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Transverse Magnetic Field Coupling Effects on the Topology of Phase Diagrams of 2-D Ising Model

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ABSTRACT

The response behavior of the topology of various phase diagrams corresponding to different physico-chemical systems has been studied. Our study relies on using the 2-D transverse field ising model and considering only distinct nearest neighbor pair-exchange interaction. We calculate phase diagrams in the polarization-temperature phase space with the aid of the Mathcad computer software. The theory is based on the simple temperature dependence of the potential parameters in the TIM within the framework of the mean field theory approximation. We developed the more complex reentrant phase diagram that is common with some binary fluids, colloids, proteins and many more systems. And by parameter modifications we obtained some common and exotic phase diagrams that corresponding to those obtained both experimentally and theoretically. A qualitative analysis of the topological influence of the transverse magnetic field coupling is discussed.

Keywords: exchange interaction, order-disorder, phase diagram, topology, transverse magnetic field, transverse Ising model (TIM).

I. INTRODUCTION

Studies of the phase diagrams associated with microscopic cooperative interaction within some physico-chemical systems have offered useful insight to the understanding of the macroscopic phenomena that are characteristic of them. Indeed a wide number of systems display phase transitions when the temperature or some other potential parameter is altered. Phase transitions are commonly observable in daily life as when water freezes to form ice or in experiments where a bar magnet loses its magnetism at high temperatures. But more complex phase transitions can be observed in optical lattices in the more complex Mott insulator-superfluid phase transition [1]. This intriguing phenomena has therefore courted lots of research work to understand its properties. Hence lots of research work on phase transitions at finite temperature [2-8] has been carried out. The Landau-Ginsburg theory, the renormalization group and the symmetry breaking concepts [9-12] have been instrumental in explaining phase transition properties in systems.

In this paper we present theoretical results and discussions on the unique influence of transverse magnetic field on the phase transition properties systems. Our focus is based on the 2-D ising model with the transverse field couplings to the energy of individual molecules at the lattice sites with only nearest neighbour exchange interaction considerations. Quite often when questions are posed about the phase transition properties of any system it stems from how phase changes are affected by the exchange interaction energy and the effect on systems in a zero external magnetic field. However the magnetic field influence is very critical on the Hamiltonian energy of a system from the point of view of the TIM, and thus affects the microscopic property changes and the topologies of phase diagrams.

Several researchers have carried out studies on the effect of the transverse field on the spin using several different approaches. For instance, Jiang et al. [13] have carried out the study of the spin-1 TIM on a honeycomb lattice with a longitudinal crystal field and discovered the presence of tricritical points whereby phase transitions change from second-order to first order. By the use of the effective field theory (EFT) and probability distribution technique, Htoutou et al.[14] did an investigation on the influence of the magnetic field on the phase diagrams of a site diluted spin-1 TIM on a square lattice. In all these studies the authors have reported the strong influence on the re-entrant behaviour of the transverse field. The longitudinal magnetic field effect on the phase transitions in spin-3/2 and spin-2 TIM has also been studied by way of both honeycomb and square lattices and using the EFT with correlations[15,16]. Recently, Yussuf et al [17], studied the phase diagrams of the spin-1 TIM with a longitudinal crystal field in the presence of a longitudinal magnetic field on a honeycomb lattice within the framework of the IEFT approximation.

Our paper is concerned with the influence of the transverse magnetic field on the topology of the phase diagrams obtained for the re-entrant behaviour exhibited by some binary fluid mixtures, colloids, proteins etc. By altering the microscopic potential field parameters for our model (TIM), we again obtain some phase diagrams that correspond to different systems commonly obtained in experiments and in theoretical calculations. These phase diagrams, thus reveal the intricate effect of the transverse field coupling force on systems.

II. METHODS AND MATERIAL

In our model (TIM) we consider a two-dimensional square lattice which has N lattice sites. At the lattice sites we have the atoms or molecules of magnetic systems which can either have a spin 'up' or spin 'down' set of orientations. In the case of binary fluids these sites can be occupied by either atoms or molecules of the mixture of two different fluids. Whatever the case maybe of magnetic systems or binary fluid systems, the model features are the same and therefore consists of a lattice of lattice site variables with two characteristic properties:

(1) Each lattice site independently takes on either the value +1 or -1; and

(2) Interaction is between only pairs of nearest-neighboring spins.

