THE PHASE DIAGRAM OF A THREE-STATE POTTS MODEL WITH COMPETING BINARY INTERACTION ON A CAYLEY TREE UP TO THE THIRD NEAREST-NEIGHBOUR GENERATIONS

BY

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

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ABSTRACT

This research is an extension of Ganikhodjaev et al. (2008), where they had generated and analysed the phase diagram consisting of the first and second nearest-neighbour binary interaction on the three-state Potts model on a Cayley tree. Therefore, in continuing the research, it is in our interest to investigate the effect of the third nearest-neighbour binary interaction to the phase diagrams of the three-state Potts model on a Cayley tree. Therefore, we generate and analyse the phase diagrams of the three-state Potts model, considering prolonged competing binary interaction J_2 and J_3 on the same branch of the Cayley tree up to the third nearest-neighbour generations. We derive the recurrence system of equations while considering some ranges of competing parameters. We carry out a numerical procedure by applying several stability conditions and characteristic points into the iteration scheme. For some non-zero parameter J_3, we found the additional phases of period 5, 6, 9, and 11, with the ferromagnetic, antiphase, paramagnetic, antiferromagnetic and modulated phase. For the modulated phase, we further study the existence of phases with period larger than 12 by conducting a numerical analysis on the variation of wavevector and Lyapunov exponent. This results in the discovery of some phases with period larger than 12, which are the phases of period 13, 16, 23, 26 and 49. From the results obtained as presented in this thesis, it is clear that the third nearest-neighbour binary interaction on the Cayley tree, considering the three-state Potts model, gives significant effect to the generation of the phase diagram.

خلاصة البحث

يهدف هذا البحث إلى دراسة عمل Ganikhodjaev وآخرين، الصادر عام (2008)، حيث قاموا بإنشاء وتحليل مخطط أطوار الذي يتكون من التداخلات الثنائي الجار الأقرب الأولى والثانية على نموذج بوتس على شجرة كايلي. تم إجراء دراسة لتأثير التداخلة الثنائي الأقرب الثالثة إلى مخططات الأطوار لنموذج بوتس على شجرة كايلي. تم إنشاء وتحليل مخططات الأطوار لنموذج بوتس من خلال النظر في التداخلات الثنائي المتنافسة المطولة J_2 و J_3 على نفس الفرع حتى الجار الأقرب الثالثة من شجرة كايلي. تم استمداد نظام معادلات متكرر حين نظر في بعض نطاقات المعلمات المتنافسة. وقام الباحث بإجراء عددي من خلال تطبيق العديد من ظروف الإستقرار ونقاظ التمييز في مخطط التكرير، فوجد في بعض المعلمات غير الصفرية J_3 للمرحلات الإضافية للفترات الخامسة والسابعة والتاسعة والحادية عشرة مع المراحل المغناطيسية الحديدية والضد الطور والشبه المغناطيسية والمغناطيسية الحديدية المضادة والمنظمة. وقام الباحث في المرحلة المنظمة بدراسة إضافية لوجود مراحل ذات فترة أكبر من الفترة الثانية عشرة عن طريق إجراء التحليل العددي على اختلاف المتجه الموجة وأس ليابونوف، حيث تم اكتشاف بعض المراحل ذات فترة أكبر من الفترة الثانية عشرة وهي مراحل الفترات الثالثة عشرة والسادسة عشرة والثالثة والعشرون والسادسة والعشرون والتاسعة والأربعون. يتضح من النتائج التي تم الحصول عليها أن التداخلات الثنائي الأقرب الثالثة على شجرة كايلي يعطي تأثيرًا كبيرًا لتوليد مخططات الأطوار لنموذج بوتس.

APPROVAL PAGE

I certify that I have supervised and 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 Science (Computational and Theoretical Sciences).

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DECLARATION

I hereby declare that this thesis is the result of my own investigations, except where otherwise stated. I also declare that it has not been previously or concurrently submitted as a whole for any other degrees at IIUM or other institutions.

