Glauber dynamics of the SK model: theory and simulations in the low-temperature phase

1998 J. Phys. A: Math. Gen. 31 10053

(http://iopscience.iop.org/0305-4470/31/50/004)

J. Phys. A: Math. Gen. **31** (1998) 10053–10063. Printed in the UK PII: S0305-4470(98)94981-2

Glauber dynamics of the SK model: theory and simulations in the low-temperature phase

Grzegorz Szamel
Department of Chemistry, Colorado State University, Fort Collins, CO 80523, USA

Received 9 June 1998, in final form 3 September 1998

Abstract. The low-temperature Glauber dynamics of the Sherrington–Kirkpatrick spin-glass model is studied using a combination of theory and computer simulations. The theoretical approach follows the spirit of Mori's continuous fraction expansion. The predicted amplitude of the long-time decay of the time-dependent equilibrium spin–spin correlation function agrees well with the Glauber dynamics simulation results. The theory predicts a universal dynamic exponent of $\frac{1}{2}$ in the low-temperature phase. The simulations cannot distinguish between a universal exponent and a temperature-dependent one.

1. Introduction

In the preceding paper [1], we presented a new approach to Glauber dynamics of the Sherrington–Kirkpatrick (SK) spin-glass model [2–4]. Our method gives very accurate results for the time-dependent equilibrium spin–spin correlation function in the high-temperature phase ($T \geqslant T_c$). Here we discuss the theoretical predictions for the low-temperature phase dynamics and compare them with the Glauber dynamics simulations results.

The motivation for this study is as follows. There are two versions of the SK model [2] that are discussed in the literature. One of them is studied theoretically and the other both theoretically and (mainly) in computer simulations. The first is the soft-spin version of the SK model with Langevin dynamics. Its studies were pioneered by Sompolinsky and Zippelius (SZ) [5] who found a continuously varying dynamic exponent in the low-temperature phase. More recently, there was a series of very interesting results concerning off-equilibrium dynamics of the soft-spin SK model [6].

The second version is the original hard(Ising)-spin SK model with Glauber dynamics. This model was a subject of early studies [2, 7] in which a universal (temperature-independent) dynamic exponent was found. Later work [8] raised a possibility of a non-universal exponent. More recently, a novel approach to Glauber dynamics has been proposed by Coolen, Sherrington, and coworkers [9] (note that these authors were not concerned with the above-mentioned dynamic exponent). This new approach was an inspiration for our work.

The main use of the SK model with Glauber dynamics is in computer simulations [2, 3, 10]. Results of such simulations are compared not only with the theoretical studies of the same model but also with those of the soft-spin model. The question then arises whether equivalence of these two models has been established. In particular, is there a continuously varying dynamic exponent in the low-temperature phase of the SK model with Glauber dynamics?

0305-4470/98/5010053+11$19.50

To the best of our knowledge, the only theoretical paper [11] that claimed to have rederived the SZ results for the hard-spin model was criticized [12] and the validity of its predictions is uncertain. In addition, although some results of the SZ theory were verified in computer simulations [10], we are not aware of any convincing simulational observation of a continuously varying dynamic exponent†. In view of these facts we consider the question of 'what is the low-temperature dynamic behaviour of the SK model with Glauber dynamics' to be an open problem.

Here we report a theoretical and simulational study of the low-temperature Glauber dynamics of the SK model. Following SZ we study time-dependent spin–spin correlations in equilibrium (we implicitly assume equilibrium within a single pure state)‡.

The theoretical analysis follows that presented in [1]. It is loosely based on Mori's [15] continuous fraction expansion. In contrast to most of the other works we study the dynamics for a given sample of coupling constants and average over the samples at the very end. The zeroth-order approximation is equivalent to a disorder-dependent version of the local equilibrium approximation of Kawasaki [16]. The first-order approximation includes an irreducible memory matrix.

Predictions of both the zeroth- and the first-order approximations are expressed in terms of the equilibrium spin correlations. In the low-temperature phase these correlations are not known explicitly and, therefore, in order to test our theoretical predictions we have to obtain them from computer simulations.

Computer simulations play a double role in this study. First, as stated in the preceding paragraph, we use them to obtain the equilibrium spin averages. More importantly, we monitor the dynamic quantities: time-dependent spin–spin correlation function and its first time derivative. We use these dynamic results to test the accuracy of our theory and also to attempt to verify the existence of a continuously varying dynamic exponent.

2. Theory

2.1. Definitions

We follow the notation of [1]. Briefly, the SK model consists of Ising spins $\sigma_i = \pm 1$ interacting via infinite-range exchange coupling constants J_{ij},

$$H = -\sum_{i<j} J_{ij}\sigma_i\sigma_j. \tag{1}$$

The coupling constants J_{ij} are quenched random variables distributed according to the symmetric distribution $P(J_{ij}) \sim \exp(-J_{ij}^2/(2J^2/N))$.

We study the time-dependent spin–spin correlation function,

$$\langle \delta\sigma_i(t)\delta\sigma_j\rangle_{\mathrm{eq}} = \langle \delta\sigma_i \exp(\Omega t)\delta\sigma_j\rangle_{\mathrm{eq}}. \tag{2}$$

Here $\delta\sigma_i$ is the fluctuation of the value of the ith local spin, $\delta\sigma_i = \sigma_i - \langle\sigma_i\rangle_{\mathrm{eq}}$ and $\langle\ldots\rangle_{\mathrm{eq}}$ denotes the equilibrium average (implicitly restricted to a single pure state). Finally, Ω is

† Note that a temperature-dependent exponent found in [13] describes off-equilibrium energy relaxation whereas the dynamic exponent studied by SZ [5] describes relaxation of *equilibrium* magnetization fluctuations.

