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Magnetic Properties and Phase Transitions in a Spin-1 Random Transverse Ising Model on Simple Cubic Lattice

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Abstract:
Within the effective-field theory with correlations (EFT), a transverse random field spin-1 Ising model on the simple cubic (z=6) lattice is studied. The phase diagrams, the behavior of critical points, transverse magnetization, internal energy, magnetic specific heat are obtained numerically and discussed for different values of p the concentration of the random transverse field.
Keywords: *Transverse Ising model, Effective-field theory, Phase transition, Magnetic properties.*

1. INTRODUCTION

Recently, a considerable attention has been paid to the investigation of the transverse Ising model (TIM). The main reason of such a great interest can be attributed to the fact that the TIM is very valuable model because of its different possible application. In fact, the TIM enables a simple explanation of the quantum properties of the hydrogen-bonded ferroelectrics, cooperative Jahn-Teller systems, as well as strongly anisotropic magnetic materials in the transverse field [see Ref.1 and references therein]. The TIM has been studied by high temperature expansions, Monte-Carlo methods, a method of combining the pair approximation with the discretized path integral representation, cluster approximation, renormalization group method, the effective-field theory (EFT) and EFT with correlations [2-12]. It has been found that the TIM has a finite temperature phase transition which can be suppressed to zero temperature where criticality still occurs for a certain value of the transverse field. Therefore, the TIM serves as a model of quantum critical phenomena at zero temperature, In addition to works on the two state spin systems, the spin-1 transverse Ising model and higher spin cases have also received attention [13,14].

Another problem of growing interest is associated with the random transverse field Ising model (RTFIM). One of the interesting phenomena in the RTFIM is the occurrence of a tricritical behavior. The RTFIM has examined by the use of various techniques, such as mean field theory, Monte-Carlo simulations, renormalization group calculations, Bethe-Peirls approximation and effective-field theories (EFT) [15-22]. It is worth noting that the analysis of the RTFIM have been almost restricted to the simple spin-$\frac{1}{2}$ system. Only very recently, some interest has been directed to understand the more complicated systems in the presence of random fields (i.e. the transverse Ising model, the amorphous Ising ferromagnet, the Blume-Capel model and spin-S Ising model). It has been shown that a very rich critical behavior can be found in these systems and many interesting phenomena can appear (i.e. the re-entrance behavior or the existence of two tricritical points).

The purpose of this paper is to investigate the effect of a transverse random field, distributed according a trimodal distribution (2), on the phase diagram and magnetic properties of a simple cubic (z=6) lattice ferromagnetic Ising system consisting of magnetic atoms with spin-1.

This study is done using the effective-field theory (EFT) with correlations method. The equations are derived using a probability distribution method based on the use of exact Van der Waerden identities. As far as we know, such a study has not been yet carried out. Section 2, described the EFT with correlations and the formulation of EFT is applied to a three-dimensional lattice (simple cubic with z=6) consisting of spin-1 atoms. In section 3, we present our numerical results and discussions, such as the phase diagrams, the thermal variations of the transverse magnetization, the internal energy, the magnetic specific heat as a function of different values of p, the concentration of the random transverse field.

2. THEORY AND FORMULATION

The random transverse field Ising model is described by the following Hamiltonian:

$$H = -J_B \sum_{\langle ij \rangle} S_i^z S_j^z - \sum_i (\Omega_B)_i S_i^x \tag{1}$$

where S_i^z, S_i^x are components of a spin-1 operator at site i, J_B is the exchange interaction at the bulk. The first and second summations are over nearest-neighbor sites and single sites located on the free space, respectively. The transverse field $(\Omega_B)_i$ is assumed to have the trimodal probability distribution:

$$P((\Omega_B)_i) = p\delta((\Omega_B)_i) + \frac{(1-p)}{2}\left[\delta((\Omega_B)_i - \Omega_B) + \delta((\Omega_B)_i + \Omega_B)\right] \tag{2}$$

where p denoted the fraction of spins not exposed to the transverse field .

