INTERNATIONAL ISLAMIC UNIVERSITY MALAYSIA

PHASE TRANSITION FOR LATTICE MODELS WITH RESTRICTED COMPETING INTERACTIONS ON CAYLEY TREE

BY

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ABSTRACT

We investigate the phenomenon of phase transition on Ising model with restricted competing interactions on Cayley tree. We first consider an Ising model with four competing interactions (external field, nearest neighbor, second neighbors and triples of neighbors) on the Cayley tree of order two. We found the analytic solution of the problem of phase transition for the case absent of external field and for the case absent of ternary interaction. Our main result is the critical curve of phase transition where for the condition satisfied, a phase transition occurs. This result is the generalization of ordinary Ising model and also other results in (Ganikhodjaev & Pah, 2003; Ganikhodjaev, 2002; Mukhamedov & Rozikov, 2004). Our investigation is based on two methods: Markov random field and recurrent equation of partition function. For general case with absent of ternary interaction, we extend the result from Ising model to Potts model. Based on the recurrent equation of the partition function derived, employing numerical method, a phase diagram is plotted with four regions i.e. Paramagnetic(P), Ferromagnetic(F), Modulated (M) and Anti-phase($< 2 >$) similar as in (Vannimenus, 1981), (Inawashiro et al., 1983) and (Mariz et al., 1985). A new region is found, we called it quasi-paramagnetic, slightly different from the ordinary paramagnetic case. Our result is different from (Vannimenus, 1981; Inawashiro et al., 1983; Mariz et al., 1985). Also using another approach, namely contour method, we show that phase transition exist in 2 component model and we describe the phase diagram of the ground state of 3 component model. The 2 component and 3 component model are generalization of the Ising model and Potts model respectively. This method was recently introduced for binary interaction on the Cayley tree (Rozikov, 2005), while our method is carried out after revising and developed from the results of Minlos's(Minlos, 2000).

ABSTRACT IN ARABIC

يتعرّض هذا البحث لظاهرة إنتقال الشكل على شجرة كيلي، وفق نموذج آيسنج (Ising model)، وذلك من خلال عمليات محصورة في الكمبيوتر. في البداية تعرض الباحث لنموذج آسنج من خلال أربع عمليات على نظام شجرة كيلي وهي :(المجال الخارجي، المجال المتجاور، المتجاور الثنائي والمتجاور الثلاثي). لقد اكتشف الباحث الحل التحليلي لغياب المجال الخارجي وغياب التفاعل الثلاثي لمسألة إنتقال المجال. كانت النتيجة الأساسية هي الإنحناء الحاد في إنتقال الشكل عند توفر كل الشرائط لحصول الإنتقال. هذه النتيجة هي تعميم لنموذج آسنج وكذلك النتائج الأخرى. قامت عملية البحث على منهجين: منهج المجال العشوائي لماركوف (Markov)، ومنهج المعادلة المطردة للعملية الجزئية. في الحالة العامة وبغياب التفاعل الثلاثي تم نقل النتيجة من نموذج آيسنج إلى نموذج بوتس (Potts). بناء على منهج المعادلة المطردة للعملية الجزئية تم استخدام المنهج العددي وتم تقطيع الشكل البياني إلي أربع مناطق هي: Paramagnetic(P), Ferromagnetic(F), Modulated (M) and Anti-phase(< 2>) similar as in(Vannimenus,1981), (Inawashiro et al.,1983) and (Mariz et al.,1985). كما وجدت منطقة أخري جديدة أسميناها (quasi-paramagnetic)، تختلف قليلاً عن (paramagnetic case) المعروف. إن النتيجة التي توصل إليها البحث تختلف عن نتيجة فانيمنيوس (Vannimenus,1981). كما استخدم الباحث مقاربة أخري وهي المنهج المقابل الذي من خلاله تم بيان أن إنتقال الشكل يظهر في نموذج العنصر الثنائي، كما تم توضيح أن الشكل البياني قائم على نموذج العنصر الثلاثي. فنموذج العنصر الثنائي والعنصر الثلاثي هما تعميم للنموذجين آيسنج وبوتس على التوالي. هذا المنهج استخدم أخيراً في التفاعل المشترك على شجرة كيلي، بينما المنهج المستخدم في هذا البحث تم تطبيقه بعد مراجعة وتطوير للنتائج التي توصل إليها منلوس (Minlos).

