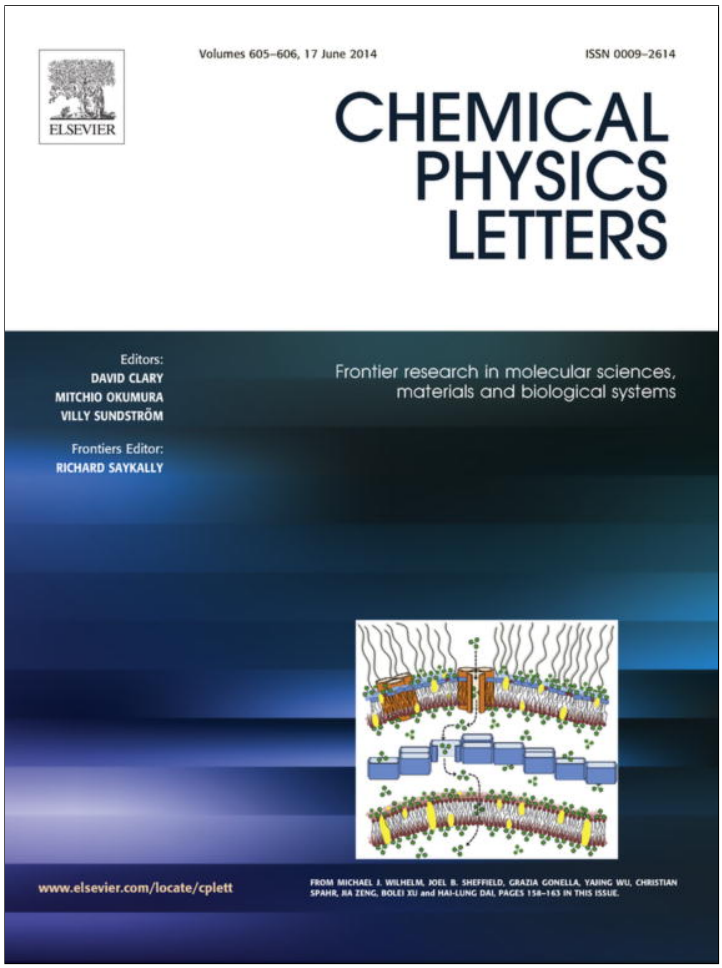

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The possible phase diagrams for the transverse Ising model with temperature-dependent parameters

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ABSTRACT

In this Letter the transition properties of the transverse Ising model with temperature-dependent parameters are investigated. By supposing the simple dependent relations of the interaction parameters on temperature, the phase diagrams are straightforwardly obtained, which may be used to describe the closed-loop behavior for the phase transition of the systems. In fact, the reentrant phase behavior of the system obtained by this Letter is to some extent coincident with the phenomena exhibited in some colloids and complex fluid mixtures as well as proteins.

1. Introduction

The study of complex fluids, like some colloids and fluid mixtures has been being an important topic in physics and chemistry, and the complexity and peculiarity of these systems have been widely investigated by the theoretical and experimental researchers [1–14]. Davies et al. studied the solubility property of nicotine-water system [6]. Walker et al. found that the phenomenon of reappearing phases is caused by the complex competition between entropy and energy in a solvent containing hydrogen bonds [7]. Moelbert et al. obtained the phase diagram for an aqueous solution of nonpolar solute particles by mean-field calculation [8]. These studies showed the complexity of the binary solutions, and indicated the strength of interaction parameters among the system may increase with temperature [9]. An increase of temperature will lead to the overcome of enthalpic contribution of the two different components [10]. Meanwhile some results generated the closed-loop phase diagrams of concentration against temperature. These shapes of phase diagrams implied that the systems may have more interesting and attractive phase behaviors. The earliest closed-loop phase diagram was obtained in the nicotine-water system [11]. Lang et al. studied the reentrant behavior of alkyl polyoxyethylene nonionic surfactants [12]. Nord et al. studied the critical phenomena in polyvinyl alcohol-acetate copolymer solutions [13]. Narayanan and Kumar reviewed some important developments regarding phenomenon of reentrant phase transitions in binary and multicomponent liquid mixtures [14]. Recently Dias studied the cold denaturation of proteins within the framework of numerical simulations of the Mercedes-Benz model for water [15], and the system also exhibits the reappearing phase behavior. In fact, the phenomenon of reentrant phase transition is intrinsically novel and is discovered in amazingly diverse systems such as binary gases, liquid crystals, microemulsions, gels, granular superconductors, proteins, organometallic compounds, crystals [14–17].