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Signature ……………………………………… Date 5th June 2020……………………..

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This thesis is dedicated to my late father, Basirudin bin Udi,

may Allah put his soul among the Believers.

And, to my mother, Azina binti Abd Rahman,

for endless support in my quest for knowledge.

Also, to my husband, Abdul Rauf bin Hamdan,

for being the fuel to my midnight oil.

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LIST OF ABBREVIATIONS

P	Paramagnetic
F	Ferromagnetic
AF	Antiferromagnetic
P3	Phase of period 3
P5	Phase of period 5
P6	Phase of period 6
P7	Phase of period 7
P9	Phase of period 9
P11	Phase of period 11
<2>	Antiphase <+ + - ->
<3>	Antiphase <+ + + - - ->
M	Modulated
PM	Paramodulated

LIST OF SYMBOLS

T	absolute temperature
$m^{(n)}$	average magnetisation
$\bar{\sigma}$	boundary configuration
Γ^2	Cayley tree of arbitrary order 2
$d(x, y)$	distance between two vertices
l	Edge
H	Hamiltonian
J_i	interaction strength
$\delta_{\sigma(x)\sigma(y)}$	Kronecker symbol
λ	Lyapunov exponent
a, b, c	Parameters
Z	partition function
$>\widetilde{x,y}<$	prolonged next-nearest-neighbour
γ, δ	ratio of interaction strength
α	ratio of temperature over interaction strength
x^0	root of semi-infinite Cayley tree
Γ_+^2	semi-infinite Cayley tree of order 2
Ω	set of all configurations
Λ	set of edges
V	set of vertices
W_n	set of vertices in *n*-th level
q	Wavevector

CHAPTER ONE

INTRODUCTION

1.1 STATISTICAL MECHANICS AND PHASE DIAGRAMS

Statistical mechanics is one of the important branches in modern physics. One of the objectives of statistical mechanics is to bring the study of microphysics and macrophysics together. It aims to derive some mathematical frameworks that account for the behaviour of macroscopic properties from the knowledge of the interaction between its microscopic constituents. This is essentially done by averaging over the large numbers of microscopic coordinates, which leaves us with only the macroscopic coordinates, such as the volume of the body, and the macroscopic variables such as temperature and pressure (Mandl, 1971).

Boltzmann (1877) and Gibbs (1902) introduced the two theoretical frameworks that dominate the realm of statistical mechanics. Interestingly, the problems formulated in each of their framework is peculiar to its own and often do not have counterpart in the other (Frigg, 2016). Consequently, a plethora of approaches to studying statistical mechanics has been developed using the variants of these two major frameworks.

One of the intriguing parts in statistical mechanics is the study of the phase transition. Phase transitions describe the transition between two different phases in a body of system. A stable phase often shares the same physical properties. During the process of transition from one phase to another, certain properties of the former phase might change due to the changes in the external conditions such as temperature and pressure.

Generally, several factors distinguish different phases of matter. One is by appearance, such that liquid water has a different appearance than crystalline water. Besides, we can differentiate the phases by noticing a presence of boundaries between the phase, which is demonstrated by the presence of meniscus between the liquid and gas in the alcohol. Other than that, the phases can be separated by categorising different internal organisation such as the spin orientation in some magnetic domain (Jaeger, 1998).

The simplest example is by describing the phase transition of water. At a certain temperature, water, which is in the liquid form, will change into ice, which is solid. This change of medium arises due to the change in the intermolecular forces between the interacting molecules and atoms. One can be inquisitive and ponder about what is happening on the boundary of the stable region, where any point on the boundary curve does not belong to any of the stable phases. Rather, the points are undergoing a transformative process. The point at where the curve terminates is called the 'critical point' as has been defined by Gibbs (1873).

Gibbs (1983) also introduced the phase diagram as a graph of thermodynamical variable. Phase diagram illustrates the different phases by putting them into different regions. Gibbs defined the boundary between regions, where distinct phases coexist as "the phase co-existence curve". This phase co-existence curve is more familiarly known as the transition line in our study. In this study, we investigate the phase diagram in detail in order to extract information about the existence of the phase transition in our model.

