THE ZEROS DISTRIBUTION OF Z_5 AND Z_6-SYMMETRIC MODELS ON TRIANGULAR LATTICE

BY

NOR SAKINAH BINTI MOHD MANSHUR

A thesis submitted in fulfilment of the requirement for the degree of Master in Science (Computational and Theoretical Sciences)

Kulliyyah of Science
International Islamic University Malaysia

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ABSTRACT

We study the Z_Q-symmetric model with the nearest neighbor interaction between molecular dipole. There were previous study on a square lattice by Martin in 1991 and also Zakaria in 2016 suggesting that the emergence of the linear arcs on the complex-temperature plane can predict the existence of multiple phase transitions. Motivated from their works, we continue to study the model on the triangular lattice specifically on the five spin directions, that is $Q = 5$ and then continue extending our study on $Q = 6$. The aim of this study is to provide more evidence on the existence of multiple phase transitions on the crystal lattice. The model is initially defined on a specific lattice which is the triangular lattice with the nearest neighbor interaction. The partition function is computed for the increasing lattice sizes by using the transfer matrix approach. By applying the Newton-Raphson method, the zeros of the partition function are computed and then plotted in the complex Argand plane for analysis. The number of linear arcs on the graph suggesting the number of phase transition. To support our claim, the specific heat equation is used for further comparison.

خلاصة البحث

يهدف هذا البحث إلى دراسة نموذج Z_Q المتماثل في (Z_Q-symmetric model) مع أقرب تفاعل بالجوار بين ثنائي القطب الجزيئي. كانت هناك دراسات سابقة على شبكة مربعة من قبل مارتن في عام 1991، وكذلك من قبل زكريا في عام 2016 تشير إلى أن ظهور الأقواس الخطية على مستوى درجة الحرارة المركبة قد يُنبئ بوجود تحولات متعددة الأطوار. دفعتنا هذه الدراسات لمواصلة دراسة النموذج على الشبكة المثلثية على وجه التحديد في اتجاهات الدوران الخمسة، أي $Q = 5$ ومن ثمَّ مواصلة توسيع دراستنا على $Q = 6$. الهدف من هذه الدراسة هو تقديم المزيد من الأدلة على وجود تحولات متعددة الأطوار على الشبكة البلورية. عُرِّفَ بالنموذج مبدئيًا على شبكة متشابكة محددة وهي الشبكة المثلثية مع أقرب تفاعل بالجوار. تم حساب دالة التقسيم لأحجام الشبكة المتزايدة باستخدام نهج مصفوفة النقل. من خلال تطبيق طريقة نيوتن–رافسون (Newton-Raphson method)، تم حساب الأصفار الخاصة بدالة التقسيم ومن ثمَّ رسمها في مستوى أرجاند (Argand) المركب للتحليل. عدد الأقواس الخطية على الرسم البياني يشير إلى عدد المراحل الانتقالية. لدعم فرضيتنا، تمَّ استخدام معادلة الحرارة المحددة لمزيد من المقارنة.

APPROVAL PAGE

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…………………………………..
Siti Fatimah Zakaria
Supervisor

…………………………………..
Nasir Ganikhodjaev
Co-Supervisor

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a thesis for the degree of Master of Computational and Theoretical Sciences.

…………………………………..
Mohd Hirzie Mohd Rodzhan
Internal Examiner

…………………………………..
Ummu Atiqah Mohd Roslan
External Examiner

This thesis was submitted to the Department of Computational and Theoretical Sciences and is accepted as a fulfilment of the requirement for the degree of Master of Science (Computational and Theoretical Sciences).

…………………………………..
Mimi Hafizah Abdullah
Acting Head, Department of Computational and Theoretical Sciences

This thesis was submitted to the Kulliyyah of Science and is accepted as a fulfilment of the requirement for the degree of Master of Science (Computational and Theoretical Sciences).