Theoretically, Ising or Ising-like model has a long and venerable tradition in the applications to order–disorder systems, such as ferromagnetic or ferroelectric systems, binary alloys, lattice gases, complex fluid, and even proteins. In ferromagnetic or ferroelectric field, Ising model has a wide and solid application [18–22]. In proteins field, Poland and Scheraga, for example, discussed a comprehensive survey of these models to deal with the coil-to-helix transition in proteins [23]. Further Badasyan et al. studied the cooperativity and stability of a helix-coil transition using a similar Ising-like model [24]. Zamparo et al. show an example for the case of Ising-like model by studying the kinetics of the Wako–Saito–Munoz–Eaton model of protein folding [25]. In complex fluid field, Campi and Krivine applied usual Ising model with temperature-dependent effective interaction to complex fluids [26], and obtained some meaningful results which can mimic the shapes of the phase diagram of complex fluids. In this Letter we will study the reentrant phase behavior of the system by using the transverse Ising model (TIM). Considering the temperature dependences of two kinds of effective interaction parameters, we will produce

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possible phase diagrams with the reentrant phase behavior and density curves against temperature with closed-loop shape.

2. The model

The Hamiltonian of the transverse Ising model is [18–22].

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

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 and J are interaction parameters, and usually called the transverse field and exchange parameters, respectively.

Within the framework of the mean-field theory, the z component of the pseudospin can be written as [18–22],

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

where $\omega_0^2 = \Omega^2 + \sigma^2$ and $\sigma = \sum_i J\langle S_i^z\rangle$. The ensemble average of the pseudo-spin $\langle S_i^z\rangle$ is understood as the order parameter of the system. In fact, $\langle S_i^z\rangle$ is used to describe the transition of the system from order ($\langle S_i^z\rangle \neq 0$) to disorder ($\langle S_i^z\rangle = 0$) state. For complex fluid system, we use usually the average occupation number or density ρ of the site i of the lattice to describe the transition properties [26], where $\rho = \langle S_i^z\rangle + 1/2$. In the following we can calculate the density ρ and analyze the transition behaviors for the square lattice system.

3. The numerical calculations and phase diagrams

Experimental studies in complex fluids demonstrated that the interaction parameters in the system may increase with increasing temperature [9,10]. Even in some crystal materials the interaction parameters showed positive relations with temperature [16,17]. Theoretically, by introducing the effective exchange interaction with temperature dependence to the usual Ising model, Campi and Krivine generated the phase diagrams of closed-loop shape, and described the reentrant phase behavior of the phase diagram of complex fluids [26]. Commonly, a microscopic Ising model cannot have a temperature-dependent parameter. However, introducing the effective model (here the T-dependence) to a microscopic theory will help to understand the physics of complicated systems in a simple way [26]. In complex fluid, for example, the solvent effect may be to bring about a renormalized, temperature-dependent effective parameter [27]. In the transverse Ising model, therefore, we suppose the effective exchange and effective transverse field parameters J and Ω have simple temperature-dependent relations as follows:

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

where T_0 are arbitrary constant. In the following the effective parameters J_0, Ω_0 and k_BT are reduced by k_BT_0, and notated still as J_0, Ω_0 and t for simplicity. In this way, we can calculate the density and phase diagrams for the transverse Ising model with effective temperature-dependent parameters. The interest of these calculations lies in three aspects. First, it is convenient to obtain the temperature dependence of the density with the closed-loop shape under the framework of the mean-field approximation. Secondly, the four kinds of the possible phase transition diagrams describing the reentrant phase behavior of the system can be obtained in the same framework without introducing supplementary assumptions. Finally, not only the exchange but also transverse field parameters are considered as effective temperature-dependence parameters, therefore the phase transition properties have obvious differences with the previous work to a large extent.