The ising model has a venerable tradition of being efficient in the calculations of the phase diagrams for complex fluids [18-22] with reentrant phase behaviour. The Hamiltonian of the 2-D model with the transverse field given as follows [18-22]:

$$H = -\sum_i \Omega S_i^x - \sum_{\langle i,j \rangle} J S_i^z S_j^z \qquad (1)$$

Where S_i^x and S_i^z are the x- and z-components of a pseudospin-1/2 operator at site i in the lattice, and $\sum_{\langle i,j \rangle}$ is the sum over only distinct nearest-neighbouring pairs. Ω is the transverse field and J is the exchange interaction constant between nearest neighbour spins.

Within the framework of the mean-field theory, the z component of the pseudospin can be written as

$$\langle S_i^z \rangle = (\sigma/2\omega_0)\tanh(\omega_0/2k_B T) \qquad (2)$$

Where $\omega_0^2 = \Omega^2 + \sigma^2$

And

$$\sigma = \sum_i J \langle S_i^z \rangle$$

The order parameter of our model is the ensemble average of the pseudo-spin $\langle S_i^z \rangle$. Mathematically, any singularity or loss in analyticity of this order parameter at any finite temperature means a change in phase. This finite temperature then defines the critical transition temperature for the system. Basically this order parameter of the system which is the ensemble average of the pseudo-spin $\langle S_i^z \rangle$ describes the transition of the system from order ($\langle S_i^z \rangle \neq 0$) to disorder ($\langle S_i^z \rangle = 0$) state [22] by our graphs. For convenience sake we shall subsequently use SS in place of $\langle S_i^z \rangle$ in labelling the graphs for the phase diagrams.

It is known from experimental research carried out with complex fluids, that temperature changes in systems may have a direct correlation with the field potential parameters of the exchange interaction and the transverse field [23-24]. Thus Campi and Krivine [25] obtained closed-loop shaped phase diagrams and described the reentrant phase behavior of complex fluids from this concept.

Dwelling on this concept as well, Simons et al [22] using transverse Ising model and assuming that the effective exchange spin and effective transverse field parameters J and Ω respectively depends directly on temperature. The proceeded further to obtain the following temperature-dependent relations:

$$J = J_0\left(\frac{T}{T_0}\right)^n \quad \text{and} \quad \Omega = \Omega_0\left(\frac{T}{T_0}\right)^m \tag{3}$$

where T_0 are arbitrary constant. Here the parameters J_0, Ω_0 and k_BT are reduced by k_BT_0 , and simply are notated still as J_0, Ω_0 and t.

We proceed further to obtain the phase diagrams by solving eqn (2) with the substitution of eqns (1) and (3). We therefore calculate graphs with polarization-as a function of J_0,n,Ω_0 and m versus effective temperature.

III. RESULTS AND DISCUSSION

The Phase diagrams

In this section we obtain the phase diagrams in polarization-temperature phase space. Graphs are plotted with the polarizations as a function of various parameters of (J_0, n, Ω_0 and m) vs. the effective temperature t. Here J_0 is the effective exchange interaction, n is the temperature exponent for J_0, Ω_0 is the effective transverse magnetic field coupling while m is the temperature exponent for the transverse field. Ω_0. By varying the effective transverse field parameter Ω_0, we can observe the effect it has on the phase transition diagram. This section therefore examines the influence of the transverse magnetic field parameter Ω_0 over the topologies of systems of constant J_0, n and m while varying Ω_0 within each figure. The trends that evolve from the polarization-temperature graphs give us a qualitative understanding of the coupling behaviour of Ω_0.

