log Z_3 - 2W_2 - 3W_1 = 0 \\ W_4 &= \log Z_4 - 2W_3 - 3W_2 - 4W_1 = 0 \\ W_5 &= \log Z_5 - 2W_4 - 3W_3 - 4W_2 - 5W_1 = 0 \\ W_6 &= \log Z_6 - 2W_5 - 3W_4 - 4W_3 - 5W_2 - 6W_1 = 0. \end{aligned} \tag{6.24}$$

Since $W_3 = 0$, $W_4 = 0$, we also learned,

$$\begin{aligned} W_4 &= \log Z_4 - 0 - 3W_2 - 4W_1 = 0 \\ W_5 &= \log Z_5 - 0 - 0 - 4W_2 - 5W_1 = 0 \\ W_6 &= \log Z_6 - 0 - 0 - 0 - 5W_2 - 6W_1 = 0. \end{aligned} \tag{6.25}$$

As shown on the above equations, in one-dimensional systems, weights for certain lattice sites after W_3 are simply linear combinations of the partition function, W_2, and W_1, with no effects from larger system sizes.

Similarly, in Bethe lattice, no matter how differently the lattices grow after three sites, the subgraphs of one site and two sites will always have the same number of embeddings on the their original graph.

As described before, for Bethe lattice, the subgraphs have different ways of embeddings resulting in multiple weight expressions for a certain lattice sites. Therefore, it is easy to assume that, due to the differences in lattice constants, the weights cannot be easily canceled out to produce nice zeros. However, it still does not mean the weights will be no longer zeros after W_3.

The lattice constants are only different when the lattice sites are more than two, which means that the different embeddings do not affect the system unless the lattice constants for W_1 and W_2 are different. If all the different constants are replaced by an arbitrary constant represented by A-F, the equations become,

$$\begin{aligned}
W_1' &= \log Z_1 \\
W_2' &= \log Z_2 - 2W_1' \\
W_3' &= \log Z_3 - 2W_2' - 3W_1' \\
W_4' &= \log Z_4 - AW_3' - 3W_2' - 4W_1' \\
W_5' &= \log Z_5 - BW_4' - CW_3' - 4W_2' - 5W_1' \\
W_6' &= \log Z_6 - DW_5' - EW_4' - FW_3' - 5W_2' - 6W_1'
\end{aligned} \tag{6.26}$$

Since the first three equations are exactly the same as W_1, W_2, W_3, in (6), $W_3' = W_3 = 0$. Rewriting 6.26 would become,

$$\begin{aligned}
W_3' &= 0 \\
W_4' &= \log Z_4 - A \times 0 - 3W_2' - 4W_1' = W_4 = 0 \\
W_5' &= \log Z_5 - B \times 0 - C \times 0 - 4W_2' - 5W_1' = W_5 = 0 \\
W_6' &= \log Z_6 - D \times 0 - E \times 0 - F \times 0 - 5W_2' - 6W_1' = W_6 = 0.
\end{aligned} \tag{6.27}$$

The derivations are exactly the same as equation (6.25), with W_3 and the rest goes to zero. Therefore, no matter what values of the lattice constants are for sites more than two, the weights after W_3' will also be zero on Bethe lattice.

From the new derivations of weights of different models on different lattices, we can see that the complex tree-like Bethe lattice, one-dimensional Potts model both behave the same as one-dimensional Ising with W_3 and the rest of the weights goes to zero. For the Bethe lattice however, the number of boundary points grows with system size unlike the one dimensional, or in fact any regular lattice. Since the LCE assumes an infinite system, we do not capture the physics of these boundary points. This aspect needs further investigation.

For all these lattice models, there is no external magnetic field, and the energy is invariant under a flipping of spins (for Ising), or a permutation of spins (for Potts). We conjecture that it is this symmetry that allows this unique feature we show above.

In the next chapter, we break this symmetry by adding an external magnetic field to the Ising model and study the resulting LCE.

Chapter 7

Effect of Reduced Symmetry

As shown in Chapter 6, the one-dimensional Ising model, one-dimensional Potts model and Bethe lattice Ising model are all symmetric systems with $W_3, W_4, W_5...$ goes to zero. However, is there any other systems that do not have this behavior? If not all their weights after two lattice sites goes to zero, at what number of lattice sites will the weights start to be trivial? Indeed, these are interesting questions to address. Therefore, we also look at weights on lattice models as two-dimensional Ising model, one-dimensional Ising model with magnetic field and these slightly more complex models showed examples of reduced symmetric.

