RESEARCH ARTICLE OPEN ACCESS

Effects oftheExchange Interaction Parameter onthePhase Diagrams fortheTransverse Ising Model

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ABSTRACT
The microscopic effect of the exchange interaction parameter for the 2-Dimensional ising model with nearest neighbor interaction has been studied. By supposing simple temperature dependent relationship for the exchange parameter, graphs were straightforwardly obtained that show the reentrant closed looped phase diagrams symptomatic of some colloids and complex fluids and some binary liquids mixtures in particular. By parameter modifications, other phase diagrams were also obtained. Amongst which are the u-shapes and other exotic shapes of phase diagrams. Our results show that the exchange interaction parameter greatly influence the size of the ordered phase. Hence the larger the value of the constant, the larger the size of the ordered phase. This means that the higher values of the exchange parameter brings about phase transitions that straddle a wider range of polarizations and temperatures.
Keywords-closed loop, exchange interaction, order-disorder, phase diagram, reentrant behavior, transverse Ising model (TIM).

I. Introduction

Phase diagrams can allow us to obtain a deeper understanding of some intriguing states of matter especially how various systems make transitions between the different states of matter. Hence while experimentally obtained phase diagrams have been helpful in the onset, they have not been tractable in disposition. The interest in phase diagrams lies in how the size and shapes of the closed loops varied with various parameters [1]. Thus with the aid of mathematical models, calculations of phase diagrams have enhanced the understanding of the underlying microscopic physical property changes that takes place within physic-chemical systems. Hence the shapes of various phase diagrams have been obtained by various models and simulations [2-27]. Teng et al [27] investigated the phase diagram for a ferroelectric thin film described by the TIM with four spin interaction. Campi et al [25] studied Ising model with temperature dependent interactions and reports that the model can generate various phase diagrams, and some having shapes as those of complex fluids.

Indeed the most intriguing aspect of phase transition phenomena is the reentrant behavior of some complex fluids and physico-chemical systems. Reentrant phase behavior offers a lot more insight into the microscopic behavior of atoms and molecules of matter. Recently the studies of reentrant behavior has gained the attention of some researchers. Redner et al [28] studied the reentrant phase behavior in active colloids with attraction. The reentrant liquid-liquid phase separation in protein solutions at elevated hydrostatic pressures was investigated by Moller et al [29]. The observation of a reentrant phase transition in incommensurate potassium was studied by Lundegaard et al [30]. While Kaneyoshi et al studied reentrant phenomena in a transverse Ising nanowire (or nanotube) with a diluted surface: Effects of interlayer coupling at the surface [31].

At this point it will be pertinent to explain the reentrants behaviors as exhibited by complex fluids especially in some binary liquids. This is because binary liquids were the medium in which were first discovered. Hence some binary mixtures of fluids show this characteristic reentrant property of reappearing phases. Thus a graph their temperature versus concentration phase diagram are closed-looped curves [32]. Earlier on the considerations of energy effects alone was not sufficient to explain the reasons why binary fluids become miscible at high temperatures. The answer to this was found in the concept of entropy. Hence a mixtures becomes miscible at high temperatures because the system tends not to minimize its energy but rather its free energy. For a system at a low temperature, entropy changes will not make much difference in its free energy. At high temperatures, on the other hand, changing the entropy by even a small amount has a large effect on the free energy, and so at high temperatures systems tend to maximize their entropy and in so doing becomes disordered.

However the question remained unanswered how the system becomes disordered again at low temperatures, since entropy influence decreases with decreasing temperature. As temperature is lowered, energy tends to dominate. Hence gradually the lowered energy becomes associated with the van der Waals attraction which has a larger effect on the free energy than the entropy does. The mixture then becomes immiscible since there are grouping of like molecules. Further lowering of the mixture's temperature brings about the immiscible phase. At sufficiently low temperature, then the low energy of hydrogen bonding tend to have a greater effect on the system's free energy. At below this point the mixture becomes miscible again. This mixture has the same macroscopic properties as the high-temperature miscible mixture [33].

Various models of this system have been studied. Using the mean-field approximation approach, Barker and Fock [34] obtained closed-looped phase diagrams with the model. However there was a difference between the observed coexistence phases and the concentration by comparison with experiment. Then, Wheeler [35] Andersen [36] presented the model called the decorated lattice-gas. This also produced closed-loop phase. In comparison with the treatment by the Ising model. It doesn't deal well with the interactions amongst the nearest neighbor molecules at each lattice as the Ising model does.

In this paper, we investigate the microscopic properties of TIM with temperature dependent potential parameters. Of particular focus is how the exchange interaction parameter affects the shapes of various phase diagrams that all commonly originate from the closed loop phase diagrams of binary fluids by parameter modification.

