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Irreversibility in Ising spin glasses in a transverse field

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Abstract. The phase diagram of the Ising spin glass model in a transverse field is studied by the local mean field method. Effects of the transverse field on specific heat, irreversibility and hysteresis are elucidated.

1. Introduction

Recently, there has been a growing interest in the theory of quantum spin glasses (SGs). Due to the non-commutativity of the spin operators one is usually bound, even within the mean field treatment, to introduce extra approximations compared to the corresponding classical problem. For instance, in the so called static approximation (see, for example, [1]–[4]) the time dependent self-interaction is assumed to be constant (corrections to this approach are discussed in [5]). Another example is that when applying the Trotter–Suzuki formalism [6] to the long-range quantum SG models [7–9] an infinite Trotter number is replaced by a finite one. Finally, the thermodynamic approach [10], used by Kopeć *et al* [11, 12] to avoid the use of replicas, requires introducing approximations that characterize all perturbative approaches. In this paper, we propose to study quantum SG systems by the local mean field approach [13, 14]. Unlike the other approaches, this method requires no additional approximations. Furthermore, it allows us to study phenomena of irreversibility and hysteresis. The latter cannot be considered with the use of the mean field method. Finally, even though this approach is very simple conceptually and operationally, it has proved itself successful in studies of classical Ising and Heisenberg random systems [13, 14]. We shall see that in the quantum case it captures the essential physics of the problem by allowing for the SG–paramagnet (PM) transition as a function of the transverse field.

In this paper, we focus on the Ising SG in the uniform transverse field. The Hamiltonian of this quantum system is given by [12]

$$\mathcal{H} = -\sum_{\langle ij\rangle} J_{ij}\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x - H\sum_i \sigma_i^z \tag{1}$$

where σ_i^x and σ_i^z are the Pauli matrices for a spin at site i. The sum in (1) is performed over nearest neighbours. The distribution of random couplings J_{ij} is taken to be Gaussian with zero mean and non-zero dispersion J. This model is believed to mimic the physics of proton glasses [15, 16] as observed, for example, in the mixed hydrogen bonded ferro- and antiferroelectric crystals such as $Rb_{1-x}(NH_4)_xH_2PO_4$ [17], and in mixed betaine phosphate–phosphite (or BP:BPI) [18]. The transverse field Γ is interpreted as the frequency of proton

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tunnelling [19] whereas the longitudinal field H corresponds to the external electric field. The quantum SG transition in a dilute dipolar coupled magnet $LiHo_{0.167}Y_{0.833}F_4$ [20, 21] also seems to be described by Hamiltonian (1).

The properties of the model without the longitudinal field have been investigated by many authors in the mean field approximation (see, for example, [22] and references therein). It has been found that there is a critical value Γ_c of Γ, below which the non-ergodic SG phase can exist at low temperatures [22, 23]. The mean field type phase diagram of model (1) in the (T, Γ, H) parameter space has been also obtained [12] using the thermodynamic approach.

The predictions of the local mean field approach discussed in section 2 can be summarized as follows. In section 3 we show that, in accord with previous results, there exists a critical value of Γ below which the SG phase is observed. Within the local mean field approximation the PM–SG transition is found to be of second order. In sections 4 and 5 we study the irreversibility and hysteresis in the longitudinal field. Both effects are found to be depressed by the transverse field. In section 6 we study the specific heat $C(T)$. The effect of the transverse field on $C(T)$ is rather different from that of the longitudinal field in a conventional SG [13, 14]. In the classical case the curves of the temperature dependence of $C(T)$ for different values of H intersect at some point. Such a behaviour is not seen in the quantum case with the transverse field, where the curves of $C(T)$ for different values of H intersect at more than one point. This may serve as an additional experimental signature of quantum effects.