7.1 2D-Ising Model Periodic Boundary Condition

In one-dimensional Ising model, the whole system is stretched in one degree freedom, and W_3, W_4, $W_5...$ goes to zero. However, for a two-dimensional Ising model system, we wonder how different the physics is from one-dimensional.

It is not hard to imagine that the first three lattice sites for two-dimensional Ising model have the same lattice constants as a one-dimensional Ising model. Even though for the graph of three lattice sites, it contains subgraphs that can be embedded the same way as one-dimensional lattice no matter which direction one of the two bonds wants to bend. Nevertheless, when there are four lattice sites, the graph can look like

a line, a zigzag, or a square. As proved in the last chapter, the embeddings of one lattice site and two lattice sites on the graph are the determining factors of whether the rest of the weights goes to zero. In this two-dimensional four lattice site case, the lattice constants for both W_2 and W_1 are 4, whereas for a symmetric system they would have lattice constants of 3 and 4 respectively. Therefore, the calculation for weights in a two-dimensional lattice Ising model becomes

$$\begin{aligned} W_1 &= \log Z_1(\beta) = \log 2 \\ W_2 &= \log Z_2(\beta) - 2W_1 = \log(e^{\beta} + e^{-\beta}) - \log 2 \\ W_3 &= \log Z_3(\beta) - 2W_2 - 3W_1 = 0 \\ W_4 &= \log Z_4(\beta) - 4W_3 - 4W_2 - 4W_1 \\ &= \log(12 + 2e^{-4\beta} + 2e^{4\beta}) - 0 - 4(\log(e^{\beta} + e^{-\beta}) - \log 2) - 4\log 2. \end{aligned} \tag{7.1}$$

As we can see, the first three equations appear to be the same as a symmetric system. However, when more than three lattice sites come into play, weights are not zeros anymore. In this case, W_4 not going to zero represents that an additional particle in the system would bring new physics into the system, whereas we do not know what it means physically yet. It is reasonable to say that, the loops produced by a two-dimensional square lattice is what results in the change in lattice constants and the break the geometric symmetry of the one dimensional lattice.

7.2 1D Ising with Magnetic Field

We can break symmetries using other methods. The previous example of one-dimensional Ising models and Potts model seemed to show that one-dimensional systems would be symmetric. However, when adding magnetic field to Ising model, we break the spin flip symmetry of the energy, and indeed, we show that the system no longer have zeros for all the weights for $n \geq 3$. Applying formula

$$E = -J \sum_{\langle ij \rangle} s_i s_j + H \sum_i s_i \tag{7.2}$$

to the partition function, one can obtain,

$$\begin{aligned} \log Z_1 &= \log(e^{H\beta} + e^{-H\beta}) \\ \log Z_2 &= \log(2e^{\beta} + e^{2H\beta-\beta} + e^{-2H\beta-\beta}) \\ \log Z_3 &= \log(e^{-3H\beta-2\beta} + e^{3H\beta-2\beta} + 2(e^{-H\beta} + e^{H\beta}) + e^{H\beta+2\beta} + e^{-H\beta+2\beta}) \end{aligned} \tag{7.3}$$

and using the equations for one-dimensional weights calculation we can obtain that

$$\begin{aligned} W_1 &= \log(e^{H\beta} + e^{-H\beta}) \\ W_2 &= \log(2e^{\beta} + e^{2H\beta-\beta} + e^{-2H\beta-\beta}) - 2\log(e^{H\beta} + e^{-H\beta}) \\ W_3 &= \log(e^{-3H\beta-2\beta} + e^{3H\beta-2\beta} + 2(e^{-H\beta} + e^{H\beta}) + e^{H\beta+2\beta} + e^{-H\beta+2\beta}) \\ &\quad - 2\log(2e^{\beta} + e^{2H\beta-\beta} + e^{-2H\beta-\beta}) - 2\log(e^{H\beta} + e^{-H\beta}) \\ &\quad - 3\log(e^{H\beta} + e^{-H\beta}). \end{aligned} \tag{7.4}$$

In this case, W_3 is obviously not zero, and neither are the rest of the weights. However, unlike the two-dimensional lattice that have different lattice constants resulting in non-cancellation of weights, adding magnetic field into a system causes Z_3 to no longer be a linear combination of Z_1 and Z_2. This prevents the three partition functions from cancelling each other out no matter what the lattice constants are.