The model that we adopted in this study is the three-state Potts model. The Potts model is the generalisation of the Ising model, where models with two or more interacting spins fall under this category. Ashkin and Teller (1943) studied the four-component version of the model earlier before Renfrey Potts formally introduced the Potts model in his 1952 doctoral thesis (Potts, 1952). It is known that the Potts model can be related to numerous important problems in the statistical lattice due to its richness content. Therefore, the Potts model has been chosen repeatedly as the model that is studied using different methods and approaches in the study of the critical point theory (Wu, 1982).

The reason why we chose to consider the three -state Potts model on a Cayley tree is that it is easier for the calculation to be evaluated by taking the tree rather than taking the whole lattice structure. The fact that the Cayley tree is a cycle-free graph makes it a very instructive example where exact calculations can be done (Baxter, 1982). The application of Cayley tree can be found as the modelling structure across many disciplines such as neural networks (Ban and Chang, 2017), chemistry (Pandey and Pande, 2014) and communication (Schibell and Stafford, 1992).

Therefore, extending the research of Ganikhodjaev et al. (2008), it is in our interest to investigate on the phase diagrams of the three -state Potts model on a Cayley tree considering the competing binary interaction up to the third nearest-neighbour generation. This is in the hope that this research would contribute to the body of knowledge of the statistical mechanics and dynamical systems.

In the following section, we have done some literature review regarding the researches that have led to our study.

1.2 LITERATURE REVIEW

The study on the phase diagram of the binary interaction on the Cayley tree has invoked a deep interest among numerous researchers. Back then, they started the research by considering the Ising setting and later extending to the Potts model.

Vannimenus (1981) pioneered the study in the phase diagrams of the Ising model nearest-neighbour and next-nearest-neighbour interaction on the Cayley tree. He introduced an iteration method, which made the study on the phase transition for more than one interaction on the Bethe lattice feasible. Furthermore, he suggested the study of the modulated phases using the variation of wavevector with temperature and the Lyapunov exponent. He found four stable phases namely ferromagnetic, paramagnetic, antiphase and modulated phase.

Inawashiro and Thompson (1983) adopted a different iteration scheme than Vannimenus (1983) and considered all interbranch next-nearest-neighbour interaction on coordination number three lattice. This was chosen as to make sure that the model undergoes frustration completely and correlates with the Beithe-Pearls approximation on the hexagonal lattices. The result is that some interesting features were found in the study. Although the phase diagram that was obtained was similar to Vannimenus (1981), at zero temperature, it revealed a chaotic phase over a finite interval of J'/J_1.

Intrigued by both of the previous studies, Mariz, Tsallis and Albuquerque (1985) produced their version of investigation by assuming the influence of external magnetic field. Instead of all interbranch next-nearest-neighbour on coordination number three lattice considered as J_2, they separated the interaction into prolonged next-nearest-neighbour J_2 and one-level next-nearest-neighbour J_3. They exhibited vanishing magnetic field $(J_1, J_2, J_3) \rightarrow -(J_1, J_2, J_3)$ isomorphism and showed that when the magnetic field is nonzero, the isomorphism is destroyed.

The richness feature of the phase diagram in the previous studies encourages the succeeding authors to shift their interest into the study of the phase diagram of the Potts model on the Cayley tree. After all, the Potts model is a generalisation of the Ising model. Therefore, Ganikhodjaev et al. (2008) studied the phase diagram of the Potts model up to the second nearest-neighbour interaction. They mentioned that the models considered on the Cayley tree and on crystal lattices often produced similar results, hence this has become the motivation for them in the research. By considering the models on the Cayley tree, the models can be formulated into dissipative mapping problems, where the methods of dynamical systems can be utilised. On the contrary, such methods do not give simpler results if they are used on the models defined on the crystal lattices. Thus, upholding the same motivation, this thesis is the continuation of Ganikhodjaev et al. (2008).