APPROVAL PAGE

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DECLARATION

I hereby declare that this dissertation 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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LIST OF ABBREVIATIONS

ANNNI	Axial Next-Nearest-Neighbour Ising
DLR	Dobrushin, Lanford and Ruelle
e.g.	for example
F	Ferromagnetic
i.e	that is
Int	interior
M	Modulated
min	minimum
nn	nearest neighbour
nnn	next nearest neighbour
P	Paramagnetic
PR	Positive Roots
QP	Quasi Paramagnetic

LIST OF SYMBOLS

Φ	spin state	2
φ	a configuration	3
$\varphi_{\Lambda}^{(i)}$	a configuration in Λ with outer constant configuration fixed at ν_i	65
q	cardinality of spin set	14
R	real line	1
S	lattice	2
T	temperature	6
u_i	reduced variables of partition function	54
V	finite volume	4
V_n	finite volume of Cayley tree at level n	21
W_n	level n of Cayley tree	21
x^0	root of semi infinite Cayley tree	20
x^*	fixed point	55
$Z, Z_{\Lambda,\omega}$	partition function	6
Z^d	d dimensional integer lattice	2

CHAPTER 1

INTRODUCTION

1.1 PRELIMINARIES

One way of understanding the law of nature is to find out how the dynamic of the microscopic components of matter, such as atoms and molecules, determine the behaviour of macroscopic objects containing many atoms, objects that we can see and touch. Due to the thermal motion, the atoms are moving randomly and freely which result in the fluctuation in measuring the macroscopic quantities. This is the main subject of statistical mechanics which provides a mathematical framework for describing how well-organized higher level structures or behaviour may result from the random, nondirected activity of a very large number of interacting lower level entities. In one case, the smallest entity can be we human, each of us, while the macroscopic correspond to our society with a large number of population.

The physical background. Consider, for example, a piece of ferromagnetic metal (like iron) in thermal equilibrium, i.e. no net flow of heat with surrounding. The piece consists of a very large number of atoms which are located at the sites of a crystal lattice. Each atom shows a magnetic moment which can be visualized as a vector in R^3. Since the magnetic moment results from the angular moments, the so called spins, of the electron. It is also called, for short, the spin of the atom. The interaction properties of the electrons in the crystal imply that only those any two adjacent atoms have a tendency to align their spins in parallel. At high temperature, this tendency is compensated by the thermal motion. The atoms acquire more kinetic energy and then moving freely, as the temperature increases. If, however, the temperature is below certain threshold value which is called the Curie temperature, the coupling of moments dominates and gives rise to the phenomenon of spontaneous magnetization, i.e. the spin system takes one of the several possible states.

As second example we consider a real gases. The gas consists of a huge number of particles which interact via van der Waals forces. To describe the spatial distribution of the particles we may imagine that the container of the gas is divided into a large number of cells which are of the same order of magnitude as the particles. To each cell we assign its occupation number i.e. the cell could be occupied by up to some n number of particle. We also replace the van der Waals attraction between the particles by an effective interaction between the occupation number. The resulting caricature of a gas is called a lattice gas. This lattice system, as well as the van der Waals forces, after modification has been applied recently to bio-information in the study of protein structure.