The starting point of the statistics of our spin system is the relation proposed by Sa'-Barreto et al [7], which is generally given by:

$$\left\langle f_i \hat{O}_i \right\rangle = \left\langle f_i \frac{Tr_i \hat{O}_i e^{-\beta H_i}}{Tr_i e^{-\beta H_i}} \right\rangle \tag{3}$$

where $\beta = \frac{1}{k_B T}$, $\hat{O}_i$ is a spin operator function at the site i, Tr_i means the partial trace with respect to the lattice site i, f_i here represents an arbitrary function of spin variables except S_i^z and S_i^x at a site i and $\langle ... \rangle$ indicates the canonical thermal average. H_i includes all parts of H associated with the lattice site i and is given by:

$$H_i = -A_i S_i^z - (\Omega_B)_i S_i^x \tag{4}$$

with $$A_i = \sum_j J_B S_j^z \tag{5}$$

By the use of (3), the longitudinal and transverse site magnetizations for the spin-1 random transverse Ising model are given by, (with $f_i = 1$),

$$\left\langle S_i^z \right\rangle = \left\langle \frac{A_i}{E_i} \frac{2\sinh(\beta E_i)}{1+2\cosh(\beta E_i)} \right\rangle \tag{6}$$

$$\left\langle S_i^x \right\rangle = \left\langle \frac{B}{E_i} \frac{2\sinh(\beta E_i)}{1+\cosh(\beta E_i)} \right\rangle \tag{7}$$

With $$B = (\Omega_B)_i \tag{8}$$

$$E_i = \sqrt{B^2 + A_i^2} \tag{9}$$

Introducing the differential operator technique [23], equations (6) and (7) can be rewritten as:

$$\left\langle S_i^z \right\rangle = \left\langle e^{A_i \nabla} \right\rangle F_B(x)\big|_{x=0}, \tag{10}$$

$$\left\langle S_i^x \right\rangle = \left\langle e^{A_i \nabla} \right\rangle G_B(x)\big|_{x=0}, \tag{11}$$

where $\nabla = \frac{\partial}{\partial x}$ is a differential operator (defined by $e^{a\nabla} F(x) = F(x+a)$). The functions $F_B(x), G_B(x)$ are defined by:

$$F_B(x) = \frac{x}{\sqrt{B^2+x^2}} \frac{2\sinh(\beta\sqrt{B^2+x^2})}{1+2\cosh(\beta\sqrt{B^2+x^2})} \tag{12}$$

$$G_B(x) = \frac{B}{\sqrt{B^2+x^2}} \frac{2\sinh(\beta\sqrt{B^2+x^2})}{1+2\cosh(\beta\sqrt{B^2+x^2})} \tag{13}$$

In order to evaluate the above equations, for spin-1, we use the decoupling approximation:

$$\left\langle S_i^z (S_j^z)^2 .. S_l^z \right\rangle \cong \left\langle S_i^z \right\rangle \left\langle (S_j^z)^2 \right\rangle ... \left\langle S_l^z \right\rangle \tag{14}$$

For $i \neq j \neq ... \neq l$, we use the generalized but approximated Van der Waerden identity [24]:

$$\exp(aS_i^z) = \cosh(\eta a) + \frac{S_i^z}{\eta} \sinh(\eta a) \tag{15}$$

With $\qquad \eta^2 = \left\langle (S_i^z)^2 \right\rangle, \qquad (16)$

then (10) and (11) are rewritten as:

$$\left\langle S_i^z \right\rangle = \prod_{j=1}^{z} \left[\cosh(\eta J_B \nabla) + \frac{\left\langle S_j^z \right\rangle}{\eta} \sinh(\eta J_B \nabla) \right] F_B(x)\Big|_{x=0} \tag{17}$$

$$\left\langle S_i^x \right\rangle = \prod_{j=1}^{z} \left[\cosh(\eta J_B \nabla) + \frac{\left\langle S_j^z \right\rangle}{\eta} \sinh(\eta J_B \nabla) \right] G_B(x)\Big|_{x=0} \tag{18}$$

where z is the coordination number, and for the simple cubic lattice z=6 .

