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Reentrancy and Dynamic Specific Heat of Ising Spin Glasses

Mai Suan Li (1,2,*), Tran Quang Hung (1,**), and Marek Cieplak (1)

(1) Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland
(2) Faculty of Engineering and Design Kyoto Institute of Technology, Sakyō-ku, Kyoto 606, Japan

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Abstract. — The dynamic susceptibility and dynamic specific heat of Ising spin glasses with non-symmetric distributions of the exchange couplings are studied by the Monte Carlo method and are compared to the results obtained previously by the local mean field method. The two methods yield qualitatively different results but they still suggest lack of any reentrancy phenomena.

One of the interesting problems of the spin glass (SG) physics is a question of the reentrancy: is there a transition from the ferromagnetic phase to the SG phase on lowering the temperature, T. The reentrancy phenomenon has been observed experimentally in many materials [1] but a theoretical justification of the phenomenon is missing. The exact Parisi solution of the infinite range SG model [2] rules the reentrancy out. Similarly, all theoretical studies of the short range Ising or anisotropic Heisenberg SG’s give no evidence for the phenomenon [3]. We have speculated [4] that the origins of reentrancy might be of a dynamical nature, i.e. resulting from finiteness of observation times. We have attempted to study this by using the Glauber dynamics [5] for Ising SG’s within the local mean field approximation [6]. This approach has yielded a double peak structure, as a function of T, in the real part of the dynamic susceptibility. The positions of these peaks, however, are such that the reentrancy is not explained and, furthermore, they merged into one peak in the static limit.

In this paper, we ask whether the dynamical origins of the reentrancy would be revealed if a more accurate treatment of the system is employed. Specifically, we use the Monte Carlo method to determine the ac susceptibility, χ′(ω) (ω is the frequency), of short range Ising systems with asymmetric couplings and again find no reentrancy. There are, however, qualitative changes compared to the local mean field method — there is no double peak structure in χ′(ω) that has been found in the approximate treatment.

Another issue of this paper is what is the temperature dependence of the dynamic specific heat c(ω). The motivation for this is as follows. Within the local mean field approximation the maxima in the real and imaginary parts move towards higher temperatures on decreasing the frequency [4] whereas an exact treatment for six-spin clusters [7] yields opposite results. Our

(*) Author for correspondence (e-mail: mali@hier.kit.ac.jp)
(**) On leave from Hanoi Technical University

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Monte Carlo results for $c(\omega)$ qualitatively agree with those obtained for the six-spin clusters, i.e. similar to that found for the susceptibility. The dynamic specific heat has been measured in glasses [8,9] but not yet in SG’s. Its experimental features remain to be determined.

We consider the Hamiltonian

$$\mathcal{H} = - \sum_{<ij>} J_{ij} S_i S_j - H \sum_i S_i,$$  \hspace{1cm} (1)

where $S_i = \pm 1$ are the spins located on the cubic lattice of $N$ sites, $<ij>$ denotes summation over nearest neighbors, the couplings $J_{ij}$ are Gaussian distributed with the mean $J_0$ and the dispersion $J$. The magnetic field considered here is time dependent and

$$H = H_0 \sin \omega t.$$  \hspace{1cm} (2)

To study dynamic quantities we employ the Monte Carlo simulation with the standard Metropolis updating. We first focus on the ac susceptibility with the eye on a possible reentrant at finite frequencies. We follow the approach taken in reference [10]. In order to determine $\chi(\omega)$ one should switch on a small amplitude field given by equation (2) and then start monitoring the magnetization after some time $t_0$ which is chosen so that all transient exponentials can be considered extinct. We study $L \times L \times L$ systems with $L=10$ and it is sufficient to choose $t_0$ as 50000 Monte Carlo steps per spins (MCS/S). Once we pass the point $t = t_0$, we average $m(t)$ over typically 2000 - 4000 periods $T_0$ ($T_0 = 2\pi/\omega$) and extract the real and imaginary parts of the susceptibility through

$$M(t) = H_0 \left[ \chi' \sin(\omega t) - \chi'' \cos(\omega t) \right]$$  \hspace{1cm} (3)