Figure 1a shows the phase diagram of the effective exchange parameter J_0 against temperature t for different n. For n not larger than 1.0 (red and blue curves), when J_0 is very small, the system is at disordered state for any given temperature, but when J_0 is large, the system is ordered at lower temperatures and disordered at higher temperatures. This situation corresponds just to the usaul phase diagram of the TIM with effective temperature-independent parameters. For the case of n larger than 1.0 (green curve), at higher temperatures the system is at disordered state for smaller values of J_0 and can be at ordered state for larger J_0 values. At lower temperatures, however, the system may be at disordered state for a large range of J_0 values. This is anomalous compared with the above property for the usual TIM with effective temperature-independent parameters because the usual system eventually ends at ordered state when J_0 is large enough. This anomaly could be attributed to the fact that at lower temperatures, the effective exchange parameter J increases with temperature so slowly that the contribution of effective exchange interaction to the ordered state is diminished to a large extent.

Meanwhile, the phase diagram shows a crossover point of temperature $t = 1$. As the parameter n increases the disordered region of the system increases at below this temperature and decreases at above this temperature.

In fact, the anomalous phase diagram corresponds to a closed-loop density curve against temperature, as shown in Figure 1b. The system is disordered at lower temperatures and becomes ordered at intermediate temperatures and again assumes disordered state at higher temperatures. As the effective exchange parameter J_0 decreases, the closed-loop region for the ordered state decreases. For the usual phase diagram, the corresponding density curves are shown in Figure 1c and d. The system is ordered at lower temperatures and disordered at higher temperatures. Maximum density of 1.0 or minimum one of 0.0 is obtainable when values of n are less than 1.0. Generally, as n decreases from Figure 1b–d (with constant J_0), on the one hand, the temperature region for the ordered state also decreases. On the other hand, the temperature region for the ordered state transforms from higher temperatures to lower temperatures, and their shape profiles change from closed-loop shape to inverted-U shape.

Figure 2a shows the phase diagram of n against temperature t for different J_0. When J_0 is small (red curve), for small values of n, the system is at ordered state at lower temperatures and at disordered state at higher temperatures. For intermediate values of n, the system is always at disordered state for any given temperature. For larger values of n, the system is at disordered state at lower temperatures and ordered state at higher temperatures.

When J_0 is large (blue curve), for small and larger values of n, the system is consistent with the situation when J_0 is small (red curve) respectively. For intermediate values of n, however, the system is at disordered state at lower temperatures, ordered state at intermediate temperatures and disordered state at higher temperatures.

The corresponding density curves are shown in Figure 2b and c. For small values of n, the system is ordered at lower temperatures and disordered at higher temperatures and maximum density of 1.0 or minimum one of 0.0 is obtainable. For a large range of n greater than 1, the system is at a disordered state at lower temperatures for certain J_0. This shows the same anamoly for the system as illustrated in Figure 1a. For intermediate values of n, the system is disordered at lower temperatures and becomes ordered at intermediate temperatures and again assumes disordered state at higher temperatures. Therefore, a closed-loop density curve was obtained. For a large value of n, the system is disordered at lower temperatures and becomes ordered at higher temperatures. Thus the figure changes from closed-loop shape to U shape.