…………………………………..
Shahbudin Saad
Dean, Kulliyyah of Science

DECLARATION

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For my parents, husband and family -

my parents Aishah binti Mohamed and Zainal Abidin bin Anon,

my beloved husband Muhammad Syaffiq bin Lias,

my brother Amin and the other families' members.

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LIST OF SYMBOLS

$\mathbb{R}$	Real Numbers
Λ	Set of Graph
$\in$	Element of Set
Q	Number of Spin Directions
β	Inverse Temperature
T	Absolute Temperature
H, H_Λ	Hamiltonian Function
$\langle i, j \rangle$	Adjacent Sites i and j
σ	Element of the Configurations
Ω, Ω_Λ	Set of All Possible Configurations
V	Vertices
E	Edges
Z	Polynomial of Partition Function
χ	Energy Level Value
C_V	Specific Heat
U	Internal Energy

CHAPTER ONE

INTRODUCTION

In this research, the Z_Q- symmetric model (Martin, 1991) is one of the models in statistical mechanics, that is an area of physics where mathematical modelling is used to study a physical system. The statistical mechanics is one of the pillars of modern physics which also can be used in the study of thermodynamic behaviour of physical system (Huang, 1987; Krieger, 1998; Yeomans, 1992).

We study a model of spin variables on graph representing the molecular spins on the crystal lattice of a physical system – such as a bar magnet. The phase transition is an example of the physical phenomena that can be benefited from the study of statistical mechanics where the analytics properties of a phase transition can be observed through this study.

The phenomena when there is a change of a thermodynamic from one phase to another phase of matter is called a phase transition (Krieger, 1998). There was a study for instance the Curie temperature that related to the prediction of critical point for a phase transition (Kittel, 2004; Kosterlitz & Thouless, 1973; Landau & Lifshitz, 1968).

The Z_Q-symmetric model is related to the Q-state Potts model (Baxter et al., 1982) where Q is the number of possible spin orientations. For $Q = 2$, this model corresponds to the Ising model (Ising, 1925). For $Q = 3$, this model corresponds to the 3-state Potts model.

For the case of one-dimensional Ising model, Ising (1925) study the ferromagnetic system and he showed that it has no phase transition. But in two or three dimension, Peierls showed that the Ising model does have ferromagnetism at sufficiently low temperature (Peierls, 1936).

The exact partition function of the square lattice is one feature to be studied in Ising model (Baxter, 2007). Kramers and Wannier (1941a, 1941b) proposed to find the solution for free energy by considering the eigenvalue of a particular matrix. That theory is applied by Onsager (1944) in his study and he successfully described the exact solution of Ising model on square lattice to show the result related to phase transition critical point. Refer a study by Kaufman (1949) which described other version of Onsager's solution. For the Q-state Potts model on lattices of three dimension, the exact result is still an open problem.

The study of the phase transition and critical properties in finite size system using the roots of the partition function was considered by many researchers such as (Fisher, 1965; Ghulghazaryan & Ananikian, 2003; Martin, 1991; Yang & Lee, 1952a, 1952b). When the phase transition occurs, the zeros are distributed in a nice pattern consists of subsets of set of zeros. This pattern gives a locus of zeros. For square lattice Ising model, the locus of zeros is given by two circles (Fisher, 1965). At the thermodynamic critical point, the locus of zeros will cut the real axis of the complex plane (Fisher, 1965; Yang & Lee, 1952a, 1952b).

Specifically for the finite system, the zeros will always lie off the real axis of the complex plane since the finite lattice partition function is a positive polynomial. But in the thermodynamic limit, it will be very close to the real axis. Thus, specifically very close to the critical point of phase transition. To support this locus of zeros, we use the theorem by Lee and Yang (1952a, 1952b) that shows the relation of the equation of states of phase transition to the root distribution of the partition function.

This theorem also known as Lee-Yang circle theorem that proved the roots must lie on a circle under certain conditions.

