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On the relaxation of infinite-range spin glasses

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Abstract. The relaxation of the Sherrington–Kirkpatrick model for spin glasses is studied at low temperatures. A recently developed numerical method is used by which an infinitely large system is simulated, hence finite size effects are avoided. For parallel dynamics the decay of the energy as well as of the magnetization is investigated. For low temperatures we find evidence for a relaxation into a state which is characterized by non-equilibrium values of the energy and a non-vanishing remanent magnetization.

1. Introduction

In thermal equilibrium the infinite-range spin glass (the Sherrington–Kirkpatrick (SK) model [1]) is characterized by infinite energy barriers and non-ergodic behaviour below the critical temperature [2]. But in a typical experiment the system is prepared in a state far from equilibrium and relaxes by thermal noise and decay of energy. At zero temperature the dynamics always decreases the energy and therefore gets trapped in metastable states [3]; hence the system decays to a state with an energy much higher than that of the ground state and with a non-zero remanent magnetization [4, 5]. For non-zero temperatures, however, the scenario is less clear. There still exists an exponentially large number of metastable states with energy values much higher than the equilibrium value [7]. But to our knowledge it is not known whether these metastable states are separated by infinitely high energy barriers from the equilibrium configuration and whether the system actually gets trapped in such states. Hence, the question remains open whether at non-zero temperatures the system approaches a state with non-zero remanent magnetization and higher energy than in thermal equilibrium.

Note that even the infinite-range Ising ferromagnet has stable states far from equilibrium with high energy and non-zero memory to the initial state. If at low temperatures a small positive magnetic field is applied, an initial state with a sufficiently large negative magnetization evolves towards a metastable state with negative magnetization and a higher energy per spin than in equilibrium. This metastable state is separated by an infinite-energy barrier from thermal equilibrium. Whether this scenario extends to spin glasses with an infinite number of metastable states is the subject of our present investigation.

While previous numerical results [5, 6] have indicated that the SK model decays to thermal equilibrium for non-zero temperatures, recent simulations have shown that some properties of the model depend strongly on the size of the system [4]. Therefore we use the method proposed in [9] to study the infinitely large system. The method combines the dynamical functional approach, which allows us to perform the limit $N \to \infty$ exactly, and a Monte Carlo simulation of the resulting stochastic single-particle equations. In [11] the approach was used to examine a variant of the Sherrington—Kirkpatrick model for spin glasses. The phase transition as a function of the asymmetry in the random couplings [10] was confirmed and investigated in detail. In the present paper, we extend the method to non-zero temperatures in order to investigate the temporal development of the energy as well as of the magnetization.

Independently, Ferraro [12] performed the same extension to non-zero temperatures in the case of symmetric couplings, using a 'trajectory scaling' (see below). His and our findings concerning the energy agree very well. Furthermore, we investigated the response function and the remanent magnetization of the system in detail. The latter was assumed to be zero from the outset in [12].

The next section gives an introduction to the mean-field Monte Carlo method of Eißfeller and Opper. In section 3 we extend the method to non-zero temperatures and derive the energy of the system. The results of the simulations are given and discussed in section 4. Section 5 contains concluding remarks.

2. Mean-field Monte Carlo method

We consider a variant of the SK model which consists of N Ising spins $S_i = \pm 1$. Every spin S_i is connected to all other spins S_j with $i < j$ by independent Gaussian couplings J_{ij} with zero mean and variance $1/N$. We allow for asymmetry in the matrix of couplings described by the parameter η:

$$\langle J_{ij} J_{ji} \rangle_J = \eta / N \tag{1}$$

where the brackets denote an average over the distribution of couplings. The couplings are fully antisymmetric if $\eta = -1$ and totally uncorrelated if $\eta = 0$. Symmetric couplings as in the SK model correspond to $\eta = 1$.

Instead of directly simulating the system of dynamical equations

$$S_i(t+1) = \text{sign}[h_i(t)] \qquad i = 1, \ldots, N \tag{2}$$

with the internal fields

$$h_i(t) = \sum_{j \neq i} J_{ij} S_j(t) \tag{3}$$

where all spins are updated in parallel, Eißfeller and Opper [9, 11] follow the dynamical functional approach [13]. This allows us to perform the average over the random couplings J_{ij} and to transform the remaining expression using saddle-point methods, which are exact in the thermodynamic limit $N \to \infty$. The result is a system of *stochastic* dynamical equations

$$\begin{aligned} S(t+1) &= \text{sign}[h(t)] \\ h(t) &= \Phi(t) + \eta \sum_s K(t,s) S(s) \end{aligned} \tag{4}$$

where the correlations of the time-dependent Gaussian noise variables $\Phi(t)$ and the response function $K(t,s)$ are determined by the saddle-point equations as

$$\begin{aligned} \langle \Phi(s)\Phi(\tau) \rangle_\Phi &= C(s,\tau) = \langle S(s) S(\tau) \rangle_\Phi \\ K(t,s) &= \langle \partial S(t) / \partial \Phi(s) \rangle_\Phi \,. \end{aligned} \tag{5}$$

For a full derivation of the dynamical single-particle equations (4), (5) and a detailed description of the Monte Carlo procedure used to simulate these equations see [11].