The mathematical model. Let S be a countable infinite set. In the case of a ferromagnetic, S consists of the sites of the crystal lattice which is formed by the position of atoms. In a lattice gas S is the set of all cells which subdivide the volume which is filled with the gas. The set S representing the sites can be expected to have some additional structure, for example we might know the distances between the sites, or we might know that certain sites are connected. We will consider structures S of the latter kind, that we suppose that the points of S are the vertices of some infinite graph $G = (S, L)$ where L is the set of edges of G. Below we will consider only two types of infinite graphs, namely integer lattice $Z^d, d > 1$ and Cayley tree J^k of order k, $k > 1$, where it is an infinite tree, i.e. a graph without cycles, from each vertex of which exactly $k + 1$ edges issue.

Secondly, let Φ be a non-empty set, which describes the possible states of each components. For a ferromagnet, Φ is the set of all possible orientations of the magnetic moments. For illustration and simplicity, we might assume that each moment is only capable of two orientations. Then $\Phi = \{-1, 1\}$, where 1 stands for "spin up" and -1 stands for "spin down". In the case of lattice gas, we can take $\Phi = \{0, 1, ..., N\}$, when N is the maximal number of particles occupy the cell. Having specified the sets S and Φ, we can describe a particular state of the total system by a suitable element $\varphi = \{\varphi(x) : x \in S\}$ of the product space $\Omega = \Phi^S$. Each of this state is called a configuration whereas Ω is the configuration space.

The physical system considered above are characterized by a sharp contrast: the microscopic structure is enormously complex and any measurement of microscopic quantities is subject to some significant statistical fluctuations. The behaviour of the atoms are random and undetermined. The macroscopic behaviour, however, can be described by means of a few parameters such as temperature and pressure respectively magnetization, and macroscopic measurements lead to apparently deterministic results. The fluctuations far from the critical point are so small which can be neglible. This contrast between the microscopic and macroscopic level is the starting point of Classical Statistical Mechanics as developed by Maxwell, Boltzmann and Gibbs. How can this be answered by mathematics? Their basic idea may be summarized as follows: the microscopic complexity can be overcome by a statistical approach in which the macroscopic determinism then maybe regarded as a consequence of a suitable law of large number. The probability measure that give rise to the microscopic property is just a 'tail' function where it become trivial when the size of number is so large.

Which kind of probability measure on Ω is suitable to describe a physical system in equilibrium? The term "equilibrium" where the kinetic energy is constant, clearly refers to the forces that act on the system. In the physical systems above, the essential contribution to the potential energy comes from the interaction of the microscopic components of the system. In addition, there maybe an external force, competing forces or external magnetic field in the case of ferromagnet. After specifying the Hamiltonian

$H(\varphi)$ and spin state Φ, we have actually defined a model on certain lattice S. The simplest of all such models is the well known Ising model (Ising, 1925). Ising model, as a highly simplified model, has greatest application not only in physics but in a very wide range of fields such as sociology, economics, genetics, network and etc.

1.2 MODEL

Generally, let $\mathcal{J}$ be the infinite set of all non-empty finite subsets of S, the lattice. A family $\{J(\varphi(V)), V \in \mathcal{J}\}$ of functions $J(\varphi(V)) : \varphi(V) \to R$ is called an interaction potential of variables $\varphi(x)$ in volume V.

For an arbitrary $W \in \mathcal{J}$ a series

$$H(\varphi(W)) = \sum_{V \subseteq W} J(\varphi(V)) \tag{1.2.1}$$

is called the energy of configuration φ in volume W. The sum

$$H(\varphi(W)|\varphi(S \backslash W)) = \sum_{\substack{V \cap W \neq \emptyset \\ V \cap S \backslash W \neq \emptyset}} J(\varphi(V)) \tag{1.2.2}$$

is called the energy of interaction configuration $\varphi(W)$ with configuration $\varphi(S\backslash W)$ (boundary configuration), and a sum,

$$H(\varphi(W)) + H(\varphi(W)|\varphi(S\backslash W)) \tag{1.2.3}$$

is called a full energy of configuration $\varphi(W)$ with boundary condition $\varphi(S\backslash W)$. Finally a sum

$$H(\varphi) = \sum_{V \in \mathcal{J}} J(\varphi(V)) \tag{1.2.4}$$

is called a Hamiltonian of given system.