2. Basic formulas

The free energy of the system is defined by

$$F = \langle H \rangle + k_B T \langle \log \rho \rangle \tag{2}$$

where the brackets denote the thermal average. In the local mean field approximation, the density matrix for model (1) is assumed to be given by

$$\rho_i = \prod_i \rho_i \qquad \rho_i = \frac{1}{Z_i} \exp[(H_i \sigma_i^z + \Gamma \sigma_i^x)/k_B T] \tag{3}$$

where

$$Z_i = \mathrm{Tr}\, \exp\{(H_i \sigma_i^z + \Gamma \sigma_i^x)/k_B T\} \tag{4}$$

and

$$H_i = \sum_j J_{ij} \langle \sigma_j^z \rangle + H. \tag{5}$$

In order to take the trace in equation (4) one has to find eigenvalues of the following operator:

$$\mathcal{H}_i = H_i \sigma_i^z + \Gamma \sigma_i^x. \tag{6}$$

These are given by

$$E_{i,\pm} = \pm\sqrt{H_i^2 + \Gamma^2}. \tag{7}$$

Thus the free energy of model (1) is as follows:

$$F = \sum_{\langle ij \rangle} J_{ij} \langle \sigma_i^z \rangle \langle \sigma_j^z \rangle - k_B T \sum_i \ln\{\exp(E_{i,+}/k_B T) + \exp(E_{i,-}/k_B T)\} \tag{8}$$

where $E_{i,\pm}$ are given by equation (7). The local magnetization $m_{zi} = \langle \sigma_i^z \rangle$ is derived from the minimum condition for the free energy: $\partial F / \partial m_{zi} = 0$. This leads to

$$m_{zi} = \frac{H_i}{\sqrt{H_i^2 + \Gamma^2}} \tanh\left(\sqrt{H_i^2 + \Gamma^2}/k_B T\right). \tag{9}$$

The local transverse magnetization m_{xi} may be obtained from the equation

$$m_{xi} = \partial F / \partial \Gamma = \frac{\Gamma}{\sqrt{H_i^2 + \Gamma^2}} \tanh\left(\sqrt{H_i^2 + \Gamma^2}/k_B T\right). \tag{10}$$

We consider systems of $L \times L \times L$ spins on a simple cubic lattice with L usually set equal to 10. At a given temperature we start from some tentative spin configuration, typically obtained by slow cooling, and solve equations (9) and (10) iteratively by proceeding from spin to spin sequentially. The local magnetic moments are obtained once the convergence is reached. The convergence is assumed to take place when

$$\sum_i [(m_{\alpha i})_n - (m_{\alpha i})_{n-1}]^2 \bigg/ \sum_i [(m_{\alpha i})_n]^2 \leqslant 10^{-6} \qquad \alpha = x, z \tag{11}$$

where n denotes the order of iteration. The SG order parameter q is defined by

$$q = \frac{1}{N} \sum_i m_{zi}^2 \tag{12}$$

where N is the number of sites considered (we can show below that no spin glass ordering occurs in the transverse direction). We average the results over 10 samples.

3. The T–Γ phase diagram

We start the iterations of equations (9) and (10) at high T by choosing $\{m_i\}$ randomly. The temperature is then decreased from $8J/k_B$ in steps of ΔT and we determine the T dependence of the order parameter q defined by equation (12). The onset of q signifies occurrence of the PM–SG transition (for $\Gamma \neq 0$ the transverse magnetization is non-zero and the conventional SG phase does not exist in this direction). The results are found to be insensitive to the choice of ΔT if $\Delta T \leqslant 0.07J/k_B$, and we use $\Delta T = 0.05J/k_B$. In this section, we put the longitudinal field $H = 0$. Figure 1 shows the critical temperature T_c as a function of Γ for an $L = 10$ system. As Γ is increased the temperature T_c decreases. Above $\Gamma_c \simeq 5.0J$ the SG like phase disappears at $T = 0$. At $\Gamma = 0$ we have $T_c \simeq 5.0J/k_B$. Therefore $\Gamma_c/k_B T_c(\Gamma = 0) \simeq 1$, which is very close to $\Gamma_c/k_B T_c(\Gamma = 0) = 1$ obtained in the mean field theory by the thermodynamic approach [12]. It should be noted that within the mean field theory the value of $\Gamma_c/k_B T_c(\Gamma = 0)$ depends on the method used. For example, the perturbative approach [24] and the numerical