II. The Model

We consider the transverse Ising model with nearest neighbor interaction only, since it has proved to be efficient in the calculation of phase diagram of complex fluids [17-20, 37] with reentrant phase behavior. Its Hamiltonian is given as follows [17-20, 37]:

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

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 $\sum_{\langle i,j \rangle}$ runs over only distinct nearest-neighboring pairs. Ω is the transverse field and J is the exchange interaction constant between nearest neighbor spins.

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

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

where $\omega_0^2 = \Omega^2 + \sigma^2$ and $\sigma = \sum_i J \langle S_i^z \rangle$ .In fact, the ensemble average of the pseudo-spin $\langle S_i^z \rangle$ is understood as the order parameter of the system (subsequently, we use SS in place of $\langle S_i^z \rangle$ in labelling the graphs).Here the order parameter of the system is the ensemble average of the pseudo-spin $\langle S_i^z \rangle$, and describes the transition of the system from order ($\langle S_i^z \rangle \neq 0$) to disorder ($\langle S_i^z \rangle = 0$) state [37].

Experimental research in complex fluids has established that temperature changes in systems may have a direct correlation with the exchange interaction parameter [10-11], while for some crystal materials the exchange parameter shows positive relationship with temperature.

With the ising model concept of an effective exchange interaction and the correlative temperature dependence was used by Campi and Krivine [25] to obtain closed-loop shaped phase diagrams and described the reentrant phase behavior of complex fluids. Therefore Simons et al using transverse Ising model and supposing that the effective exchange and effective transverse field parameters J and Ω developed the simple temperature-dependent relations as follows [37]:

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

where T_0 are arbitrary constant. Here the effective parameters J_0, Ω_0 and $k_B T$ are reduced by $k_B T_0$, and simply are notated still as J_0, Ω_0 and *t*. By this therefore, we can calculate the phase diagram on the polarization-effective temperature space with effective temperature-dependent exchange interaction parameters.

III. The Phase diagrams

In this section we obtain the phase diagrams in polarization-temperature space. Graphs are plotted with the polarizations for various parameters of (J_0, n, Ω_0 and m) vrs the effective temperature t. By varying the effective exchange parameter J_0, we can observe the effect it has on the phase transition diagram.

In fig.1, we see the effect of changing the effective exchange parameter (J_0) while keeping all other parameters constant. The plots are closed looped curves that are symmetrical along the horizontal axis and shows typical phase diagrams for reentrant phase behavior. Thus at very low temperatures, the system is in disordered state, while at intermediate temperatures it is in the ordered state then at high temperatures it is again in the disordered state. When J_0 is high (J_0= 1.6), the closed looped curves are broader and covers a wider spectrum of concentration and temperature. This means the region for which the system is ordered is bigger. As J_0 decreases to 1.05, the closed loop profiles also progressively decrease, and as a result the ordered region diminishes while the disordered region becomes more dominant.

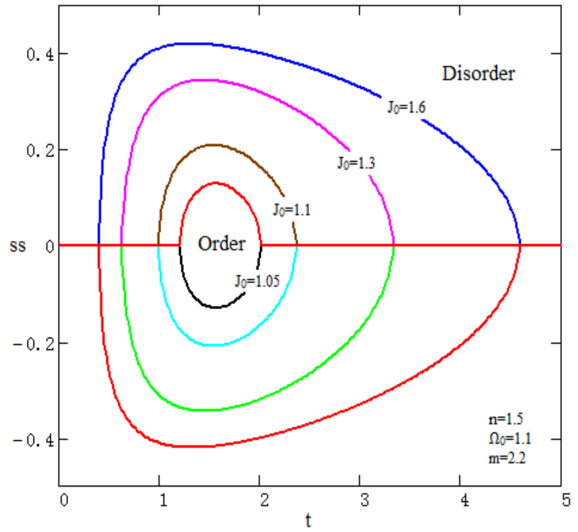

Fig.1. Phase transition diagram showing the polarization ss for various J_0 parameters given n=1.5., Ω_0=1.1 and m=2.2 vs temperature t.

Fig. 2 shows a system with mixed fortunes when it comes to the property of reentrant behavior. First of all for this system, when J_0 is large, the system has only two transition states, and is ordered at low temperatures and disordered at high temperatures. But when J_0 is small, then the reentrant phase property appears similar to fig. 1 above. Hence the system is disordered at high temperatures, ordered at intermediate temperatures and again becomes disordered at low temperatures. For these systems, the bigger the J_0 values, the bigger the ordered phase.