The study of complex-temperature zeros of partition function was first discussed on a square lattice Ising model by Fisher (1965) and also by Abe (1967), Katsura (1967) and Ono et al. (1967). In addition, the study was also made by Liu and Sinclair (2019). The arc in the zeros distribution is observed to discuss the singularity of specific heat which corresponds to the existence of phase transition. The phase transition was observed by Onsager (1944) in his square lattice Ising model when there is a singularity in the graph of the specific heat (Machek, 1965). In a finite size system, the analytic properties of the phase transition is investigated from a study of the zeros of the partition function.

For the Z_Q-symmetric model on square lattice, Martin (1988, 1991) and supported by Zakaria (2016) suggested that the existence of multiple phase transitions can be predicted by the emergence of line curves on the complex-temperature plane. We extend their study to different type of Z_Q-symmetric model and on different lattice in order to provide more evidence to the existence of multiple phase transitions.

We focus on the Z_Q-symmetric model on a triangular lattice with the nearest neighbor interaction for two types of spin direction and we assume no external magnetic field is present. We also consider the two magnetic dipole interaction only if they are close together (nearest neighbour) and other interaction at larger distance is negligible. We first investigate this model on five spin directions between molecular dipole, i.e $Q = 5$ and then continue with the six spin directions, i.e $Q = 6$.

1.1 PRELIMINARIES

The Z_Q-symmetric model is a model on discrete variables represents the magnetic dipole moment of the atomic spins. The spin particles are represented by a graph of lattice where the vertices of the graph represent the spin variables that are embedded to the Euclidean space $\mathbb{R}^3$. The spins will interact with its nearest neighbor represented by an edge of graph. The graph is defined as below.

Definition 1.1 A directed graph Λ is a triple $\Lambda = (V, E, f)$. V is a set of vertices and E is a set of edges, that is $v \in V$ and $e \in E$. The f is a function $f : E \to V \times V$. Given $e \in E$ and $v_1, v_2 \in V$, the images $f(e) = <v_1, v_2>$ gives the `*source*' and `*target*' vertex of edge e.

Definition 1.2 The distance $d_\Lambda(u, v)$ is the number of edges in the shortest path from u to v. Two vertices $u, v \in V$ are called nearest neighbours if $f(e) = <v_1, v_2>$ for some $e \in E$, i.e. when $d_\Lambda(u, v) = 1$.

Definition 1.3 Consider a set V of lattice sites, each site with a set of adjacent sites forming a d-dimensional lattice. For each lattice site $k \in V$ there is a discrete variable σ_k such that $\sigma_k \in \{1,2, \dots, Q\}$, representing the site's spin. A spin configuration, $\sigma = (\sigma_k)_{k \in V}$ is an assignment of spin value to each lattice site.

1.2 THE ISING MODEL AND THE POTTS MODEL

The Ising model is a mathematical model of ferromagnetism in statistical mechanics. The model consists of discrete variables that can be in one of two states (+1 or −1) which represent spin up and spin down respectively. Ising showed that there is no phase transition in one dimensional Ising model case (Baxter et al., 1982). However, Ising assumed for higher dimension, the phase transition also does not exist due to the no phase transition in one-dimensional case (Ising, 1925). The Ising model configuration is defined as below (This result was proven wrong by Peierls (1936)).

Definition 1.4 Consider a set V of lattice sites, each site with a set of adjacent sites forming a d-dimensional lattice. For each lattice site $k \in V$ there is a discrete variable σ_k such that $\sigma_k \in \{+1, -1\}$, representing the site's spin. A spin configuration, $\sigma = (\sigma_k)_{k \in V}$ is an assignment of spin value to each lattice site.