Indeed, when only the bond energy is considered for the partition function, the system is very predictable with a regular behavior. However, why is adding the individual property (in this case the magnetic field) affects the symmetric we assume? And what exactly is happening within the system? If we break down all the equations, we are able to understand it more clearly.

For a typical one-dimensional Ising model without magnetic field, we obtained partition function for the first three lattice sites as,

$$\begin{aligned} \log Z_1(\beta) &= \log[(2) \times 1] \\ \log Z_2(\beta) &= \log[(2)e^{\beta} + (2)e^{-\beta}] \\ \log Z_3(\beta) &= \log[(2)e^{-2\beta} + 2 \times (2) \times 1 + (2)e^{2\beta}] \end{aligned} \tag{7.5}$$

where we can take out the number "2" in the equations and change them into,

$$\begin{aligned} \log Z_1(\beta) &= \log(2) + 0 \\ \log Z_2(\beta) &= \log(2) + \log(e^{\beta} + e^{-\beta}) \\ \log Z_3(\beta) &= \log(2) + \log(e^{-2\beta} + 2 \times 1 + e^{2\beta}). \end{aligned} \tag{7.6}$$

The reason why W_3 can go to zero is because all the terms have the same coefficients, allowing the partition functions to be simpler.

When the calculation of weights is applied, the $\log 2$ get cancel out with each other, which leads to W_3 being zero. So, as was expressed in the previous chapter,

$$\begin{aligned} W_1 &= \log Z_1(\beta) = \log 2 \\ W_2 &= \log Z_2(\beta) - 2W_1 = \log(e^{\beta} + e^{-\beta}) - \log 2 \\ W_3 &= \log Z_3(\beta) - 2W_2 - 3W_1 = 0. \end{aligned} \tag{7.7}$$

However, When magnetic field is considered, the partition functions start to contain terms that have inconsistent coefficients, (rearranging Equations 7.3)

$$\begin{aligned} \log Z_1 &= \log[(e^{H\beta} + e^{-H\beta}) \times 1] \\ \log Z_2 &= \log[(e^{0H\beta} + e^{0H\beta})e^{\beta} + (e^{2H\beta} + e^{-2H\beta})e^{-\beta})] \\ \log Z_3 &= \log[(e^{-3H\beta} + e^{3H\beta})e^{-2\beta} + 2 \times (e^{-H\beta} + e^{H\beta}) \times 1 + (e^{H\beta} + e^{-H\beta})e^{2\beta}]. \end{aligned} \tag{7.8}$$

As we can see that the coefficients in the parenthesis here are numbers wit H in the exponents,$(e^{H\beta} + e^{-H\beta}), (e^{2H\beta} + e^{-2H\beta}), (e^{-3H\beta} + e^{3H\beta})$. In order to do the same trick as the previous example, we should expect being able to take out the coefficients from the equations. However, H here in the exponents are with different coefficients themselves because they are produced by different lattice sites of the Ising Model, making all of them unequal to each other and cannot be taken ot. From this scenario, we could also observe that in order for these coefficients to be the same, the only possible way is to make all the H be zero, then $(e^{H\beta} + e^{-H\beta}) = (e^{2H\beta} + e^{-2H\beta}) = (e^{-3H\beta} + e^{3H\beta})$. When they are equal to each other, they could be taken out from the equation and be canceled out. Regarding to the previous case of Ising Model without magnetic field, we can also consider it having the magnetic coefficient $H = 0$. This explains why adding all these individual magnetic energies to the system would break the balance.

In situation as Ising model without magnetic field, W_3 drops to zero so does the rest of the weights. Therefore, we can look at the values for the weights including and after W_3.

7.3 Convergence Plots

Due to the complexity of the Ising model with magnetic field and the break of its symmetry, we are interested in knowing if there are other patterns we can obtain

from all the results of linked-cluster expansion. This section includes plots of the change in the weights for the log of the partition function related to the number of lattice sites contained in the system, that happens to both open boundary and periodic boundary conditions.

Open Boundary Ising model with Magnetic Field

For open boundary condition, if W_3 and the rest of the weights do not go to zero at all for Ising model with magnetic field, then it is also interesting to see if the weights will converge to a certain number. Equation 7.9 is just a reminder as how we calculate all the weights in all the previous calculations, and is identical as the formula (equation 6.7) introduced in the previous chapter.

$$W_o(c) = O(c) - \sum_{s<c} W_o(s). \tag{7.9}$$

In here, we use all the partition functions of different numbers of lattice sites for $O(c)$, and subtract all the previous weights. Setting β to 1, we are able to obtain specific weights through different arbitrary magnetic fields. By plotting out weights from W_1 to W_2, we can see the trend of how different magnetic field would affect the behaviors of the system.