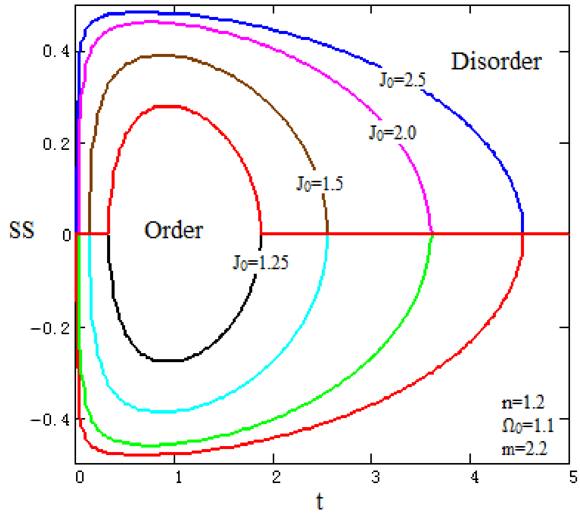

Fig. 2Phase transition diagram showing the polarization ss for various J_0parameters given n=1.2, Ω_0=1.1 and m=2.2 against temperature t.

Fig. 3 shows the category of phase diagrams which have the U-shape profiles. The phase profiles are concentric half circles and these systems exhibit the normal sequence of phase transitions with temperature. Hence at low temperatures the system is ordered and at high temperatures it is disordered. The smaller the value of J_0 becomes, the smaller the region of the ordered phase. This means that the range of polarization and temperature for the ordered phase gets smaller while that of the disordered phase gets larger. This phase diagram is synonymous with ferromagnetic-paramagnetic phase transition systems.

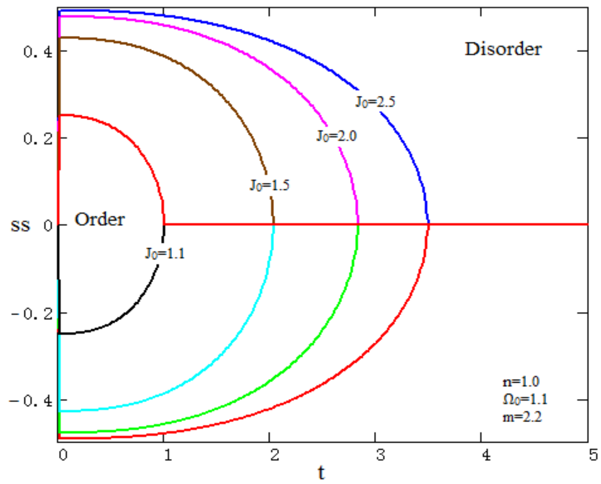

Fig. 3. Phase transition diagram showing the polarization ss for various J_0parameters given n=1.0, Ω_0=1.1 and m=2.2 against temperature t.

The fourth category of phase behavior can be found in fig. 4. Here at temperature t=0, all the various systems are equally polarized. The phase profiles are crescent-shaped half circles. This therefore means that they have two distinct phase states. At low temperatures, the system is at the ordered state and at high temperatures it is in the disordered state. As J_0 decreases from 2.5 to 1.1, the region for the ordered phase also decreases and as a result only the temperature range for the ordered phase decreases.

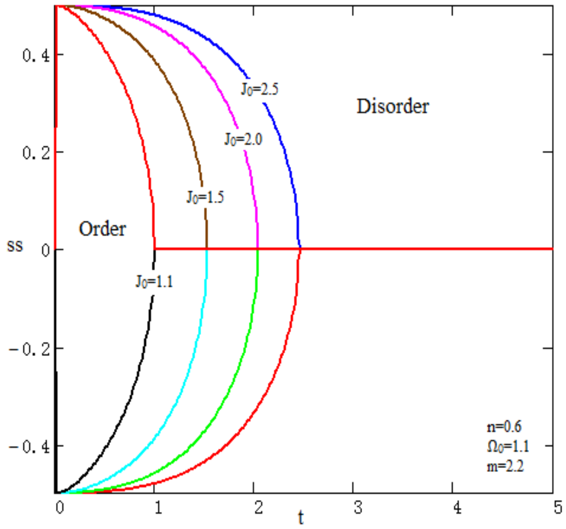

Figure 4. Phase transition diagram showing the polarization ss for various J_0parameters givenn=0.6, Ω_0=1.1 and m=2.2) against temperature t

IV. Conclusions

This paper studies the effect of the exchange interaction parameter J_0 on the mathematical framework of the ising model with temperature dependent relations. Graphical plots were obtained by theoretical formulations from the model 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.

By obtaining the more complex phase diagram of the reentrant closed loop phase behavior in the first category, other phase diagrams were obtained by parameter modifications of the first category systems. Other exotic shapes such as U shape and the D-shape and crescent-shaped were obtained and analyzed.

Our results basically show that systems become more disordered when the exchange interaction parameter is decreased. As a result, the ordered phase ranges of polarization and temperatures diminishes with a decrease in the exchange interaction parameter influence.

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