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Time and length scales in spin glasses

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Abstract

We discuss the slow, nonequilibrium, dynamics of spin glasses in their glassy phase. We briefly review the present theoretical understanding of the spectacular phenomena observed in experiments and describe new numerical results obtained in the first large-scale simulation of the nonequilibrium dynamics of the three-dimensional Heisenberg spin glass.

1. Why do we study spin glass dynamics?

Spin glasses can be seen as one of the paradigms for the statistical mechanics of impure materials. Experimentally, however, the spin glass phase is always probed via nonequilibrium dynamic experiments, because the equilibration time of macroscopic samples is infinite. Simulations can probe equilibrium behaviour for very moderate sizes only, so the thermodynamic nature of the spin glass phase is still a matter of debate. It is also as a model system that the glassy dynamics of spin glasses has been studied very extensively in experiments, simulations, and theoretically in the last two decades [1, 2]. Although many theories account for the simplest experimental results, such as the ageing phenomenon, early experiments revealed several other spectacular phenomena (rejuvenation, memory, etc) that are harder to explain, allowing one to discriminate between various approaches [3].

In recent years, several theoretical descriptions of the slow dynamics of spin glasses described the physics in terms of a distribution of length scales whose time, t, and temperature, T, evolution depends on the specific experimental protocol, as reviewed in [3]. Ageing is described as the slow growth of a coherence length, $\ell_T(t)$, reflecting quasi-equilibrium/nonequilibrium at shorter/larger length scales. Sensitivity to perturbations of quasi-equilibrated length scales accounts then for rejuvenation effects, while the strong temperature dependence of the growth law $\ell_T(t)$ explains memory effects [4–8]. If early numerical studies revealed the existence of such a distribution of length scales [9], its physical relevance was critically discussed only relatively recently [10, 11]. A major problem, however, is that most studies focused on the Edwards–Anderson model of an Ising spin glass, defined by the Hamiltonian

$$H = -\sum_{\langle i,j\rangle} J_{ij} S_i S_j, \tag{1}$$

where $S_i = \pm 1$, the sum is over pairs of nearest neighbours of the chosen lattice, and J_{ij} is a quenched random interaction, drawn from a symmetric distribution. The interest of the model (1) is that it has been studied very extensively so some—but only very few!—issues have been settled, most notably the existence, for space dimensions $d \geqslant 3$, of a second-order phase transition to a spin glass phase [12, 13]. The nonequilibrium dynamics of the Ising spin glass has also been quite extensively studied. Unfortunately, for $d = 3$, some of the key experimental observations are not reproduced [11, 14], although simulations in $d = 4$ have been more successful [11]. This may not be too surprising, since real spin glasses are made not of Ising spins but vector spins. When the interaction between spins is isotropic, the system is therefore best described by the Heisenberg spin glass Hamiltonian

$$H = -\sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{2}$$

where the $\mathbf{S}_i$ are now three-component vectors of unit length. The Heisenberg spin glass has been far less studied than the Ising one, both statically and dynamically, presumably because it was hoped that the understanding of the apparently simpler Ising case would be sufficient to interpret experiments. Very recent experiments systematically comparing Ising (i.e. very anisotropic) and Heisenberg samples have shown substantial quantitative differences between the two types of sample, the nonequilibrium effects being indeed much clearer in Heisenberg samples [15, 16].

Hence, it can reasonably be hoped that dynamic studies of the Heisenberg spin glass in $d = 3$ will reproduce the key experimental effects, with the result that deeper theoretical knowledge of the nature of the nonequilibrium dynamics of spin glasses can be gained. In this paper, we extract some preliminary results from the first large-scale numerical simulation of the nonequilibrium dynamics of the three-dimensional Heisenberg spin glass [17].

2. Simulation details

We simulate the Heisenberg spin glass (2) for $d = 3$. The sum in (2) runs over nearest neighbours of a cubic lattice with periodic boundary conditions. We use a heat-bath algorithm [18] in which the updated spin has the correct Boltzmann distribution for the instantaneous local field. This method has the advantage that a change in the spin orientation is always made. We use a rather large simulation box of linear size $L = 60$, and study several temperatures $T = 0.16, 0.15, 0.14, 0.12, 0.10, 0.08, 0.04$ and 0.02. Although all the quantities we shall study are self-averaging, we use several realizations of the disorder, typically 15, to increase the statistics of our data.

Contrary to the Ising case, the phase transition of the Heisenberg spin glass is still an open problem. A decoupling between spin and chiral degrees of freedom was theoretically suggested [19], while early simulations even questioned the mere existence of a phase transition [18]. Very recent simulations involving the most efficient tools used to study the Ising spin glass conclude that the model is characterized by a phase transition, at $T_c \simeq 0.16$, where both spins and chirality simultaneously freeze [20]. This motivates our choice for the upper temperature studied in our dynamical approach and our use of spin variables as dynamical objects of study.