So for the Ising model (Ising, 1925) interaction potentials of variables $\varphi(x)$ in volume V is defined following way:

$$J(\varphi(V)) = \begin{cases} 0 & \text{if} \quad |V| \geq 3 \\ -J\varphi(x)\varphi(y) & \text{if} \quad V = \{x, y\} \quad \text{and} \quad x, y \quad \text{are nearest neighbours.} \\ 0 & \text{if} \quad V = \{x, y\} \quad \text{and} \quad x, y \quad \text{are not nearest neighbours.} \\ -h\varphi(x), & \text{if} \quad |V| = 1, V = \{x\} \end{cases} \tag{1.2.5}$$

where $J, h \in R$. Now, we can introduce the well known Ising model (Ising, 1925) which is a ferromagnetic system with simplest state space $\Phi = \{-1, 1\}$, namely "spin down" and "spin up" respectively. Similarly, let $\varphi(x)$ be a function to $\varphi : S \to \Phi$, where S is the set of sites of the lattice. The collection of $\varphi(x)$ on all $x \in S$ is denoted by $\varphi = \{\varphi(x) : x \in S\}$ which is called a configuration. To each configuration φ a potential energy $H(\varphi)$, Hamiltonian, is assigned by a real function

$$H(\varphi) = -J \sum_{<x,y>} \varphi(x)\varphi(y) - h \sum_{x \in S} \varphi(x). \tag{1.2.6}$$

where $J, h \in R$. Ising (Ising, 1925) made the simplifying assumption that only interactions between neighbouring spins need to be taken into account. Here the first sum is taken over all pairs x, y of points which are the nearest neighbour, i.e. there is an edge connecting them, and it is denoted by $< x, y >$. The first term represents the energy caused by the interaction between the neighbouring spins and J measures the strength of this interaction. The product spin in the first term is $+1$ if both has same spin and -1 if both has different spin. For the ferromagnetic case, which J is positive, spins are tend to be aligned to the same spin for nearest neighbour. When J has opposite sign, it is called anti-ferromagnetic and it is tends to antialign them. The second term is external magnetic field where h measures the strength of the external magnetic field. Magnetic interaction tends to align in spin in single value of the spin state. The strength of the interaction measures the tendency of the alignment while the the thermal energy tries to destroy the order.

We will consider the generalization of Ising model, such that

$$J(\varphi(V)) = 0, \quad \text{if} \quad |V| \geq 4$$

which $J(\varphi(V)) \neq 0$ for $|V| = 3$, that is to consider the interactions between triples of spins. In Ising's case, only nearest neighbour binary interaction being considered. By specified $J(\varphi(V))$ and Φ, we are actually defining a model, i.e. each model is characterized by the definition of $J(\varphi(V))$ and Φ.

1.3 GIBBS MEASURE

Let S be a infinite lattice and Φ is a state space. For any finite subset Λ of S, denote $\Omega_\Lambda = \Phi^\Lambda$. As before Ω_Λ is the set of all configuration φ_Λ on Λ and ω be configuration on $S \backslash \Lambda$, $\omega \in \Phi^{S \backslash \Lambda}$. Assume a Hamiltonian H is given on $\Omega = \Phi^S$. A probability measure P is called a *Gibbs measure* with Hamiltonian H if it satisfies the DLR equation (see Sinai, 1982): $\forall$ finite $\Lambda \subset S$ and $\varphi_\Lambda \in \Omega_\Lambda$:

$$P\left(\left\{\varphi \in \Omega : \left.\varphi\right|_\Lambda = \varphi_\Lambda\right\}\right) = \int_\Omega P(\mathrm{d}\omega)\mu_\omega^\Lambda(\varphi_\Lambda), \tag{1.3.1}$$

where μ_ω^Λ is the conditional probability defined by:

$$\mu_\omega^\Lambda(\varphi_\Lambda) = \frac{1}{Z_{\Lambda,\omega}} \exp\left(-\beta H\left(\varphi_\Lambda \middle| \omega\right)\right).$$