Because of randomness of transverse fields, we should perform the random average of $(\Omega_B)_i$ with using the probability distribution function $P((\Omega_B)_i)$. We can define $\mu^z = \left\langle \left\langle S_i^z \right\rangle \right\rangle_r$ and $\mu^x = \left\langle \left\langle S_i^x \right\rangle \right\rangle_r$ and $\overline{\eta}^2 = \left\langle \left\langle (S_i^z)^2 \right\rangle \right\rangle_r$, where $\langle ... \rangle_r$ denotes the transverse field average.

Thus, doing the random average, (17) and (18) can be transformed into the forms:

$$\mu^z = \left[\cosh(\overline{\eta} J_B \nabla) + \frac{\mu^z}{\overline{\eta}} \sinh(\overline{\eta} J_B \nabla) \right]^z \overline{F_B}(x)\Big|_{x=0} \tag{19}$$

$$\mu^x = \left[\cosh(\overline{\eta} J_B \nabla) + \frac{\mu^z}{\overline{\eta}} \sinh(\overline{\eta} J_B \nabla) \right]^z \overline{G_B}(x)\Big|_{x=0} \tag{20}$$

On the other hand, for a spin S higher than $S = \frac{1}{2}$, one has to evaluate the parameter $\overline{\eta}$ (for $S = \frac{1}{2}$ parameter $\overline{\eta}$ is given by $\overline{\eta} = \frac{1}{2}$). It can be derived in the same way as S_i^z and S_i^x by the use of (3):

$$\overline{\eta}^2 = \left\langle \left\langle e^{A_i \nabla} \right\rangle H_B(x)\Big|_{x=0} \right\rangle_r$$
$$= \left[\cosh(\overline{\eta} J_B \nabla) + \frac{\mu^z}{\overline{\eta}} \sinh(\overline{\eta} J_B \nabla) \right]^z \overline{H}_B(x)\Big|_{x=0}, \tag{21}$$

Here, the function $H_B(x)$ for spin-1 is defined by:

$$H_B(x) = \frac{B^2 + (x^2+y^2)\cosh(\beta y)}{y^2\left[1+2\cosh(\beta y)\right]} \tag{22}$$

Where $\quad y = \sqrt{B^2+x^2} \qquad (23)$

and the functions $\overline{F}_B(x)$ and $\overline{G}_B(x)$ and $\overline{H}_B(x)$ are obtained as follows:

$$\overline{F}_B(x) = \int P((\Omega_B)_i) F_B(x) d((\Omega_B)_i) \tag{24}$$

$$\overline{G}_B(x) = \int P((\Omega_B)_i) G_B(x) d((\Omega_B)_i) \tag{25}$$

$$\overline{H}_B(x) = \int P((\Omega_B)_i) H_B(x) d((\Omega_B)_i) \tag{26}$$

The random averaged internal energy $\overline{U}$ is given by:

$$\frac{\overline{U}}{N} = -\left\langle \left\langle A_i S_i^z \right\rangle \right\rangle_r - \left\langle (\Omega_S)_i \left\langle S_i^z \right\rangle \right\rangle_r \tag{27}$$

where N is the number of magnetic atoms. Here, by substituting $f_i = A_i$ into (3), the first term of this relation can be written as:

$$\left\langle \left\langle A_i S_i^z \right\rangle \right\rangle_r = \left(\frac{\partial}{\partial y} \left\langle \left\langle e^{yA_i} \right\rangle \right\rangle_r\right)\Big|_{y=\nabla} \overline{F_B}(x)\Big|_{x=0} \tag{28}$$

The expressions $\left\langle \left\langle A_i S_i^z \right\rangle \right\rangle_r$ and $\left\langle (\Omega_B)_i \left\langle S_i^z \right\rangle \right\rangle_r$ can be evaluated by the same way as that of μ^z and μ^x and $\overline{\eta}^2$. After this procedure, one obtains:

$$\left\langle \left\langle A_i S_i^z \right\rangle \right\rangle_r = zJ_B \overline{\eta} \left[\sinh(\overline{\eta} J_B \nabla) + \frac{\mu^z}{\overline{\eta}} \cosh(\overline{\eta} J_B \nabla) \right] \times$$
$$\left[\cosh(\overline{\eta} J_B \nabla) + \frac{\mu^z}{\overline{\eta}} \sinh(\overline{\eta} J_B \nabla) \right]^{z-1} \overline{F_B}(x)\Big|_{x=0} \tag{29}$$