The periods we have considered are 10, 20 and 100 MCS/S multiplied by 2$\pi$. The results of our calculations for the standard SG’s ($J_0 = 0$) are presented in Figure 1. We take $H_0$ to be equal to 0.01$J$: smaller values of $H_0$ leave the result almost unchanged. In all our calculations we choose the cubic system with the linear size $L = 10$. For large $\omega$’s the maximum of $\chi'(\omega)$ is rather broad. On decreasing $\omega$ the position, $T_\omega$, of the maximum moves towards lower temperatures and it sharpens up. In the dc limit the maximum acquires a cusp-like appearance and $T_\omega \rightarrow T_g$, where $T_g$ is the equilibrium transition temperature. The absorptive susceptibility $\chi''$, on the other hand, has a small but distinct anomaly around $T_\omega$. To obtain the dc susceptibility we follow Bhatt and Young [11] using 10$^5$ MCS/S for equilibration and another 10$^5$ MCS/S for averaging. The results are averaged over 10 samples. It should be noted that the corresponding maximum of the static susceptibility $\chi(\omega = 0)$ is located at $T \approx 1.2J$ (more accurate Monte Carlo calculations involving the finite size scaling give an estimate of $T_g \approx 1.1J$ [1]). The results presented in Figure 1 are very similar to those obtained for the standard SG Au$_{1-x}$Mn$_x$ with $x = 0.0298$ [12] and for Eu$_{0.2}$Sr$_{0.8}$S [13] and also to what happens in the local mean field approximation [4].

The question we ask now is whether reentrancy phenomenon can take place on short time scales when only some partial equilibration of the system can be achieved. To answer this question we study the equilibrium phase diagram first. The results of our calculations are presented in Figure 2. The paramagnet (PM) - SG and ferromagnet (FM) - SG boundary lines are obtained from the maxima of the static susceptibility $\chi(0)$ (see Fig. 3). The SG - FM transition boundary is obtained from the dependence of $\chi(0)$ on $J_0$ for various temperatures (see Fig. 4). Clearly, there is no reentrancy in the static regime. We now calculate the ac susceptibility for various values of the mean, $J_0$, of the couplings. Our Monte Carlo simulations indicate that (see Fig. 2) the ferromagnetically ordered phase exists at low $T$’s for $J_0 > 0.45J$. Figure 5 shows the $T$-dependence of $\chi'$ and $\chi''$ for $J_0 = 0.5J$ for 3 different frequencies. The
Fig. 1. — The static and dynamic susceptibility of the standard SG ($J_0 = 0$). The values of frequency are indicated. The system size $L = 10$ and the results are averaged over 10 samples. The open squares, black triangles, squares and circles correspond to $\omega \tau_0 = 0, 0.01, 0.05$ and 0.1 respectively. On decreasing $\omega$ the maxima of $\chi'(\omega)$ moves towards the equilibrium value of the critical temperature $T_g \approx 1.2J$.

Fig. 2. — The $T - J_0$ phase diagram. The solid lines correspond to the equilibrium case (the curves are obtained from maximum of the susceptibility). PM, FM and SG denote the paramagnet, spin glass and ferromagnetic phases respectively. Within indicated error bars the SG - FM transition boundary is a straight line. The black triangles, squares and hexagons correspond to $T_{\text{max}}$ of $\chi'(\omega)$ obtained for $\omega \tau_0 = 0.1, 0.05$ and 0.01 respectively (see Fig. 5 and 6 below).

Similar plots for $J_0 = 0.7J$ is shown in Figure 6. In all cases we observe only one peak in $\chi'(\omega)$ as a function of $T$ (the positions of these peaks for various $\omega$ and $J_0$ are plotted in Fig. 2) and the reentrancy phenomenon does not arise. It appears that the double peak structure in $\chi'(\omega)$ predicted by the local mean field method applied to the Glauber dynamics is either a fallacy of the approximate method or it is real but at the same time too weak to be detected by
Fig. 3. — The temperature dependence of the static susceptibility $\chi(0)$ for various values of $J_0$. The open squares, black triangles, squares and circles correspond to $J_0 = 0, 0.3J, 0.4J$ and $0.7J$ respectively. Depending on $J_0$ the maxima of these curves correspond to the PM - SG and PM - FM phase transition shown in the phase diagram in Figure 2.

Fig. 4. — The dependence of $\chi(0)$ on $J_0$ for various values of $T$. The open squares, black triangles, squares and circles correspond to $k_B T/J = 0.3, 0.5, 0.7$ and 0.9. The maxima correspond to the SG-FM transition shown in Figure 2.

the Monte Carlo averaging process. In any event, the origins of any reentrancy in SG systems remain obscure.