Similar to this research, they had considered a three-state Potts model defined on the semi-infinite Cayley tree of order 2. By deriving the recurrence equations, they had generated a phase diagram that is similar to the one found in Vannimenus (1981), only that they had found a new phase in the modulated region which demonstrate the paramagnetic activity. However, this new phase is different from the paramagnetic phase since the paramagnetic phase occurs at high temperature, whereas this new phase only occurs at low temperature. Due to the fact that this new phase exists in the modulated region while exhibiting the paramagnetic behaviour, this brings them to name the new phase as the paramodulated phase. The paramodulated phase marks the significance of this research as compared to the previous ones.

They also had linearised the system and derived the eigenvalue equation in order to determine the stability limit line of the paramagnetic region. This method however is a limitation of our study as will be explained in the conclusion.

In the following year, Ganikhodjaev et al. (2009) continued the study on the phase diagram of the Potts model. However, in this study, they included one-level next-nearest-neighbour interaction on the Cayley tree. In contrary to the previous study on both Ising and Potts settings, the phase diagram that was generated in this study showed that the multicritical Lifshitz point is shifted to a finite temperature rather than stayed on the zero temperature. Not only that, the paramagnetic phase disappears as soon as the one-level interaction becomes nonzero.

Continuing the research, Ganikhodjaev and Rodzhan (2015) had studied the phase diagram of the Ising model on the Cayley tree with competing interactions up to the third nearest-neighbour. This paper demonstrated the existence of a new phase, which is the paramodulated phase, as well as the ferromagnetic, antiferromagnetic and paramagnetic phases. Other than that, in this study, they had considered spins, which are belonging to different branches of the tree. Ganikhodjaev (2016) would later define this interaction as the ‘Uncle-Nephew’ interactions.

Ganikhodjaev and Rodzhan (2016) had extended the research by examining the phase diagram of the Ising model on the Cayley tree with competing first, second and third nearest-neighbour interactions. They had managed to show that the third nearest-neighbour interactions give rise to the existence of antiphase $< 3 >$ with its magnetisation of successive generation behaves with structure $< + + + - - - >$.

Many researchers soon after embarked on similar investigations, extending each study by an important factor in the hope to discover new and interesting feature of the phase diagram. Yet, to the best of the author’s knowledge, most of the studies, considering the three-state Potts model on the Cayley tree, have only considered the binary interaction up to the second nearest-neighbour generation. Hence, it is in our keen interest to investigate how the consideration of the third nearest-neighbour binary interaction would have affected the generation of the phase diagram.

1.3 RESEARCH OBJECTIVES

The objectives of this research are:

i. To derive the recurrence system of equations (nonlinear dynamical systems) for the three-state Potts model up to the third nearest-neighbour interactions
ii. To study the phase diagrams of three-state Potts model with competing binary interactions up to the third nearest-neighbour interactions
iii. To investigate in detail the modulated phases by investigating the wavevector and Lyapunov exponent.

1.4 THE ORGANISATION OF THE THESIS

In this first chapter, we have introduced the background and motivation of this study, where the previous researches that have led to this study are discussed. The literature review has also been presented chronologically. On top of that, we have presented the objectives of this research in Chapter One.

In Chapter Two, we will provide the methodology of this research. This includes all the important definitions and mathematical formula utilised for the purpose of this study. We will also provide the general methods on how the period phases are characterised. Then, we will present the basic equations of this research and start to derive the recurrence equations in detail.

The results and discussions will then be presented in Chapter Three and Chapter Four. In Chapter Three, we will present all the phase diagrams generated using the derived recurrence equations. The morphology of the phase diagrams will also be discussed in detail.

On the other hand, Chapter Four discusses about the existence of the phases of period larger than 12 in the modulated region by employing the method of the variation of wavevector and the Lyapunov exponent. We will start the chapter by introducing the average magnetisation that will be utilised in generating the wavevector as well as the Lyapunov exponent. Then, the diagrams of the wavevector will be presented and discussed in searching for the phases of period larger than 12. Finally, we will present the Lyapunov exponent and discuss its results in determining the stability limit cycle of the found period phases in the modulated region.