$$\left\langle\left\langle(\Omega_B)_i S_i^z\right\rangle\right\rangle_r =$$

$$\left[\cosh(\bar{\eta}J_B\nabla)+\frac{\mu^z}{\bar{\eta}}\sinh(\bar{\eta}J_B\nabla)\right]^z \overline{(\Omega_B)_i G_B(x)}\Big|_{x=0} \qquad (30)$$

It is clear that for the evaluation of averaged internal energy $\bar{U}$, we must know μ^z , μ^x and $\bar{\eta}$. Then these quantities can be easily obtained by solving (19)-(21) numerically. Finally, the averaged magnetic specific heat can be determined from the relation:

$$\bar{C} = \frac{\partial \bar{U}}{\partial T}, \qquad (31)$$

3. SUMMARY AND DISCUSSION

In this section, the results for the spin-1 random transverse Ising model are shown. At first, in Figure 1, there are presented the phase diagrams in the $\Omega - T$ plane for various values of p in the case of the simple cubic (z=6) lattice. From this figure we can see that the effect of a random transverse Ising model. Namely, the critical temperature gradually decreases from its Ising value at $\Omega = 0$ and rapidly vanishes when the transverse field approaches some critical Ω_c depending on the value of p. It can be also seen that the value of Ω_c in spin-1 is greater than Ω_c in spin-$\frac{1}{2}$ system. When the transverse field is bimodally distributed (p=0), the critical temperature decrease gradually from its value of $T_c(\Omega = 0)$ ($\frac{T_c}{J_B} = 3.5287$), to vanish at some critical value of Ω_c ($\frac{\Omega_c}{J_B} = 5.2865$). As shown in the figures, when we consider a trimodal random transverse field distribution (i.e. $p \neq 0$), a finite critical transverse field Ω_c also exists for $p \cong 0$. The appearance of such a finite critical value Ω_c for , can be explained by the existence of a small cluster of zero transverse field sites, which, at the ground state, can not keep order in the system for any Ω . On the other limit, if only a small fraction of spins is exposed to Ω (i.e. $p \cong 1$), the cluster of zero transverse field sites includes nearly all sites of the lattice. From the above limit behaviors obtained for $p \cong 0$ and $p \cong 1$, one can reasonably expect that there appears a critical value p^* of the concentration of zero transverse field sites ($p^* = 0.4375$) showing two different behaviors of the system which depends on the range of p.

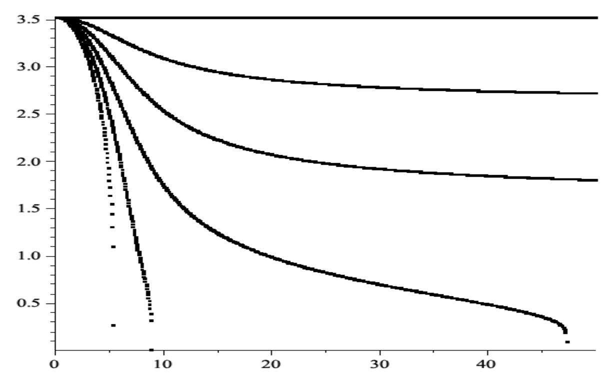

Figure 1: *The phase diagram (T/JB versus Ω) of spin-1 random transverse Ising model in the simple cubic lattice for various p (from left to right, p=0, 0.2, 0.4, 0.6, 0.8, 1).*

Indeed, for $0 \le p \le p^*$, the cluster of zero transverse field sites is small and hence the order, at T=0, is destroyed beyond a finite critical value Ω_c . But for $p^* \le p \le 1$, such a cluster is sufficiently large to keep order in the system at very low temperature, even in the limit of infinitely large values of the transverse field. Thus, we conclude that the existence of a finite critical value Ω_c at the ground state is related to the size of the cluster of zero transverse field sites.