For any two adjacent sites $i, j \in V$, there is an interaction J. Also a site $j \in V$ has an external magnetic field h interacting with it. The energy of a configuration σ is given by the Hamiltonian function,

$$H(\sigma) = -J \sum_{<i,j>} \sigma_i \sigma_j - \mu\, h \sum_{j} \sigma_j\,, \tag{1.1}$$

where J is a constant that represents the strength of interaction. The first sum is the summation of all pairs of adjacent spins. The notation $< i, j >$ indicates that the sites i and j are nearest neighbours. While μ represent the magnetic moment. The magnetic moment is the interaction strength of an object with an applied field that produces a magnetic field. If $J > 0$, then the interaction is called ferromagnetic. Conversely, if $J < 0$, then the interaction is called antiferromagnetic. However, if $J = 0$, then the spins are not interacting to each other.

For Ising model, two spin variables spin in the same direction has energy 1 and -1 otherwise. For two or more spin states, the generalisation of this Ising model is called the Q-state Potts model (also known as Potts model for simplicity) (Baxter, 1973; Potts, 1952). It is a model of interacting spins on a crystalline lattice with Q is the number of spin directions. The behaviour of the ferromagnetism and other certain solid-state physics may be gained from this model. The Q-state Potts model is a representation of a physical system in which spins are allowed to be oriented from Q possible spin directions.

The energy of a configuration of σ is defined by the Hamiltonian function as follows. Let $\sigma = (\sigma(0),\ \sigma(1),\ \sigma(2), \dots,\ \sigma(n)) \in \Omega$ where n is the number of vertices and Ω is the set of all possible configurations.

Definition 1.5 The Hamiltonian of Potts model on graph $\Lambda = (V, E, f)$ is defined as

$$H(\sigma) = -J \sum_{\substack{<i,j>=f(e),\\ e \in E}} \delta_{\sigma(i)\sigma(j)}, \tag{1.2}$$

where the Kronecker delta function is given by

$$\delta_{\sigma(i)\sigma(j)} = \begin{cases} 1, & if\ \sigma(i) = \sigma(j) \\ 0, & if\ \sigma(i) \neq \sigma(j) \end{cases},$$

with the sum running over all the nearest neighbour interaction in Λ and J is the interaction strength.

For Potts model, two spin variables spin in the same direction will have energy 1 and 0 otherwise. As the Ising model, if $J > 0$, then it is corresponded to a ferromagnetic state. It means that the energy on the system is in the lowest energy where all the spins variables are oriented in the same direction. Conversely, if $J < 0$, then it is corresponded to an antiferromagnetic state, where the nearest neighbour of each spin variable is oriented in anti-align to each other.

1.3 THE Z_Q- SYMMETRIC MODEL

The Z_Q-symmetric model is a model that related to the Q-state Potts model (Baxter et al., 1982) by the number of Q spin directions. This model sometimes is called a clock model due to the arrangement of the energy which is illustrated by a literal clock that has 12 point marked around the clock face. Z_Q refers to the symmetry group being

Z/QZ, the discrete rotation group of order Q. The Hamiltonian is invariant under global Z_Q transformation (related to gauge theories (Martin, 1991)) (Martin, personal communication, September 3, 2019). The spin directions of this model is represented by the idea of clock-like circle. Due to that, this model also known as a clock model. The example of the spin interaction that are using this idea can be referred in Figure 2.3 (Chapter 2.1.2). The interaction between one spin to another will produce a Hamiltonian energy. Furthermore, the difference of the energy is always remains the same when any pair of the direction is moved with fixed angle around the clock. This arrangement is associated to the symmetrical properties of the model. We define the Hamiltonian function of the Z_Q- symmetric model as follows.

Definition 1.6 For any microstate $\sigma \in \Omega$, the Hamiltonian of Z_Q- symmetric model is defined as below and noted that Ω is the set of all possible configurations.

$$H_{\chi}(\sigma) = -J \sum_{\substack{\langle i,j\rangle = f(e). \\ e\in E}} \chi[\sigma(i) - \sigma(j)]$$

$$= -J \sum_{\substack{\langle i,j\rangle = f(e)\,. \\ e\in E}} \sum_{r=1}^{\left[\frac{Q}{2}\right]} \gamma_r \cos\left(\frac{2\pi r\big(\sigma(i) - \sigma(j)\big)}{Q}\right) + \check{\gamma}_r, \tag{1.3}$$

where $\left[\frac{Q}{2}\right]$ is the integer value of the division and $\gamma_r, \check{\gamma}_r \in \mathbb{R}$ are model parameters fixed for a given model.