Lastly, in Chapter Five, we present the conclusion for this thesis. We will review the results of this research to determine whether the objectives of this research are achieved or not. Then, we will present the limitations of this study and recommend some open problems for future researches related to this study.

We have also attached the list of references that are used in this study. Appendix I is also provided for the readers to check the periodicity behaviour of the phases presented in Chapter Four. The last page of this thesis includes Appendix II, where the publications of this research are mentioned for the readers' perusal.

CHAPTER TWO

METHODOLOGY

2.1 INTRODUCTION

In this study, we carry out an investigation on the three-state Potts model on the Cayley tree of order-2 with competing interactions up to the third nearest-neighbour generations. We employ the line of methodology that was introduced by Vannimenus (1981). This is crucial for us to observe the behaviour of our dynamical system as well as study in detail the local properties of our model.

Ganikhodjaev et al. (2008) has presented the phase diagrams of the three-state Potts model, where they considered the competing nearest-neighbour J_1 and prolonged next-nearest-neighbour J_p interactions. There are five phases discovered in the phase diagrams, which are paramagnetic, ferromagnetic, paramodulated, antiphase and modulated. All these phases meet at the point $\left(T=0,\ J_p/J_1=1/3\right)$.

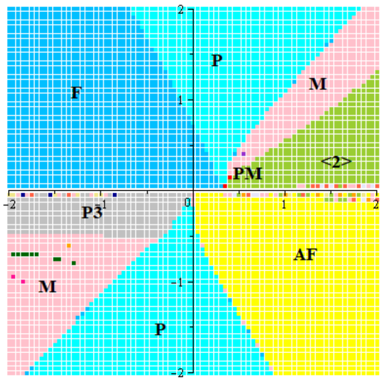

Figure 2.1: Phase Diagrams Derived from The Recurrence Equations in Ganikhodjaev (2008), where $J_3 = 0$. (F- Ferromagnetic, P-Paramagnetic, M-Modulated, PM-Paramodulated, <2>-Antiphase, AF-Antiferromagnetic, P3-phase of period 3)

The paramodulated phase was a new phase discovered which set their study apart from the rest. We can see this phase in Figure 2.1 where it is represented by the small red dots. This phase is an essential discovery in the case of the Potts model.

Therefore, we are intrigued to find out whether the presence of the third nearest-neighbour interaction will give a significant effect on the generation of the phase diagrams. We also would like to know if there is any additional phase that would be discovered if the third nearest-neighbour binary interaction is considered in the model. We will also carry out a detailed investigation on the modulated phase by applying the variation of the wavevector with temperature as well as evaluating the Lyapunov exponent.

2.2 DEFINITIONS

Before we delve further, we would like to first clarify the definition of some terms that are relevant in this study. As we have mentioned before, we consider our model on a Cayley tree.

Definition 2.1. *Cayley tree Γ^k of order $k \geq 1$ is an infinite tree, which is a graph without cycles with exactly $k+1$ edges exiting each vertex. We denote the Cayley tree as $\Gamma^k=(V, \Lambda)$, where V is the set of vertices and Λ is the set of edges on Γ^k .*

Two vertices x and y, where $x, y \in V$, are the first nearest-neighbour if there is only one edge $l \in \Lambda$ in between them that is denoted as $l = \langle x, y \rangle$. The distance $d(x, y)$ on Γ^k, where $x, y \in V$, represents by the number of edges which make up the shortest path from x to y.

For a fixed set $x^0 \in V$, we denote

$$W_n = \{x \in V \mid d(x, x^0) = n\}, V_n = \{x \in V \mid d(x, x^0) \leq n\},$$

and L_n *is the set of edges in* V_n*. The fixed vertex* x^0 *is called the* 0*-th level and other vertices x defined in* W_n *are the n-th levels. Further, we define* $|x| = d\,(x, x^0)$, *where* $x \in V$.