In figures 2, 3, 6, 7, the temperature dependences of the transverse magnetizations as well as the parameter q ($q = \bar{\eta}^2$) for the simple cubic lattice are depicted, when the transverse field is fixed at some typical values. Finally, in figures 4, 5, 8, and 9, the temperature dependences of the internal energy ($\frac{-\bar{U}}{NJ_B}$) and the magnetic specific heat ($\frac{\bar{C}}{k_B N}$) are plotted for various p in the same system. We can see that, if the transverse field increases, then the absolute value of internal energy in the systems increases. On the other hand, the magnetic specific heat is gradually depressed by increasing the transverse field strength Ω. It can also be seen that the jump at the critical temperature gradually disappears with the increasing value of Ω.

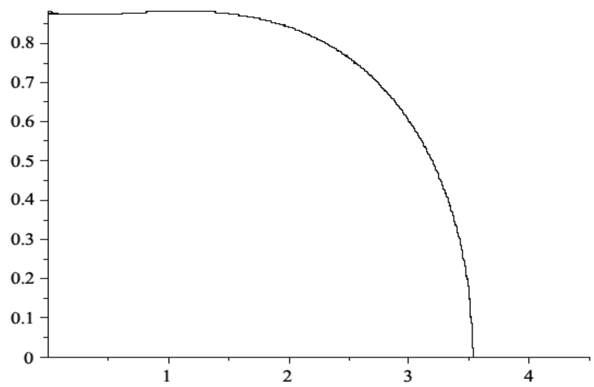

Figure 2: *The temperature dependencies of transverse magnetization* $M_z = \frac{\mu^z}{J_B}$ *for various p and* Ω *=0.1*

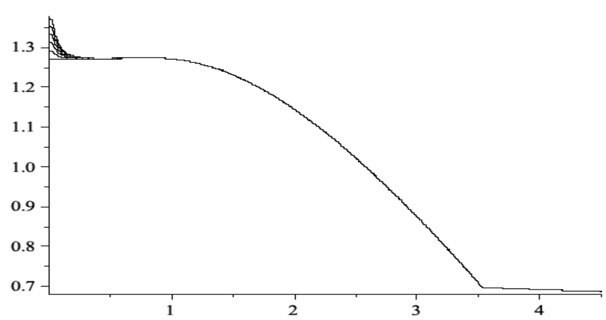

Figure 3: *The temperature dependencies of* $q = \overline{\eta}^2$ *for various p and* Ω *=0.1*

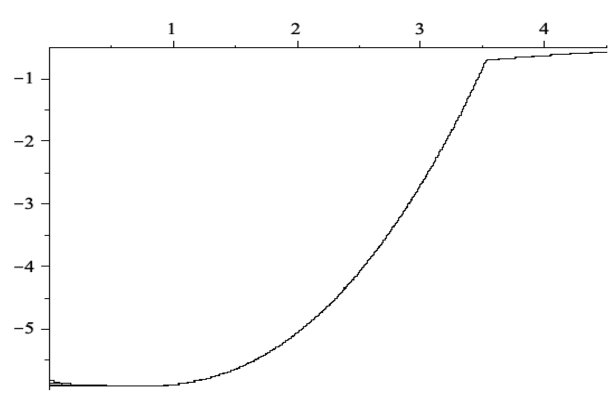

Figure 4: *The internal energy* $(\frac{-\overline{U}}{NJ_B})$ *versus temperature T/JB for various p and* Ω *=0.1*

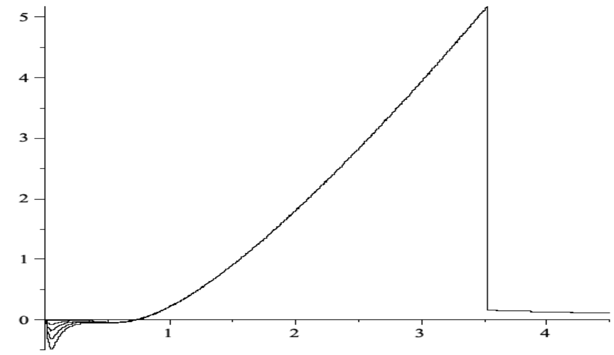

Figure 5: *The magnetic specific heat* $(\frac{\overline{C}}{k_B N})$ *versus T/JB for various p and* Ω *=0.1*