3. Extension to non-zero temperatures

In order to include noise in the dynamical single-particle equations, we add an independent random variable $r(t)$ to the internal field

$$S(t+1) = \text{sign}[h(t) + r(t)] \tag{6}$$

where $r(t)$ is generated according to

$$r(t) = \frac{1}{2\beta} \ln \left[\frac{1 - x(t)}{x(t)} \right] \qquad \text{with } x(t) \text{ equally distributed in } [0, 1]. \tag{7}$$

In the following the asymmetry η is set to 1. In this case the dynamics obeys detailed balance and the noise parameter β can be interpreted as the inverse temperature $\beta = 1/T$. In thermal equilibrium, it leads to a Gibbs distribution of the spin configurations with the partition function [14, 15]:

$$Z = \text{Tr}_S \exp \left[\sum_i \ln \left\{ 2\cosh \left(\beta \sum_j J_{ij} S_j \right) \right\} \right]. \tag{8}$$

In equilibrium, the mean energy per spin of the system is given by

$$\langle E/N \rangle_\beta = -1/N \ \partial \ln Z / \partial \beta = \langle \tanh[\beta h_i] \ h_i \rangle_\beta \,. \tag{9}$$

Using the Monte Carlo procedure mentioned above, the time-dependent energy can be calculated from

$$e(t) = E(t)/N = -\langle \tanh[\beta h(t)] h(t) \rangle_\Phi = -\langle \text{sign}[h(t) + r(t)] h(t) \rangle_{\Phi,r} \,. \tag{10}$$

In order to compare the energy of the system extrapolated to infinite times $e_\infty = \lim_{t\to\infty} e(t)$ with results of equilibrium statistical mechanics, the free energy of the system with the partition function (8) should be derived using replica theory. We performed the replica symmetric calculation following Fontanari and Koeberle [16] and found that the parallel SK model (or Little model [17]) follows the same thermodynamics as the sequential SK model, but that the free energy is twice the original one. This result gives further evidence for the conjecture [18, 12] based on numerical findings [18] that the full hierarchical solution of the SK model is—up to a factor of two—also valid for the Little model (equation (8)).

4. Results and discussion

Using the Monte Carlo procedure described in [11] we simulate the single-particle equations (6) with the internal fields given by (4). The decay of the energy is calculated for the first 130 time steps for various values of the temperature. In order to estimate the averages over the random Gaussian variables Φ, occurring in the saddle-point equations (5), we simulate $N_T = 10^6$ trajectories, starting from a fully magnetized state $S(t=0) = 1$ for all trajectories. In the following all fits were done in the temporal range from $t = 20$ to 130. The results could be fitted well by the function

$$e(t) = \text{constant} \times t^{-a} + e_\infty \tag{11}$$

where the parameters a and e_∞ are functions of the temperature. Figure 1 shows $a(T)$. The resulting extrapolated values e_∞ are displayed in figure 2 together with the replica symmetric solution and the solution of the full replica symmetry breaking equations [19]. The latter was taken from [12] (figure 3). As expected, for $T = 0$ the energy e_∞ is higher than the corresponding equilibrium value. This is consistent with the remanent magnetization $m_{\text{rem}} \simeq 0.18$, which was found, for example, in [9, 11]. Also for low (but non-zero) temperatures the equilibrium values are not reached. Surprisingly, the simulated

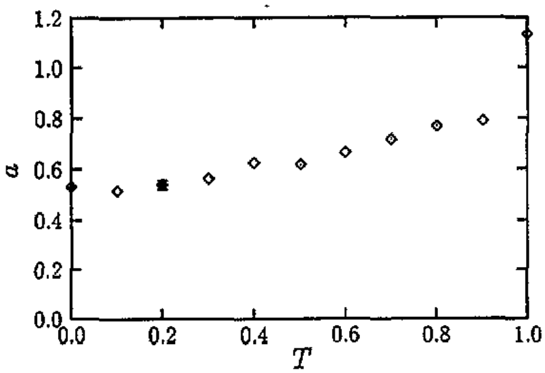

Figure 1. The temperature dependence of the exponent a. The error bar is estimated from ten independent runs (3σ).