The constants $\beta = 1/kT$ is known as inverse temperature, $T > 0$ is temperature and k is

Boltzman's constant which could be omitted throughout the thesis. $Z_{\Lambda,\varphi}$ stands for the partition function in Λ, with the boundary condition ω:

$$Z_{\Lambda,\varphi} = \sum_{\varphi_\Lambda \in \Omega_\Lambda} \exp\left(-\beta H\left(\varphi_\Lambda \,\middle|\, \omega\right)\right). \tag{1.3.2}$$

The Gibbs measure gives directly the probability of a given configuration φ to occur in the configuration space Ω_Λ. It is not surprise that Gibbs measures is widely use in simulating physical system, this is due it is the generalization of Markov chain and also it's property of strictly positivity. Dobrushin (Dobrushin, 1968; Dobrushin, 1968) was who introduced a class of Markov random fields generalizing the definition of the Markov Chain. Then, Spitzer (Spitzer, 1970) showed that the translation invariant Markov random field are precisely the Gibbs measure of nearest-neighbour interactions.

The limiting Gibbs measure is referred to the Gibbs measure when the limit of the finite volume is tends to the entire graph $\Lambda \to \infty$, this limit also known as thermodynamic limit. Most of the thermodynamic properties can be expressed directly in terms of the partition function, e.g. free energy, entropy and pressure. Once the explicit form of the limiting Gibbs measure or the partition function is obtained, most of the problem centered on it could be solved directly as well. However, this is known to be a difficult task.

1.4 PHASE TRANSITION

The set $\mathcal{M}(H)$ of all Gibbs measures for H can, and should, be regarded as a proper mathematical description of the set of all possible equilibrium states for a physical system that consists of a huge number of components which are coupled together by the Hamiltonian H. In fact, the Gibbs measures exhibit a rather strong equilibrium property that even each microscopic, i.e. finite, subsystem is in conditional equilibrium, when the "surrounding" is frozen.

According to this interpretation, the non-uniqueness of the Gibbs measure for a given Hamiltonian H means that the physical system may "choose" from these equilibrium states. Such a free choice is the characteristic of a physical system which undergoes a phase transition. This fact suggests the following terminology:

A Hamiltonian H is said to exhibit a phase transition if $|\mathcal{M}(H)| > 1$.

In many standard texts on statistical mechanic (see e.g. Georgii, 1988; Preston, 1974; Simon, 1993), the phenomenon of phase transition was commented not to be regard as an observation of a mixture of the states in physical world. We do not see a mixture of liquid and solid form of water at frozen point, rather we see only one of the phases subject to what phase we approach this point from, namely boundary condition. In the case where we start above frozen point, we shall see liquid form of water at frozen point or we will see ice at frozen point if we start below frozen point. The two (or more) states actually do not co-exist at a given parameter, rather phase transition reflects that the system can takes any one of the multiple states which still subject to the boundary condition. The free choice is actually not really free. The co-existence is refer to the co-existence of more than one distribution for a given same parameter, most of the time is temperature. For the case of ferromagnetism (see Figure 1.1) in the absence of magnetic field $h = 0$, the magnetization is either positive or negative which subject to is the initial condition, when ever it is below the Curie temperature $T < T_c$. When $T > T_c$ in the absence of magnetic field $h = 0$, the magnetization is zero, which characterize absence of phase transition.