The value of the Hamiltonian are depending on the angle between two spins or by the distance between them. If the angle between two spin directions are small, it will has less energy losses as compared to the large size of angle. This energy loss is called the energy penalty (Zakaria, 2016). This energy representation is equivalent to the Potts model when the pair of spin variables $(\sigma(i), \sigma(j))$ are pointed in the same direction.

The study of Z_Q-symmetric model was previously studied on a square lattice especially by Martin (1991) and Zakaria (2016). Their study highlighted that the emergence of line curves on the complex-temperature plane can predict the existence of multiple phase transitions. To provide more evidence to the research, we study the Z_Q-symmetric model on different lattice pattern that is the triangular lattice. The comparison with other type of model and lattice aims to provide more evidence of the existence of multiple phase transitions. For this purpose, we will focus on the triangular lattice.

We study this type of model with five directions, i.e. $Q = 5$ which we call as the Z_5-symmetric model and six directions. i.e. $Q = 6$ which we call as the Z_6-symmetric model with the nearest neighbour interaction between molecular dipole on increasing lattice sizes. The Figure 1.1 below shows three fixed size triangular lattices as example.

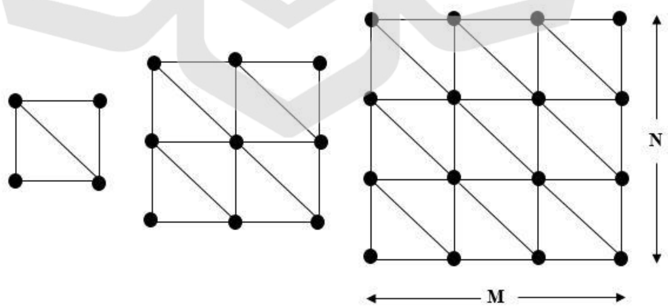

Figure 1.1 Triangular Lattices with Different System Size N by M.

1.4 THE PARTITION FUNCTION

Partition function is a function that relates temperature and other parameters with the states of a spin system. It describes the statistical properties in the thermodynamic system. Total energy, free energy, entropy and pressure are all the aggregate thermodynamic variables and it can be expressed in terms of partition function or its derivatives (Baxter, 2007; Berlinsky & Harris, 2019; Zakaria, 2016). We study the partition function as our main function in this research.

Consider a system A, with a temperature T, both the volume and the number of particles fixed in all times, where the transfer of heat energy to its neighbour and environment is allowed. So any system in contact with the system A will eventually reach the thermal equilibrium at the temperature of the system A. This kind of system is called a canonical ensemble. The partition function for this system that allows the energy transfer to its neighbour and environment with the other fixed parameters in a system is called the canonical partition function or simply a partition function. We define the partition function as follows.

Definition 1.7 For a given H_Λ and graph Λ, where H_Λ here is the Hamiltonian function for the microstates σ of the graph Λ. The partition function is defined as

$$Z_\Lambda(\beta) = \sum_{\sigma \in \Omega_\Lambda} exp(-\beta H_\Lambda(\sigma)) \tag{1.4}$$

where the summation is over all possible microstate σ of a system. The β is the inverse temperature, $\beta = 1/k_B T$ in which k_B is the Boltzmann's constant, T is the absolute temperature, and Ω_Λ is the all possible configurations of the graph Λ.

1.5 PHYSICAL MOTIVATION

Many cases that related to the model on crystal lattice has yet to be solved and studied. One of the successfully solved cases that has been done by the previous