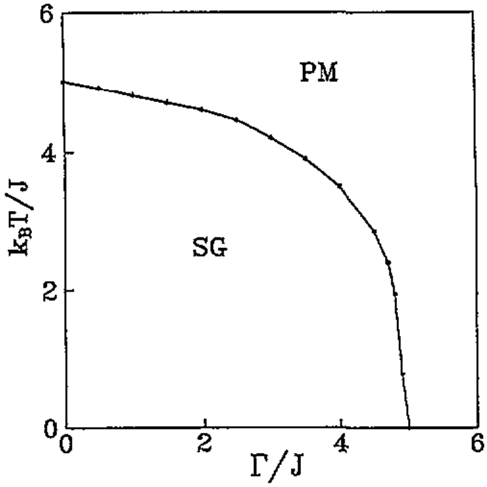

Figure 1. The T–Γ phase diagram of model (1) with $H = 0$. PM and SG denote the paramagnet and spin glass phases respectively. We have $T_c(\Gamma = 0) \simeq 5.0J/k_B$. The critical transverse field Γ_c above which the SG phase disappears at any T is given by $\Gamma_c \simeq 5.0J$.

Trotter–Suzuki method [7] give $\Gamma_c/k_BT_c(\Gamma = 0) \simeq 1.5$ whereas the static approximation [7, 24] yields $\Gamma_c/k_BT_c(\Gamma = 0) \simeq 2.0$. The discretized path integral method [16] leads to $\Gamma_c/k_BT_c(\Gamma = 0) \simeq 1.33$. Note, however, that the mean field theories are meant for the infinite-dimensionality limit whereas our result is meant for $D = 3$.

In order to clarify the kind of quantum SG transition we calculate the free energy at the critical line for spin configurations derived from various starting states and find essentially no difference. This suggests that the transition is second order. This result could be at odds with recent experimental results of Wu *et al* [21], who observe no divergence of non-linear susceptibility, suggesting that the quantum SG transition might be of the first order. More studies are needed to elucidate this point.

It should be noted that the finite-size effect on the phase diagram has also been investigated. For $L > 10$, where L is the linear size of sample, the topology of the Γ–T phase diagram does not change significantly compared to the $L = 10$ case.

4. FC and ZFC magnetizations

In this section, we discuss the effect of the transverse field on the field cooled (FC) and zero field cooled (ZFC) magnetizations

$$M_\alpha = \frac{1}{N}\sum_i m_{\alpha i} \qquad \alpha = z, x. \tag{13}$$

During the cooling process in the longitudinal field Γ is always kept fixed. To simulate the ZFC and FC situations, we follow the procedure used in experiments. For example, in order to determine $M_{z,x}^{\mathrm{ZFC}}$ we set the longitudinal field to zero and then cool the system from a high temperature (of about $8J/k_B$) down to a very low temperature, which we chose to be $T = 0.05J/k_B$. Subsequently, we switch the longitudinal field on and equilibrate the system at this lowest T. We then fix the strength of H and increase T slowly to a required value and determine the corresponding magnetization. In the FC case we simply lower the temperature from the PM regime and the longitudinal field is held fixed. The temperature step ΔT is taken to be $0.05J/k_B$. Figure 2(*a*) shows the T dependence of M_z^{FC} and M_z^{ZFC} for several values of H and for $\Gamma = J$. The two magnetizations coincide only at high temperatures. As for the classical Ising SG [13] the longitudinal field reduces the irreversibility effect. The temperature T_{irr}, where the FC and ZFC magnetizations begin to differ, decreases with H. The effect of the transverse field may be seen in figure 2(*b*) where the T dependences of M^{FC} and M^{ZFC} for indicated values of Γ and $H = J$ are plotted. Clearly the irreversibility effects are also suppressed by the transverse field (the difference between FC and ZFC magnetizations is enhanced and T_{irr} increases with decreasing Γ). For values of Γ greater than the critical Γ_c the FC and ZFC longitudinal magnetizations would coincide. The finite-size effect on the irreversibility has been also studied for several values of $L > 10$. No qualitative departure from the results shown in figure 2 is observed. We can show that no irreversibility effect has been observed for the transverve magnetization: M_x^{FC} and M_x^{ZFC} always concide. Figure 3 shows the temperature dependence of M_x for selected values of Γ at $H = J$.