The specific-heat spectroscopy has been demonstrated to be a useful tool for studying relaxation processes in supercooled liquids [8,9]. In a typical experiment [8] one immerses a heater into the liquid and applies a sinusoidal current at frequency $\omega$. The power dissipated contains a dc component and an ac component at frequency $\omega$, ranging between 0.2 Hz and 6 kHz. The ac component results in phase-shifted temperature oscillations and defines the complex specific heat.
Fig. 5. — The dynamic susceptibility for different frequencies (black triangles, squares and circles denote $\omega_0 = 0.01, 0.05$ and $0.1$ respectively) and $J_0 = 0.5$. The results are averaged over 10 samples.

Fig. 6. — The same as in Figure 5 but for $J_0 = 0.7$.

Birge and Nagel [8] pointed out that in unfrustrated materials and standard liquids the real part of the specific heat $c'(\omega)$ does not practically depend on $\omega$ and the imaginary part is almost zero. In the case of SG’s, however, and presumably of other systems with many modes of configurational relaxation, the dynamic specific heat may be used as another probe of SG dynamics [7]. Indeed the dynamic specific heat couples to the time evolution of even-spin correlations whereas the dynamic susceptibility is given in terms of odd-spin correlations. By working with a six-spin cluster Cieplak and Szamel demonstrated [7] that the temperature and frequency dependence of the dynamic specific heat is similar to that of the dynamic
susceptibility except that the former is not affected by processes coupled to the very longest relaxation time in the system. When one fixes $\omega$ and plots $c'$ and $c''$ as a function of $T$ then one gets a curve with a maximum. On decreasing $\omega$ the position of the maximum moves towards lower temperatures and it sharpens up. The studies of clusters are illuminating but the clusters do not display any finite critical temperature. In [4] we studied the dynamic specific heat of the system undergoing the transition to the SG phase at $T \neq 0$ using Glauber dynamics and the local mean field approximation. Contrary to the results for clusters the maxima of $c(\omega)$ moves towards higher temperature on decreasing $\omega$. In this paper we reconsider this problem by Monte Carlo simulations.

In the experiments on liquids, an oscillatory heat causes temperature oscillations. For a theoretical study of SG's it is more convenient to define the same dynamic specific heat by inverting the situation. We thus propose that the temperature of the spin system varies periodically with time:

$$ T(t) = T + \delta T \sin(\omega t) , $$

where $\delta T$ is assumed to be small relative to $T$.

The perturbation in $T$ results in a oscillatory evolution of the internal energy. The oscillatory part of the average Hamiltonian, $< H >$, will be denoted by $\delta < H >$. When transients die out one can define $c'$ and $c''$ as follows

$$ \delta < H > /N = \delta T [ c'(\omega) \sin(\omega t) - c''(\omega) \cos(\omega t) ] . $$

Fig. 7. — The real and imaginary parts of the dynamic specific heat for the 3D system ($L = 10$) as a function of $T$. The solid line corresponds to the equilibrium specific heat which is obtained by using $10^5$ MCS/S for equilibration and another $10^5$ MCS/S for averaging. The black triangles, circles and squares correspond to $\omega T_0 = 0.01, 0.025$ and $0.05$, respectively. The results are averaged over 10 samples.

Similar to calculations of susceptibility we skip first $10^5$ MCS/S and average $\delta < H >$ over 2000 - 4000 periods. The periods we have considered are 20, 40 and 100 MCS/S multiplied by $2\pi$. Our calculations have been carried out for the 3D system of size $L = 10$. Averaging of $c'(\omega)$ and $c''(\omega)$ is performed over 10 samples. The amplitude $\delta T$ is taken to be equal to $0.01 J/k_B$ (the results remain almost the same for smaller $\delta T$).

Figure 7 shows the temperature dependence of the dynamic specific heat for selected values of $\omega$. The longer the period of oscillations, the closer $c'$ resembles the equilibrium specific
heat. The maxima of $c'$ and $c''$ move toward lower temperatures as $\omega$ is decreased. It should be noted that the same tendency has been observed in the 6-spin cluster and in experiments on glasses. It is, however, opposite to what observed within the dynamic local mean field approximation [4]. The failure of the latter approach in predicting correct positions of minima should be related to the fact that the energy ought to be determined from two-spin correlations but not from the local magnetizations.

It would be interesting to compare the results on dynamic specific heat with experiments and to clarify the origins of reentrancy. On the theoretical side, we observe that the local mean field approach applied to the dynamics offers apparent advantages over the Monte Carlo method — calculational speed and large signal to noise ratio — but is shown here to be qualitatively unreliable for frustrated systems.

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References