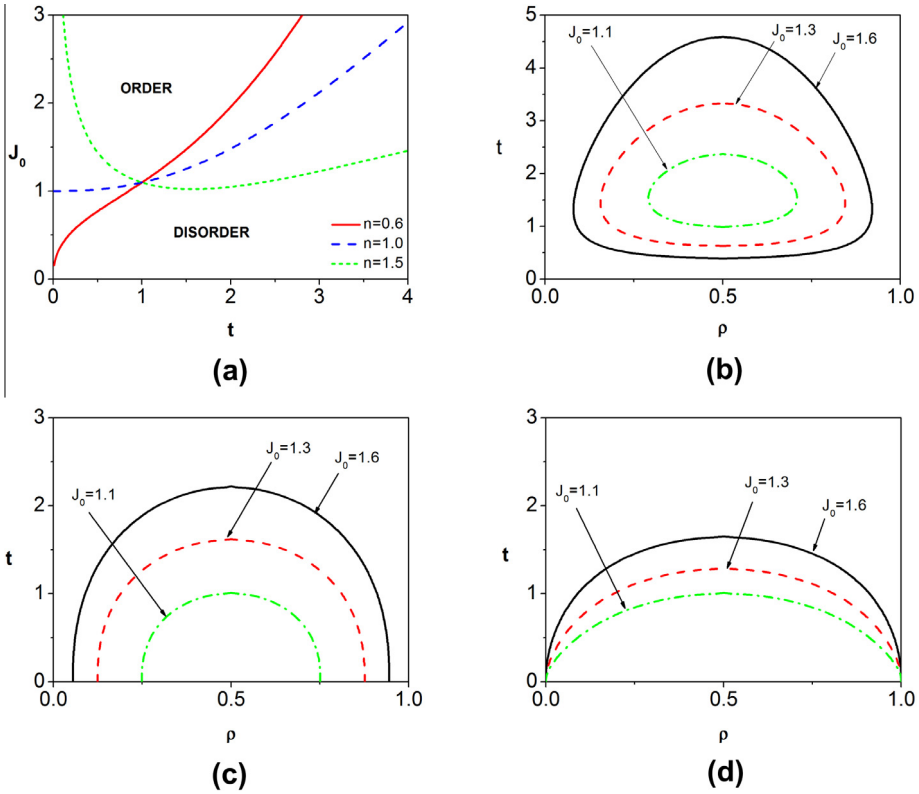

Figure 1. (a) The phase diagram of the exchange parameter J_0 against temperature t for different exponents n ($\Omega_0 = 1.1, m = 2.2$). (b–d) The density curves for different exchange parameter J_0 in relation to the above phase diagram (for $n = 1.5$, 1.0 and 0.6, respectively).