Due to the very small change in weights after three, the following figures are the log plots for all the weights from one lattice site to twelve lattice sites. When H is 0, it is identical to the Ising model without magnetic field and W_3 and after should go to zeros. When H is very small, say $H = 10^{-5}$ W_3 starts to be slightly above zero.

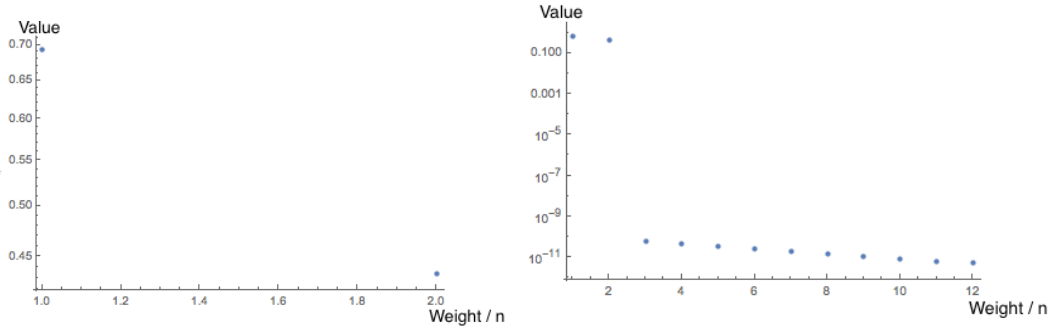

Figure 7.1: $H = 0$, $H = 10^{-5}$, since W_3 and the rest go to zero for $H = 0$, there are no log values for weight number after three

As H goes up to 10^{-1}, the log plot converges very fast and close to zero.

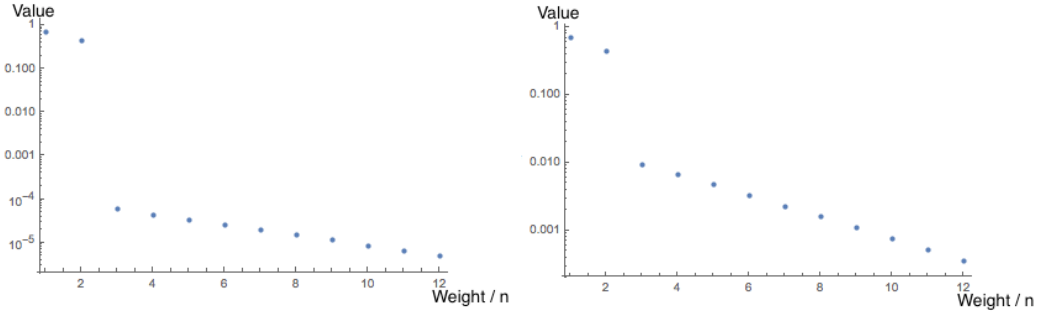

Figure 7.2: $H = 0.1$, $H = 0.13$

As H becomes larger as $0.13 < H < 0.3$, the convergence becomes relatively slow.

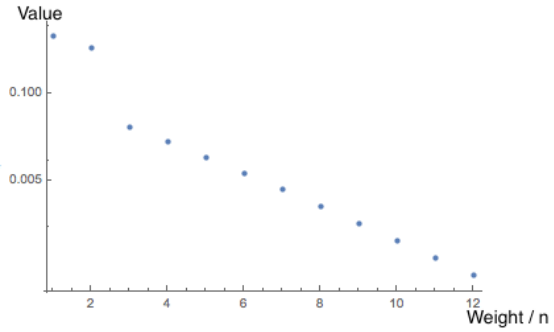

Figure 7.3: $H = 0.26$

An assumption can be made that as H goes higher, convergence goes slower. However, when giving bigger values to H, the situation goes back to having fast convergence.