3. What has to be measured?

Before embarking in the complex phenomenology of spin glasses, it is worth discussing the simplest protocol one can think of to probe the spin glass phase. A 'simple ageing' experiment

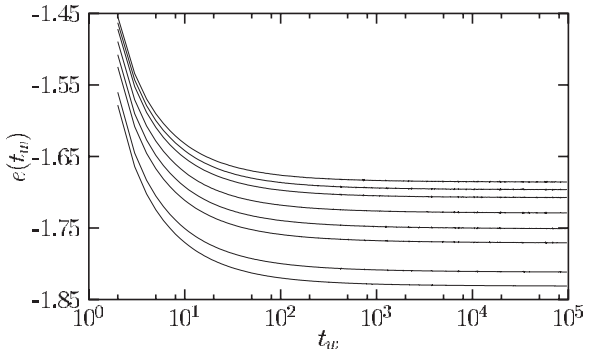

Figure 1. Time evolution of the energy density (3) after a quench from infinite temperature at the initial time t_w for $T = 0.16$, 0.15, 0.14, 0.12, 0.10, 0.08, 0.04, and 0.02 (from top to bottom).

consists of a sudden quench at initial time $t_w = 0$ from a temperature well in the paramagnetic phase, $T \gg T_c$, to a constant, low temperature below the spin glass transition, $T < T_c$. Ageing means a very slow evolution with time t_w (called the 'age') of the physical properties of the system. To study this behaviour, we record two types of quantity. First, 'one-time' quantities can be studied, such as the energy density of the spin glass,

$$e(t_w) = \frac{1}{N} H. \tag{3}$$

The time evolution of $e(t_w)$ for various low temperatures is presented in figure 1, from which the slow decrease of the energy towards an asymptotic equilibrium value is indeed observed, the sign that the dynamics is non-stationary.

We also study 'two-time' dynamic quantities. While experiments usually record response functions, it is easier to measure the corresponding correlation functions in numerical work. Here, we record the spin–spin autocorrelation function defined as

$$C(t + t_w, t_w) = \frac{1}{N} \sum_i \mathbf{S}_i(t + t_w) \cdot \mathbf{S}_i(t_w). \tag{4}$$

The qualitative behaviour of this function is well known, and a prototypical example is shown in figure 2. As usual, the time decay of $C(t + t_w, t_w)$ can be decomposed into two parts. For short time separations, $t \ll t_w$, the dynamics is almost independent of t_w, while the later decay, $t \gg t_w$, becomes slower as t_w becomes larger. Nonstationarity is reflected in the fact that $C(t+t_w, t_w) \neq C(t)$. The physical interpretation is simple: since the relaxation time of the sample is infinite, the only relevant timescale is the age of the sample t_w which imposes an age-dependent relaxation time: the older the sample, the slower its relaxation becomes. A careful analysis of short- and long-time behaviours of $C(t + t_w, t_w)$ and comparison to experimental data is described in [17].

4. Understanding ageing in real space

The key problem is to understand the subtle slow changes that the system undergoes: what does 'old' or 'young' really mean for the sample? The answer necessarily connects to equilibrium, since the system eventually equilibrates for $t_w \to \infty$. Moreover, the decomposition of the decay $C(t + t_w, t_w)$ between a fast stationary process and a slow non-stationary one directly suggests the existence of some sort of local equilibrium within the sample: a spin appears

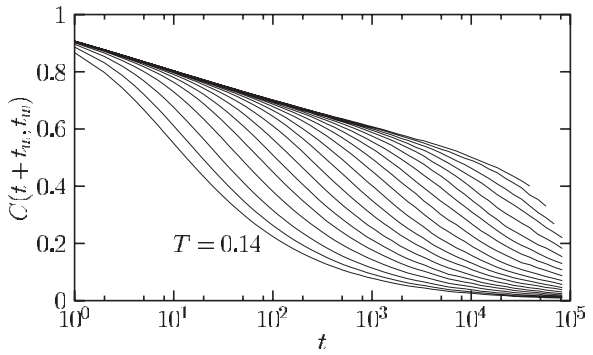

Figure 2. Spin–spin autocorrelation function (4) as a function of the time difference t for various t_w logarithmically spaced in the interval $t_w \in [2, 57\,797]$; t_w increases from left to right. The temperature is $T = 0.14$.

Figure 3. The orientation variable $\cos\theta_i$ defined in equation (5) is encoded in a greyscale in a $60 \times 60 \times 60$ simulation box at three different times $t_w = 2$, 27, and 57 797 (from left to right) and temperature $T = 0.04$. The growth of a local random ordering is evident.

locally equilibrated (short-time dynamics) although the sample as a whole is still far from equilibrium and evolves towards equilibrium (long-time dynamics).