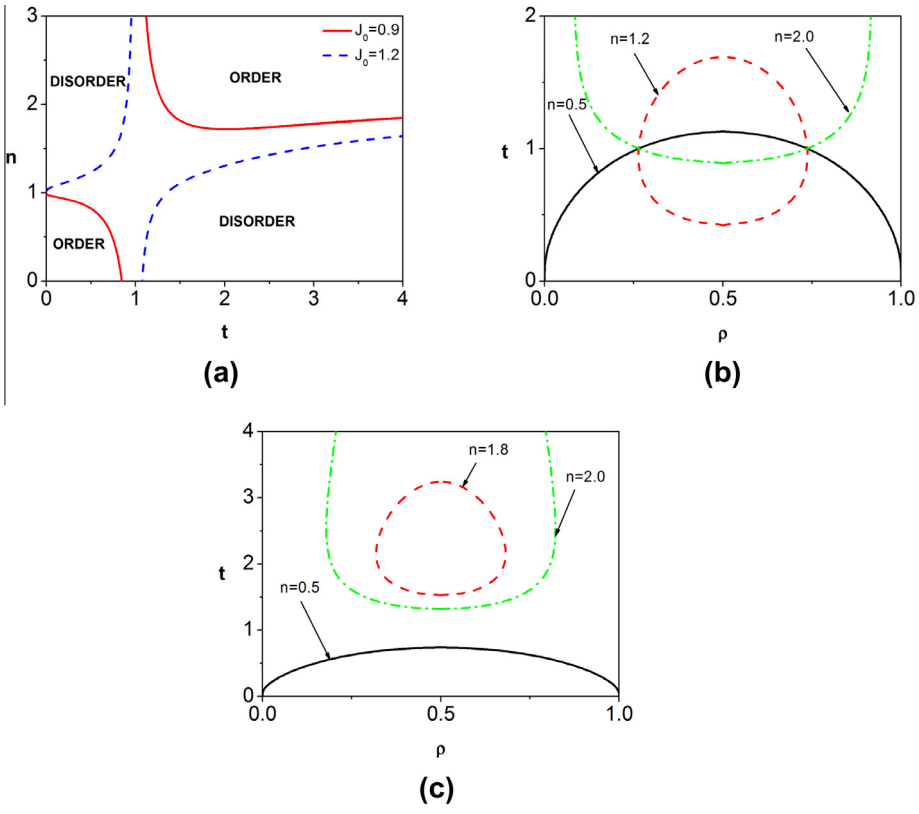

Figure 2. (a) The phase diagram of the exponent n against temperature t for different exchange parameter J_0 ($\Omega_0 = 1.1$, $m = 2.2$). (b–c) The density curves for different n in relation to the above phase diagram (for $J_0 = 1.2$ and 0.9, respectively). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

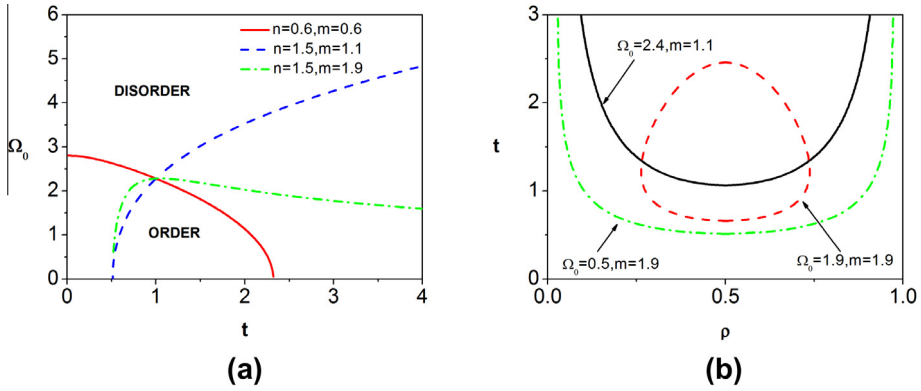

Figure 3. (a) The phase diagram of the transverse field parameter Ω_0 against temperature t for different exponent m (for $J_0 = 1.4$), and (b) The density curves in relation to the above phase diagram (for $J_0 = 1.4$ and $n = 1.5$).

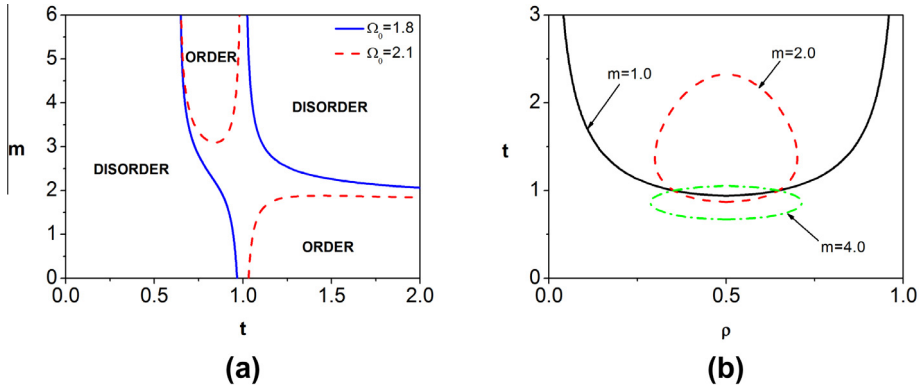

Figure 4. (a) The phase diagram of the exponent m against temperature t for different transverse field parameter Ω_0 (for $J_0 = 1.3$, $n = 1.6$), and (b) The density curves in relation to the above phase diagram (for $\Omega_0 = 1.8$).

Figure 3a shows the phase diagram for Ω_0 against temperature t for various m. For the smaller n and m (red curve), the usual phase behavior is exhibited. This is the same as the phase diagram of the transverse Ising model with temperature-independent parameter, i.e., the system is ordered at lower temperatures and disordered at higher temperatures [22]. But when m is intemediate (blue curve), for small values of Ω_0 the system is at disordered state at lower temperatures and ordered state at higher temperatures. For larger values of Ω_0, the system is always at disordered state for any given temperature. When m is larger (green curve), for small and large values of Ω_0, the system is consistent with the situation when m is intemediate (blue curve) respectively. For intemediate values of Ω_0, however, the system is at disordered state at lower temperatures, ordered state at intermediate temperatures and disordered state at higher temperatures. Hence the disordered region becomes dorminant with the increase of Ω and a reentrant phase behavior can be described.