Figure 1 give the polarization-temperature phase diagram for systems with J_0=1.6, n=1.6 and m=2.0. This system shows the phenomenon of the re-entrant behaviour associated with some complex fluids, binary mixtures, colloids, proteins etc. For these systems, at a narrow range of low temperature close to zero, the system is completely susceptible to being in the disordered state. As temperature is increased, for intermediate temperatures, the system has the likelihood of becoming ordered. For these intermediate temperatures, the bigger the value of Ω_0, the smaller the ordered phase region. Hence the polarization and temperature range for which the ordered phase is stable becomes smaller and diminishes as Ω_0 is increased. At higher temperatures the system once again becomes disordered for all polarization ranges. One noticeable trend about this figure is the egg-shaped profile. As Ω_0 is decreased this egg-shape profile is being enhanced. As Ω_0 is increased however, the profile is distorted from egg-shape and appears as oval shape until incompletely diminishes.

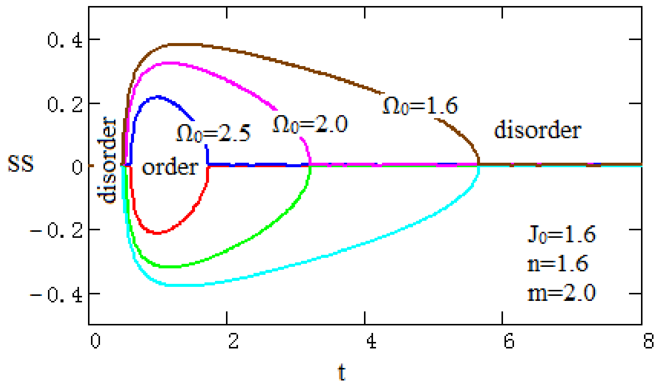

Figure 1: Phase transition diagram showing the polarization SS against temperature t for various effective transverse field parameter Ω_0 for a system where J_0=1.6, n=1.6, and m=2.0.

Fig. 2 shows common features as fig. 1. They all show the phenomenon of re-entrant behaviour. For fig. 2 the model is that for systems with J_0=1.1, n=1.6 and m=2.0. When J_0 was reduced, it was observed that Ω_0 had to be correspondingly reduced in order to mimic the re-entrant behaviour. All other properties associated with fig. 1 are same with fig.2. And it corroborates the influence of Ω_0 being an inveterate modifier of the shape profile by skewing it in towards egg shaped when it is smaller.

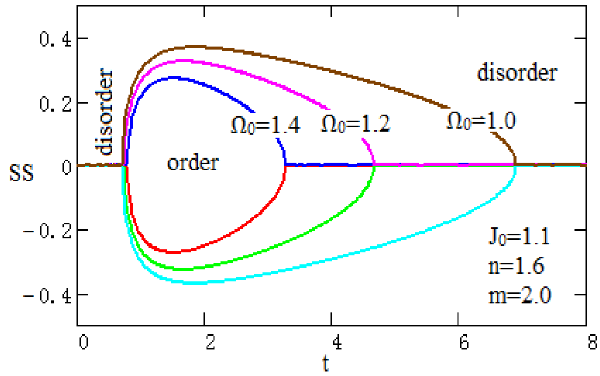

Figure 2: Phase transition diagram showing the polarization SS against temperature t for various effective transverse field parameter Ω0 for a system where J0=1.1, n=1.6, and m=2.0.

Fig. 3 shows the phase diagrams for systems with J_0=0.9, n=1.6 and m=1.0. These graphs have the U shaped profile that is commonly symptomatic with ferromagnetic to paramagnetic Curie temperature phase transitions. Thus at lower temperatures, the system is in the ordered state. As temperature increases, the system is stable in the disordered state. It can be observed that the smaller the value of Ω_0 the smaller the region of the ordered phase. Also the range of polarizations for transitions can occur is larger when Ω_0 is smaller. As Ω_0 gets bigger, the region for the disordered state gets smaller while ordered phase region gets larger.