It is possible to illustrate this last statement, as was done in the Ising case [9]. Because of the disorder, the spin orientations in an equilibrium configuration are random, so it is impossible to detect any domain growth by simply looking at the spin directions. However, two systems, (a, b), evolving independently but with the same realization of the disorder will reach correlated equilibrium configurations [13], so the orientations of the spins in the two copies will be similar, up to a global rotation. In figure 3, we present pictures where the 'orientation' variable

$$\cos\theta_i(t) = \mathbf{S}_i^{\mathrm{a}}(t) \cdot \mathbf{S}_i^{\mathrm{b}}(t) \tag{5}$$

is encoded in a greyscale. Comparing three successive times, it becomes clear that ageing involves the growth with time of a local random ordering imposed by the disorder of the Hamiltonian.

It is of course possible to go beyond simple pictures of black and white domains and measure the growing coherence length $\ell_T(t)$ corresponding to the mean domain size in figure 3. For this purpose, the spatial decay of the following correlation function is recorded:

$$C_4(r,t) = \frac{1}{N}\sum_i \mathbf{S}_i^{\mathrm{a}}(t) \cdot \mathbf{S}_{i+r}^{\mathrm{a}}(t)\mathbf{S}_i^{\mathrm{b}}(t) \cdot \mathbf{S}_{i+r}^{\mathrm{b}}(t). \tag{6}$$

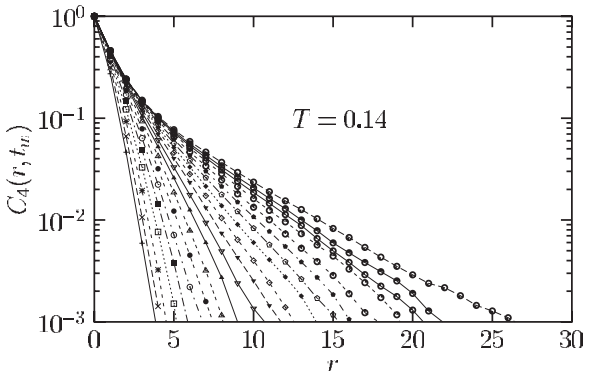

Figure 4. Two-spin, two-replica correlation function (6) as a function of the distance r between the spins for various t_w logarithmically spaced in the interval $t_w \in [2, 57\,797]$; t_w increases from left to right. The temperature is $T = 0.14$.

This function is a straightforward generalization of the two-spin, two-replica correlation function studied in the Ising case which measures spatial correlations of the random relative orientation of two spins [9]. In figure 4, we show this function for the same parameters as for the correlators of figure 2. The spatial decay of $C_4(r, t)$ is clearly slower for larger t, in agreement with the pictures in figure 3. Physically, this means that a larger time t_w implies a slower relaxation due to a larger coherence length, very much as in standard coarsening phenomena.

Note that due to periodic boundary conditions, the function (6) in figure 4 is symmetric about $L/2 = 30$. In [19], it was argued that spin and chirality degrees of freedom undergo different ageing dynamics because they are statically decoupled. The numerical support for this statement was the observation, for a system of linear size $L = 15$, that the autocorrelation (4) becomes stationary at large t_w. From figure 6, we immediately recognize that the data of [19] are plagued by severe finite size effects, so the conclusions of previous ageing studies of the Heisenberg spin glass [19, 21] must be treated with some care and this justifies our numerical effort of simulating a very large system, $L = 60$. The scaling properties of $C_4(r, t)$ and the properties of the coherence length are further discussed in [17]. We make here the important remark that much larger length scales can be reached in the same numerical time window for the Heisenberg spin glass than for the Ising case, which may indicate that richer behaviour can be seen in nonequilibrium simulations of the Heisenberg spin glass than the Ising ones.

5. Conclusion

We have motivated the need for large-scale numerical simulations of the three-dimensional Heisenberg spin glass in order to fill the gap between spatial theoretical descriptions of spin glass dynamics and experimental observations. The results presented here for the dynamics of the model (2) show that spin variables qualitatively follow the same type of ageing behaviour as in the Ising case, which is due to the slow growth with time of a dynamic coherence length. In [17], we analyse in detail the scaling properties of the dynamic functions reported here. The observation that very large length scales can be reached in the numerical time window, see figure 4, gives us the hope, also confirmed by preliminary work, that the model will allow us to reproduce most of the experimental effects, with the advantage that simulations have direct access to the distributions of length scales involved in phenomenological theories, providing further understanding of spin glass dynamics.

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