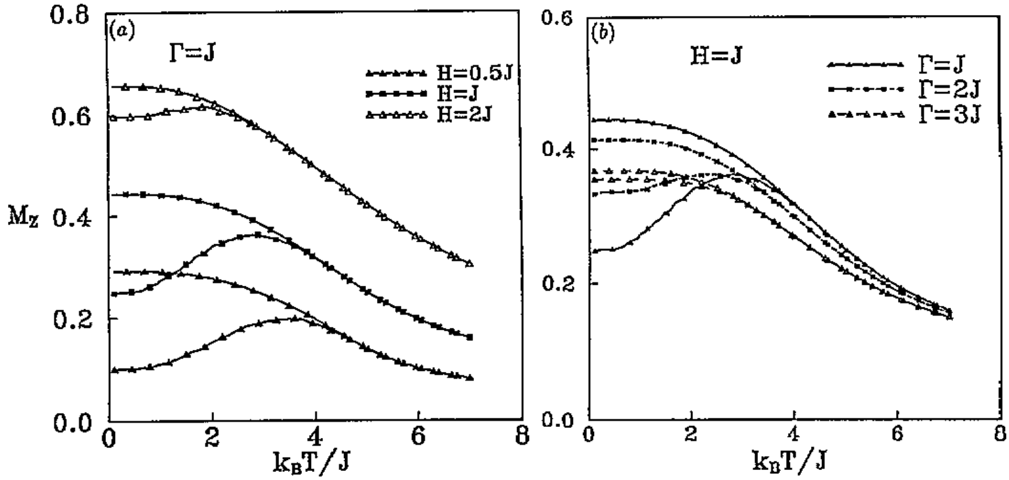

Figure 2. The temperature dependence of FC and ZFC longitudinal magnetizations (upper and lower branches respectively): (*a*) various H and $\Gamma = J$; (*b*) various Γ and $H = J$. The results, as in the remaining figures, are averaged over 10 samples for the $L = 10$ system.

It should be noted that the effect of the transverse field on the irreversibility is very similar to that of the single-ion easy plane anisotropy in the $S = 1$ classical Ising model [25]. This appears to be because the transverse field and the anisotropy both tend to make the system paramagnetic.

Fixing H, we have considered the FC and ZFC regimes in a transverse field (experimentally this is easy to realize for magnets [21] by varying the field applied to the transverse direction). No difference between FC and ZFC magnetizations is shown up.

5. Hysteresis effect

To study the hysteresis the temperature ($T < T_c$) and the transverse field are held fixed. We start from $H = 4J$ and decrease it to $-4J$ and then increase it up to the initial value.

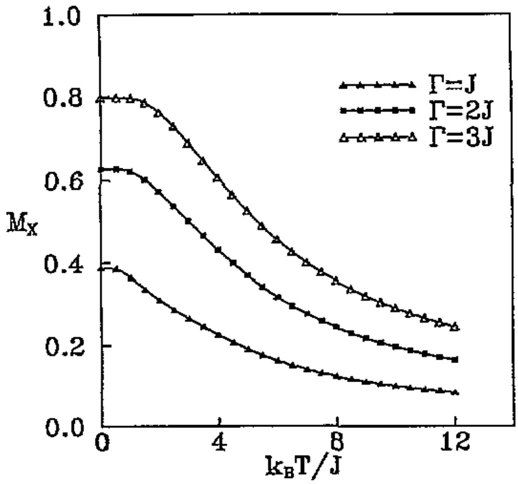

Figure 3. The temperature dependence of the transverse magnetization M_x for several values of Γ and $H = J$. M_x^{FC} and M_x^{ZFC} are the same.

As before, the system size $L = 10$. The field step ΔH is chosen to be $\Delta H = 0.01J$ (the results are found to be unaffected on varying ΔH between $0.005J$ and $0.05J$). The resultant longitudinal magnetization at $T = 0.5J/k_B$ is shown in figure 4 for selected values of Γ (there is no hysteresis effect in the transverse direction). The conventional SG case corresponding to Γ=0 has been considered by Soukoulis *et al* [13]. Varying the starting and ending longitudinal field H one can show that the results do not change significantly. At high fields H the magnetization assumes a unique value, so the resulting loop is independent of the way it was generated. Clearly, the transverse field depresses the hysteresis phenomenon: an increase in Γ makes the loop narrower. This conclusion remains valid for other system sizes. For $L = 10$ the hysteresis effect disappears at $\Gamma \simeq 4.5J < \Gamma_c$.