Two vertices x, y $\in V$ *are the second nearest-neighbour if* $d(x, y) = 2$*. They are called prolonged second nearest-neighbour if* $|x| \neq |y|$*, where they are denoted by* $>\widetilde{x, y}<$*. Two vertices x, y* $\in V$ *are the third nearest-neighbour if* $d\,(x, y) = 3$*. They are called prolonged third nearest-neighbour and is denoted by* $<x, \widetilde{y}>$ *if* $x \in W_n$ *and* $y \in W_{n+3}$.

If the path from x^0 *to y goes through x, then it is denoted as* $x \prec y$*. The vertex y is a direct successor of x given that* $y \succ x$ *and x and y are nearest neighbours. We denote the set of the direct successors of x as S(x), which is if* $x \in W_n$*, then*

$$S(x) = \{y_i \in W_{n+1} \mid d(x, y_i) = 1, i = 1, \ldots, k\}.$$

For any vertex where $x \neq x^0$*, x has k direct successors and* x^0 *has* $k + 1$.

For the purpose of this study, we consider our model on a semi-infinite Cayley tree of order two.

A semi-infinite Cayley tree Γ_+^2 of order two is an infinite graph without cycles with $k + 1$ edges exiting each vertex except for x^0 which consists of k edges. The model that we have chosen for this study is the 3-state Potts model. The Q-state Potts model was introduced as a generalisation of the Ising model, extending to two ($Q = 2$) or more interacting spins.

Specific to our study, we chose to employ the 3-state Potts model; therefore, our model has a set $\phi = \{1, 2, 3\}$ on the Cayley tree of order two, Γ^2.

Let us present a general definition of the Q-state Potts model,

Definition 2.2. *The Q-state Potts model is a spin system, which consists of a set* $\phi = \{1, \ldots, Q\}$ *of spins values and by the Cayley tree* Γ^k. *A configuration* $\sigma \in \phi^{\Gamma^k}$ *assigns a spin value* $\sigma(x) \in \phi$ *to each of the vertex x. We let* $\Omega \in \phi^{\Gamma^k}$ *to be the set of all configurations on* Γ^k.

Let Ω be the set of all configurations, and then we have that

Definition 2.3. *A function* $H: \Omega \to R$ *is called a Hamiltonian corresponding to the energy of a configurations.*

Now we would like to define some terms that will be used in the analysis of the phase diagram, which is an important part in order to understand a dynamical system. Suppose that we have a mapping such that $f: X \to X$ where $X \subset R^n$.

Definition 2.4. *If* $f: X \to X$ *is a mapping and* $f(c) = c$, *then c is a fixed point of* f.

Using a graphical representation, a mapping has a fixed point at c if it has a graph which intersects at the point (c, c) on the line $y = x$. *The fixed point is denoted as Fix(f).*

Definition 2.5. *Let* $f^{((k))(x)} = f(f^{(k-1)}(x))$ *with* $f^{(1)}(x) = f(x)$, *where* $k = 1, 2, \ldots$. *The point* x *is a periodic point of* f *with period k if* $f^{(k)}(x) = x$.

This means that if x is a fixed point of $f^{(k)}$, then x is a periodic point of f with period $k = 1$. Moreover, the point x has a prime period k^0 if $f^{(k^0)}(x) = x$ and $f^{(n)} \neq x$ where $0 < n < k^{(0)}$. This implies that the point x is said to have a prime period $k^{(0)}$ if x returns to the initial value after being iterated exactly $k^{(0)}$of f.

Consequently, we can gather all the iterations of a fixed point x into a set and call it the orbit of x. Furthermore, if x is a periodic point, then the orbit is called the periodic orbit or the periodic cycle of x.

Definition 2.6. *Suppose* $\hat{f}: R^m \to R^n$*is a vector-function* $\hat{f} = (f_1, f_2, \ldots, f_n)$ *and* $x = (x_1, x_2, \ldots, x_m)$ *given by n real-valued component functions*