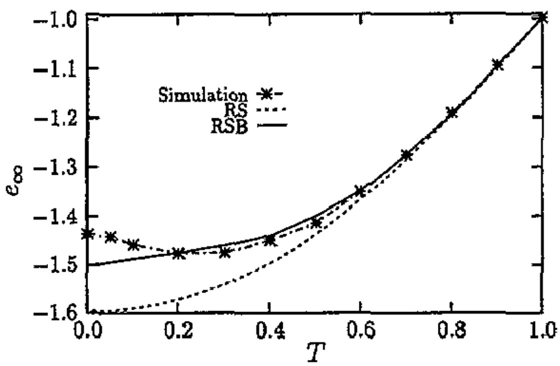

Figure 2. The extrapolated values of the energy (stars) as a function of the temperature. The error bar as a result of ten independent runs for $T = 0.2$ is smaller than the symbol size. The broken curve represents the replica symmetric solution, whereas the full curve shows the numerical solution of the replica equations [19] and was taken from [12].

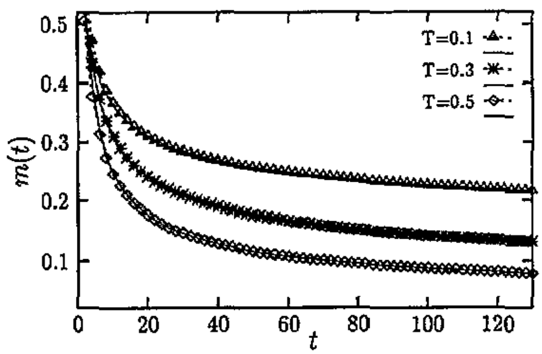

Figure 3. The decay of the magnetization for different temperatures. The full curves display the corresponding fit functions.

energy e_∞ shows a non-monotonic behaviour as a function of the temperature, which contradicts equilibrium theory. On the other hand, the simulations are in good agreement with equilibrium theory for temperatures $T \gtrsim 0.6$. Note that the number of metastable states (solutions of the TAP equations) drastically decreases at $T \simeq 0.6$ [7].

The same non-monotonic behaviour of e_∞ at low temperatures was found by Ferraro, who assumed a linear dependence of the time-dependent energy on the inverse of the number of trajectories N_T [12]. Using $N_T = 8000$ and 16 000 he could not calculate the value for zero temperature, since the system freezes after a short time for these small numbers of trajectories. He explains the deviation from the equilibrium values by a further (very slow) relaxation with the consequence of a non-universal exponent a. Looking at the relaxation of the magnetization and the behaviour of the response function we suggest a different interpretation (see below).

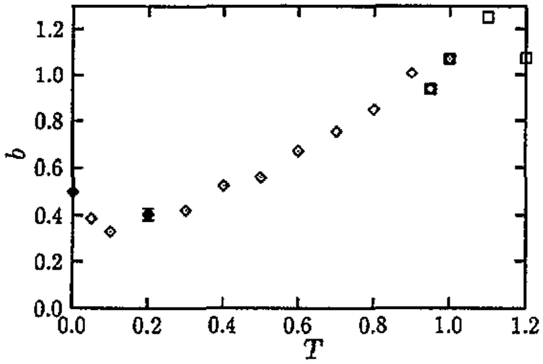

Figure 4. Temperature dependence of the exponent b. The error bar is estimated from ten independent runs (3σ). Up to the temperature $T = 1$ the power law was fitted; for higher temperatures an additional exponential factor had to be included. At the temperatures $T = 0.95$ and $T = T_c = 1$ the exponents b for both fits coincide.

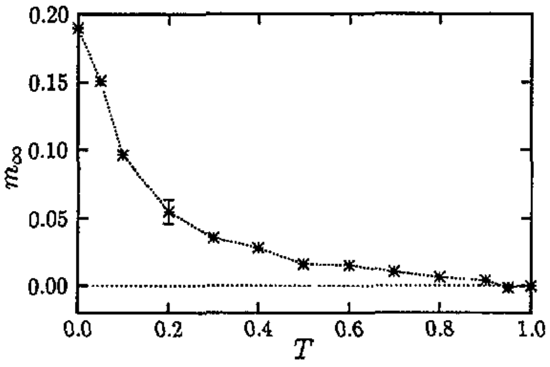

Figure 5. The remanent magnetization as a function of the temperature. The error bar is estimated from ten independent runs (3σ).

The magnetization describes the system's memory of its initial state

$$m(t) = \langle S(0)S(t)\rangle_\Phi \,. \tag{12}$$

In equilibrium the system should be completely independent of its initial configuration or in other words: the equilibrium state is characterized by a zero remanent magnetization $m_\infty = \lim_{t\to\infty} m(t) = 0$.