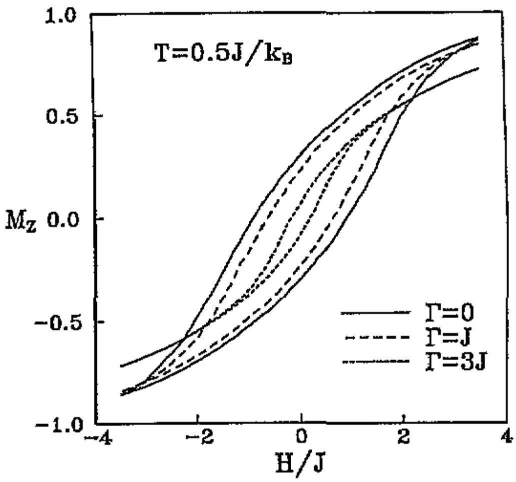

Figure 4. The hysteresis effect for various values of the transverse field Γ and for $T = 0.5J/k_B$.

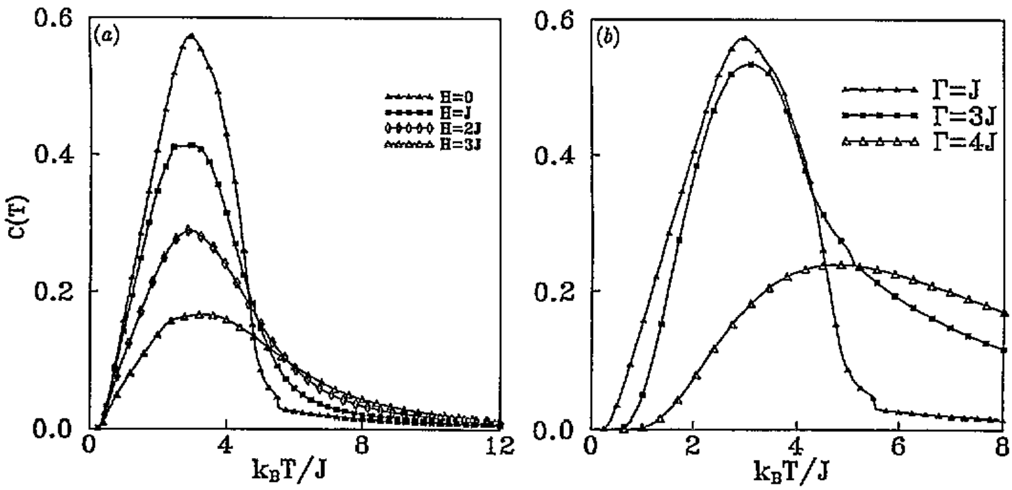

Figure 5. The specific heat of the Ising SG in longitudinal and transverse fields: (*a*) various H and $\Gamma = J$; (*b*) various Γ and $H = 0$.

6. Specific heat

The temperature dependence of the specific heat $C(T)$ has been studied for various values of H and Γ in the FC mode. In this configuration all the usual thermodynamic relations are satisfied and $C(T)$ is defined as a first derivative of the internal energy with respect to the temperature. Figure 5(*a*) shows that for a fixed value of Γ the dependence of $C(T)$ on H and on T differs from that for the standard SG case [13]. In the latter case $C(T)$ for different H intersect at some temperature somewhat above $T_{\max}$, at which $C(T)$ has a maximum. Obviously, in the quantum case these curves do not meet at one temperature. This may be a signature of the quantum effect. The maximum of the specific heat is found to be shifted towards higher temperature as Γ is increased. The influence of the transverse field is found to be similar to that of the longitudinal one (see figure 5(*b*)).

The simple approach of the local mean field allows us to study quantum effects in spin systems in a fruitful way and without any additional approximation. The local mean field method could also prove to be useful in studies of more complicated quantum systems such as the XY model in a transverse field [26], the proton glass model with a random field [27], etc.

Acknowledgments

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