In summary of above, the physical phenomenon of phase transition is reflected in mathematical model by the non-uniqueness of the Gibbs measure. Fortunately and somewhat surprisingly, the model developed above is indeed realistic enough to exhibit this non-uniqueness of Gibbs measures in an overwhelming number of cases in which a

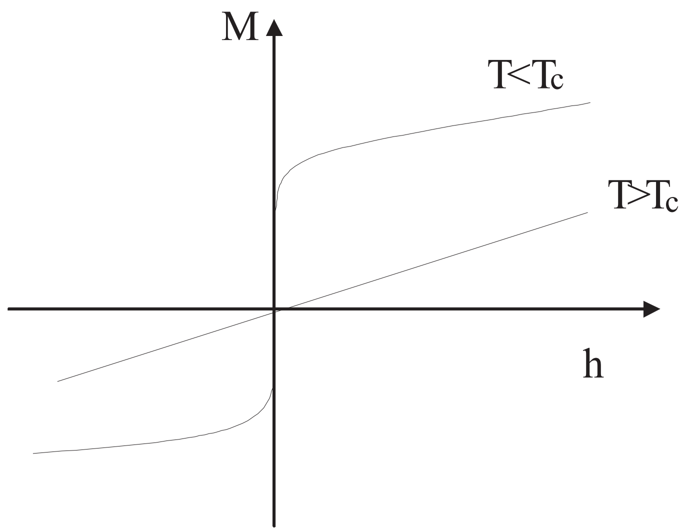

Figure 1.1: Magnetization (M) versus magnetic field strength (h).

phase transition is predicted in physics. This fact is one of the main reason for the physical interest in Gibbs measure. The phase transition usually occurs at low temperature, namely if it is possible to find an exact value of temperature T^* such that a phase transition occurs for all $T < T^*$, then T^* is called a critical value of temperature. Finding the exact value of the critical temperature for some models means to analytically solve the model, or the model is exactly solved.

1.5 LITERATURE REVIEW

The phenomenon of phase transition is one of the most interesting topic of statistical physics. There are many solved and unsolved problems in various models, such as different integer square lattice model and Cayley tree, denoted by Z^d and J^k respectively. A Cayley tree J^k (see also (Baxter, 1982)) of order $k \geq 1$ is an infinite tree, a graph without cycles, from each vertex of which exactly $k + 1$ edges issue. Unfortunately, the Cayley tree is not a realistic one. This is due to Cayley tree's infinite dimensionality i.e. the ratio of the number of boundary sites to the interior sites of Cayley tends to a constant in the law of large number. The boundary tends to grow in the same order as the volume grows. In other words the measure of thermodynamic limit is not trivial for the Cayley tree model. However, the solvability of the tree model provide us an greater advantage to obtain an exact solution, over it's counter part the regular lattice, where for the other lattice certain assumptions or approximation has to be made. The exact solution is rarely seen in the problem of phase transition on regular lattice. Despite the fact that Cayley tree has constant thermodynamic limit, one can find a good approximation for regular lattice through the exact solution of tree model to gain a qualitative picture of the phase diagram. The corresponding properties in tree model then could be expected to be exist for regular lattices, and consequently be of relevance for some real system e.g. spin-glasses. In fact, the thermodynamic limit is not the absolute answer as a bridge between the microscopic entity and macroscopic behaviour. The law of the thermodynamic limit was merely voted, a tight win, and accepted by the community of science in the early of 20th century. Nowadays, the emerging science of networks in the information technology era has attracted a new wave of interest in such models (Dorogovtsev and Mendes, 2002; Pastor-Satorras & Vespignani, 2004; Albert & Barabasi, 2002; Dorogovtsev and Mendes, 2003). Moveover, one could also see the motivation of the research on Cayley tree through a series of papers which will be mentioned later.

The existence of phase transition for the Ising model on Cayley tree for order $k \geq 2$ was solved independently by Katsura and Takizawa (1974) and Preston (1974). In the measure theoretic approach, the study on the description of the limiting Gibbs measures are carried out in a series of papers (Ganikhodjaev, 1990; Bleher & Ganikhodjaev, 1990; Ganikhodjaev & Rozikov, 2000). The full analysis on all limiting Gibbs measures respect to a given Hamiltonian for any lattice is a difficult problem. In above mentioned papers, some transformation groups and automorphisms of the Cayley tree was intro-