The corresponding density curves are shown in Figure 3b. For certain Ω_0, when m is large, the system is disordered at lower temperatures and becomes ordered at intermediate temperatures and again assumes disordered state at higher temperatures. Therefore, a closed-loop density curve was obtained. Further calculation indicates that with increasing Ω_0 the closed-loop region for the ordered state decreases. As m decreases, the closed-loop shape is lost.

Figure 4a is the phase diagram of m against temperature t for various Ω_0. When Ω_0 is small (blue curve), for small values of m, the system is at disordered state at lower temperatures and ordered state at higher temperatures. For larger values of m, the system is at disordered state at lower temperatures, ordered state at intermediate temperatures and disordered state at higher temperatures. It represents the reentrant phase behavior of the system.

When Ω_0 is large (red curve), for small and large values of m, the system is consistent with the situation when Ω_0 is small (blue curve) respectively. For intermediate values of m, however, the system is always at disordered state for any given temperature.

The corresponding density curves are shown in Figure 4b. A closed-loop density curve was obtained when m is large. With increasing m, the reentrant phase region decreases and shifts to the lower temperature obviously.

4. Conclusions

In this Letter the transition properties of the transverse Ising model with temperature-dependent parameters are studied. With the help of supposed exponent dependent relations of the effective interaction parameters on temperature, the possible phase diagrams have been obtained by using the mean-field approximation. Among these phase diagrams, there exist the normal and anomalous phase diagrams. The anomaly in the phase diagram is completely determined by the closed-loop shapes of the density curves.

The numerical calculations indicate that the phase diagrams depend sensitively and dramatically on the exponents n and m, and the strength of effective interaction parameters J and Ω. With changing the effective exchange and effective transverse field parameters, the system is translatable between disordered and ordered states which exhibit the reentrant phase behavior. Although these results are qualitative and have not been compared

with experiments for specific materials, they show a tendency that may be useful in future theoretical and experimental investigations of the complex fluid systems.

Appendix

Considering that $\langle S_i^z \rangle$ will be very small while the temperature is near the transition temperature, we have the following equation with respect to the transition temperature and interaction parameters:

$$1 = (zJ/2\Omega)\tanh(\Omega/2k_BT) \tag{A-1}$$

where z is the coordination number of a site in the lattice system, and for the square lattice z is 4. Substituting Eq. (3) into Eq. (A-1), we have obtained a transcendental equation as follows:

$$1 = [zJ_0(T/T_0)^{n-m}/2\Omega_0]\tanh[\Omega_0(T/T_0)^m/2k_BT] \tag{A-2}$$

Obviously, the phase diagrams showing the relations between the transition temperature and interaction parameters can be determined from Eq. (A-2). In fact, Eq. (A-2) can be calculated numerically by Monte Carlo simulation or common software such as Mathcad. Here we take the phase diagram of Ω_0 against temperature t for example to show Monte Carlo calculation, where $J_0 = 1.4$, $n = 1.5$ and $m = 1.1$. It can be found that when the size of random number reaches 10^6 the results of Monte Carlo simulation are in complete agreement with ones of Mathcad. The calculating program of Monte Carlo simulation is as follows:

```
n = 1.5; m = 1.1;
N = 1000000;
f = inline('Ω-2.8*t^0.4*tanh(0.5*Ω*t^0.1)');
rand('state', sum(100*clock));
Ωt = rand(N,2);
Ωt (:,1) = Ωt (:,1)*4;
Ωt (:,2) = Ωt (:,2)*6;
for k = 1:N
  fΩt (k) = f(Ωt (k,1), Ωt (k,2));
end
fabs = abs(fΩt);
id0 = find(fabs<1e-4);
plot(Ωt (id0,1), Ωt (id0,2),'*')
axis([0406])
```

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