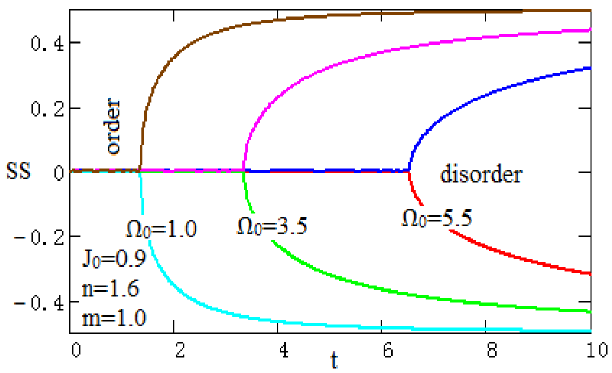

Figure 3: Phase transition diagram showing the polarization SS against temperature t for various effective transverse field parameter Ω_0 for a system where J_0=0.9, n=1.6, and m=1.0.

Fig. 4 shows the phase diagrams for systems with J_0=1.6, n=0.8 and m=2.0. These are commonly known as the reverse U-shapes. Here also we have the possibility two distinct phase transitions. At lower temperatures, the system is stable in the ordered phase. However as temperature is gradually increased, the range polarization of transitions to the disordered phase also progressively decreases. At high temperatures, the system is in the disordered state. As Ω_0 is progressively decreased, the region for the ordered phase increases while that for disordered phase decreases. Also as Ω_0 is decreased one can observe appearance of the shape of jet-plane nose protuberance fashioning out.

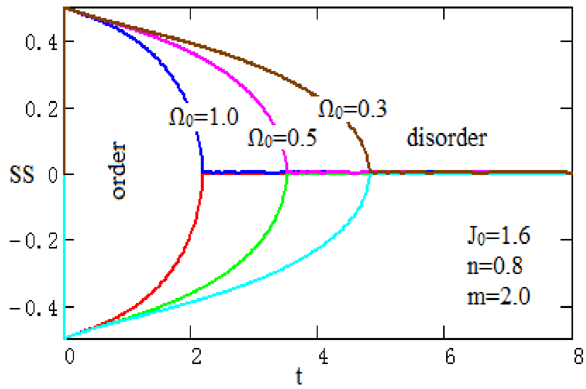

Figure 4: Phase transition diagram showing the polarization SS against temperature t for various effective transverse field parameter Ω_0 for a system where J_0=1.6, n=0.8, and m=2.0.

IV. CONCLUSION

This paper studies the coupling effect of the transverse field parameter Ω0 on the Hamiltonian of the Ising model. It develops a theory on simple temperature dependent relationship between the potential field parameters in the model and this is used to calculate phase diagrams in the polarization-temperature phase space. The topology of these diagrams then reveal a qualitative depiction of the influence of the transverse field coupling effect by simple parameter modification using the Mathcad software. First of all the graphs obtained were categorized according to the various shapes of phase diagrams that have been observed for systems both theoretically and experimentally.

Our calculation was able to model the more complex phase diagram of the reentrant egg-shaped closed loop phase behavior in the first category, other phase diagrams were obtained by parameter modifications as well. Such as f the first category systems. Other exotic shapes such as U shape and the reverse U-shape were obtained and analyzed.

Our results basically show that there is a direct influence of the transverse magnetic field on all systems that exhibit phase transitions. First of all, for all these systems, as the exchange interaction energy is decreased, there is a corresponding decrease in the transverse field coupling energy in order for system to showcase phase transitions between phases. Also the transverse field has a sharp influence on the egg-shaped protuberance commonly found in systems with reappearing phases as well as the jet-plane nose shape of some systems. It is observed that the region for order or disorder in systems dramatically changes when the transverse magnetic field coupling parameter is altered. As a result, the range of polarization and temperatures for which phase transitions occur is also affected with changes in the transverse field coupling parameter influence. Finally, as the transverse magnetic field influence is increased, the systems begin to lose the property of having any phase transitions and so only single phases (of either ordered or disordered) subsists.

Thus this study has succeeded in explaining some trends observable on phase diagrams. This is important because it gives another angle to the important influence of the transverse field parameter, which is an important component of the Hamiltonian of the Ising model. Thus any cursory consideration on any experimental or theoretical phase diagram, will reveal the benign influence of the transverse field coupling constant and so a qualitative description in these terms can be made.
We recommend that future work be carried on the combined effect of the temperature exponents m and n.

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