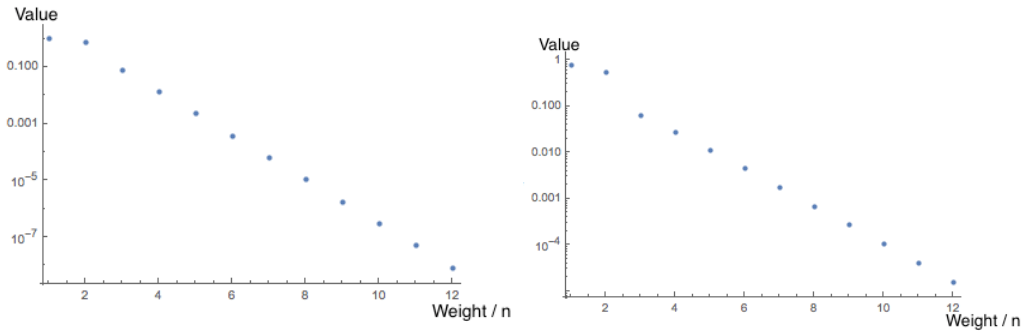

Figure 7.4: $H = 0.36$, $H = 0.45$

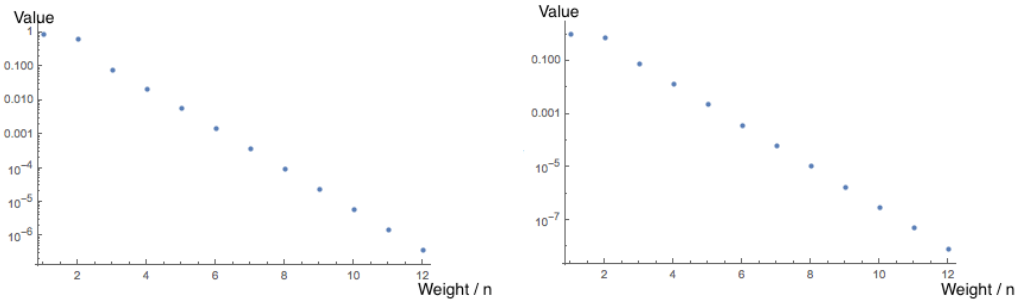

Figure 7.5: $H = 0.67$, $H = 0.98$

As shown on the log plots, convergence appears to be very fast on both high magnetic field and low magnetic field. As the magnetic field approaches 0.3, the convergence becomes the slowest. It makes sense that when magnetic field contributes to the balance of polarization, meaning the number of up spins is closer to the number of down spins, there would be decreased energy on the right part of equation 2 to slow down the convergence of the original energy on the left part. Therefore, the weights would not converge as fast as it should be. Meanwhile, the polarization causes the increase of the energy on the right part that quickly cancels out the left part, inducing a fast convergence of the weights.

Chapter 8

Conclusion

The study of different model systems could be applied to multiple areas such as innovation of material utilization, dynamics of particles movements and even analysis of societal phenomena. For a certain model system, the properties of the individuals and their relationships with the neighbors are specifically defined, so the system gets more complicated as the size grows. In our part of the study, we want to know how and when we can obtain the final result for the infinite size system with only a small size system. In other words, we want to find the fastest way to approximate the infinite size system. Linked-cluster expansion method is shown to be the most efficient approximation method.

The purpose of this thesis research is to apply the study of weight in linked-cluster expansion to models and lattices that have not been studied before. Weight, meaning the additional contribution in adding an extra particle to physical observable of the system, shows whether a system is symmetric.

In this thesis research, we show that – similar to one-dimensional Ising model, for Ising model on Bethe lattice and one-dimensional Potts model, we can obtain results for the infinite size system with only three lattice sites in the system, meaning weights go to zero include and after n= 3. We have also studied the effect of breaking an internal symmetry on the weights in the LCE and showed that reducing the symmetry removes the unique property that the weights vanish above $n = 3$.

However, for two-dimensional Ising model, and Ising model with magnetic field, we cannot obtain results for the infinite size system with finite number of lattice sites in the system. For the case of the 2D-Ising model, we show that it is the presence of loops in the lattice that destroy a certain geometric symmetry. For the case of the Ising model with a magnetic field, we further showed that for very small or very large values of the external field H, we go back to a situation where W_3 and onwards are almost 0 (not exactly). This is consistent with the fact that the maximum competition from the external magnetic field with the spin ordering happens around $H = 1$.

This means that we still have not found the exact solutions for the two-dimensional Ising model or one-dimensional Ising model with magnetic field. It seems that the loop in two-dimensional model is what is causing the change of physics, but how the break of symmetry happens is still unknown. For Ising model with magnetic field, the similar question arises, as how the addition of individual magnetic property can fail maintaining the symmetry. Therefore, the future study of this research would be to develop further generalizations into how symmetries impact the LCE in more complex models, and how we can potentially exploit this knowledge to develop a more efficient linked-cluster expansion.

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