The decay of the magnetization for the first 130 time steps is displayed in figure 3 for various temperatures. Note, that the magnetization vanishes at uneven times [11], which is not shown in figure 3. The non-zero part of the magnetization reveals the following relaxation behaviour:

$$m(t) = \begin{cases} \text{constant} \times t^{-b}(+m_\infty) & \text{for} \quad 0 < T \lesssim 1 \\ \text{constant} \times t^{-b}\exp[-t/\tau] & \text{for} \quad T \gtrsim 1 \end{cases} \tag{13}$$

where the parameters b, τ and m_∞ are again functions of the temperature—as displayed in figure 4 for the exponent b. At a temperature $T \simeq 1$ we find a transition in the relaxation behaviour of the magnetization from an algebraic decay to one with an additional exponential factor, in agreement with the critical temperature $T_c = 1$ predicted by equilibrium theory. In contrast to [12] we allow—also in the case of non-zero temperatures—for an additional parameter corresponding to the remanent magnetization. Doing so, we find a non-zero remanent magnetization m_∞ which slowly decays to zero with increasing temperature (figure 5). Up to the critical temperature a memory of the initial state remains, which indicates a relaxation into a non-equilibrium state.

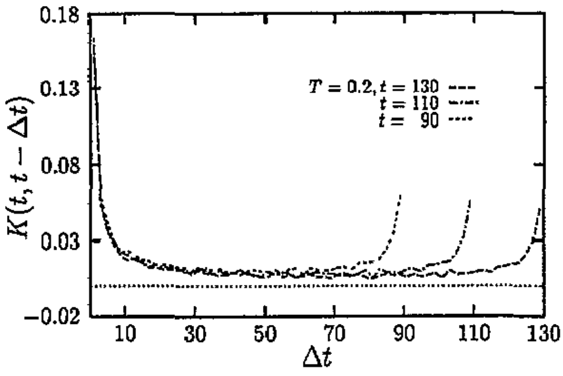

Figure 6. The response function for $T = 0.2$ and different times t as a function of the time difference $\Delta t = (t - s)$—averaged over ten independent runs. The fluctuations at intermediate times (due to numerical noise) have been smoothed down by this average, which accentuates the memory effect.

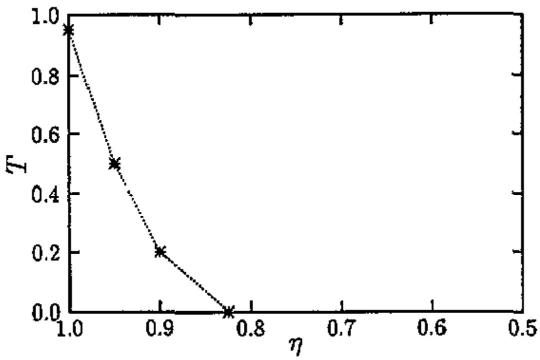

Figure 7. Phase diagram as a function of the asymmetry parameter η and the temperature T. Below the broken curve the remanent magnetization is found to be different from zero $m_\infty \neq 0$.

We have investigated another quantity which gives further evidence for a non-zero remanent magnetization at low temperatures. The memory effect to the initial conditions at low temperatures is also reflected in the behaviour of the response function $K(t, s)$. As can be seen from (5), this function describes the average response of the magnetization at time t to small variations of an external field at a previous time s. In figure 6 the response function $K(t, t - \Delta t)$ at low temperature ($T = 0.2$) is displayed as a function of the time difference $\Delta t = t - s$ for various times t and averaged over ten independent runs. The system responds strongly to variations at times s close to time t, whereas intermediate times do not influence the system. But a significant increase of K at large Δt can be observed, indicating a stronger memory to the initial conditions. For high temperatures, memory effects are short range and K decays after a few time steps Δt. Moreover, the fact that the response functions are identical at large times s (small Δt) for all displayed times t reflects a stationary behaviour, i.e. a dependence on time differences only.

We extended our investigations of the remanent magnetization at non-zero temperatures to the asymmetric case $\eta < 1$. In a region of temperatures $T \lesssim 1$ and values of the asymmetry parameter $\eta > 0.825$ (figure 7) we find the same behaviour as described above, namely a non-vanishing remanent magnetization and a memory effect in the response function K.

Furthermore, we studied the dependence on the number of trajectories in the range $10^4 \leqslant N_T \leqslant 3.2 \times 10^5$. For high numbers of trajectories ($3.2 \times 10^5, 1.6 \times 10^5$) we find clear deviations from a linear dependence of the time-dependent energy (or respectively magnetization) on $1/N_T$ which was suggested in [12]. These deviations may be responsible for the quantitative differences concerning the values of the exponents a.

5. Conclusion

In conclusion, we have examined parallel non-equilibrium dynamics of the SK model and find evidence for a relaxation into a state characterized by a non-zero remanent magnetization and a non-equilibrium value of the energy for low but non-zero temperatures. This indicates that spin glasses relax to stable states far from thermal equilibrium.

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