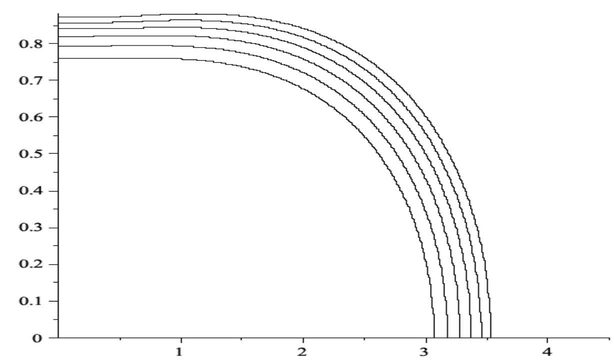

Figure 6: *The temperature dependencies of transverse magnetization* $M_z = \frac{\mu^z}{J_B}$ *for various p (from left to right, p=0, 0.2, 0.4, 0.6, 0.8, 1) and* Ω *=3*

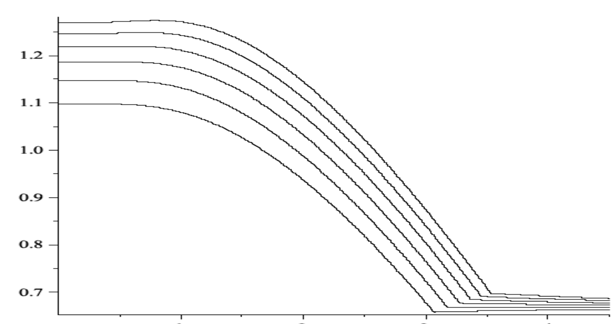

Figure 7: *The temperature dependencies of* $q = \overline{\eta}^2$ *for various p (from left to right, p=0, 0.2, 0.4, 0.6, 0.8, 1) and* Ω *=3*

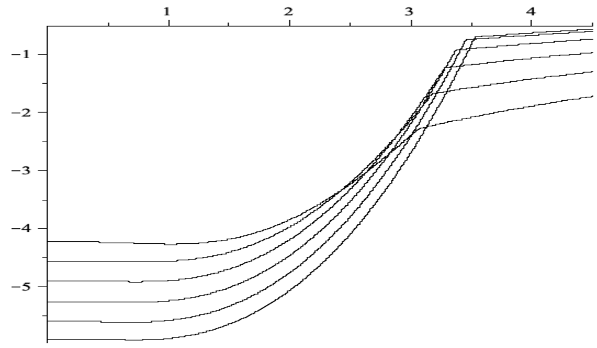

Figure 8: *The internal energy ($\frac{-\bar{U}}{NJ_B}$) versus temperature T/Js for various p (from left to right, p=0, 0.2, 0.4, 0.6, 0.8, 1) and* Ω *=3*

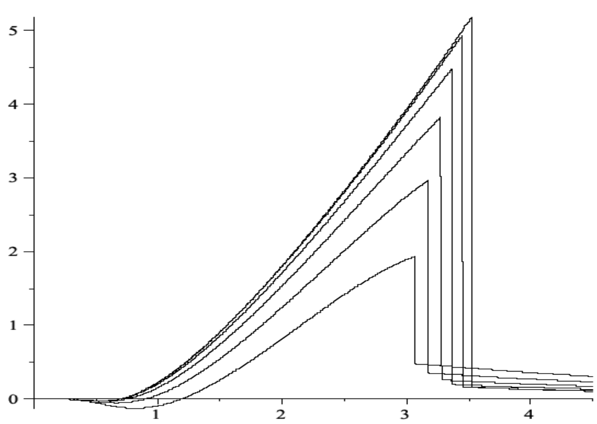

Figure 9: *The magnetic specific heat ($\frac{\bar{C}}{k_B N}$) versus T/Js for various p (from left to right, p=0, 0.2, 0.4, 0.6, 0.8, 1) and* Ω *=3*

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