‡ Note that the problem that we address is different from that addressed by the off-equilibrium studies [6]. In particular, we assume that the system is in equilibrium and therefore time-translational invariance of the correlation functions is valid. Alternatively, in the language of the off-equilibrium papers [6, 14], we study spin–spin correlations $\langle\delta\sigma(t_w + t)\delta\sigma(t_w)\rangle$ in the regime $0 \leqslant t \ll t_w$, $t_w \to \infty$. In this regime equilibrium within a given pure state is established and time-translational symmetry is satisfied. We carefully check that our Glauber dynamics simulations are in the same dynamical regime (see section 3).

the evolution operator,

$$\Omega = -\sum_i (1 - S_i) w_i \tag{3}$$

with S_i being the spin-flip operator, $S_i \sigma_i = -\sigma_i$, and w_i being the transition rate,

$$w_i = (1 - \sigma_i \tanh(\beta h_i))/2 \tag{4}$$

where h_i is a local magnetic field acting on the ith spin,

$$h_i = \sum_{j \neq i} J_{ij} \sigma_j. \tag{5}$$

2.2. Zeroth-order approximation

To derive a zeroth-order approximation for the equation of motion for the time-dependent spin–spin correlation function we follow [1, section 2.2] and obtain

$$\partial_t \langle \delta\sigma_i(t) \delta\sigma_j \rangle_{\mathrm{eq}} = -\langle 1 - \sigma_i \tanh(\beta h_i) \rangle_{\mathrm{eq}} \sum_l A_{il} \langle \delta\sigma_l(t) \delta\sigma_j \rangle_{\mathrm{eq}}. \tag{6}$$

Here A is the inverse matrix of spin correlations,

$$\sum_j A_{ij} \langle \delta\sigma_j \delta\sigma_k \rangle_{\mathrm{eq}} = \delta_{ik}. \tag{7}$$

Note that A is equal to the Hessian of the Thouless–Anderson–Palmer [17] free energy. Above T_c the Hessian is known explicitly. Below T_c it can be expressed in terms of local (sample-dependent), equilibrium site magnetizations [4],

$$A_{ij} = -\beta J_{ij} + \delta_{ij} \left(\sum_k (\beta J_{ik})^2 (1 - m_k^2) + \frac{1}{1 - m_i^2} \right) \tag{8}$$

where m_i is the local magnetization at site i, $m_i = \langle \sigma_i \rangle_{\mathrm{eq}}$.

To get explicit results we have to solve (6). To this end we decompose the matrix of the spin correlations,

$$\langle \delta\sigma_i(t) \delta\sigma_j \rangle_{\mathrm{eq}} = \sum_{\lambda\nu} a_{\lambda\nu}(t) t_\lambda^i t_\nu^j \tag{9}$$

where t_λ^i and t_ν^i are the eigenvectors of the matrix of inverse spin correlations (Hessian) and λ and ν are the corresponding eigenvalues. Note that at an initial time $a_{\lambda\nu}(t = 0) = \lambda^{-1} \delta_{\lambda\nu}$. Substituting (9) into (6) we get the equation of motion for the amplitudes,

$$\partial_t a_{\lambda\nu}(t) = -\sum_\mu \mu \sum_i t_\lambda^i \langle 1 - \sigma_i \tanh(\beta h_i) \rangle_{\mathrm{eq}} t_\mu^i a_{\mu\nu}(t). \tag{10}$$

At this point we make two assumptions. At present, the only way to check them is *a posteriori*. First, since at the initial time the matrix of amplitudes, $a_{\lambda\nu}$, is diagonal, we shall assume that we can neglect off-diagonal terms at later times. This amounts to the following approximation in the equation of motion (10)

$$\sum_i t_\lambda^i \langle 1 - \sigma_i \tanh(\beta h_i) \rangle_{\mathrm{eq}} t_\mu^i \approx \delta_{\lambda\mu} \sum_i t_\lambda^i \langle 1 - \sigma_i \tanh(\beta h_i) \rangle_{\mathrm{eq}} t_\lambda^i. \tag{11}$$

Now we can write down a formal solution for the spin–spin correlation function. In the following we will restrict ourselves to the diagonal part, i.e. $\langle \delta\sigma_i(t) \delta\sigma_i \rangle_{\mathrm{eq}}$,

$$\langle \delta\sigma_i(t) \delta\sigma_i \rangle_{\mathrm{eq}} = \sum_\lambda t_\lambda^i \frac{1}{\lambda} \exp(-t/\tau(\lambda)) t_\lambda^i. \tag{12}$$

The off-diagonal part vanishes after sample averaging. Here the relaxation time $\tau(\lambda)$ is given by

$$\tau(\lambda)^{-1} = \lambda \sum_i t_\lambda^i \langle 1 - \sigma_i \tanh(\beta h_i)\rangle_{\rm eq} t_\lambda^i. \tag{13}$$

Since the spectrum of the eigenvalues of the Hessian extends to zero as $\rho(\lambda) \sim \lambda^{1/2}$ [18] it follows from equation (12) that the dynamic exponent describing the long-time decay of the spin correlations is temperature independent and equal to $\frac{1}{2}$.

To calculate expression (12) explicitly for all times we need the whole spectrum of the eigenvalues and eigenvectors of the Hessian. However, in order to get the amplitude of the $t^{-1/2}$ tail in the spin–spin correlations we need only the low-λ behaviour of the distribution of the eigenvalues and the eigenvector corresponding to the zeroth eigenvalue,

$$\langle \delta\sigma_i(t)\delta\sigma_i\rangle_{\rm eq} \approx \alpha\sqrt{\pi} t_0^i t_0^i \left(\sum_i t_0^i \langle 1 - \sigma_i \tanh(\beta h_i)\rangle_{\rm eq} t_0^i \right)^{-1/2} t^{-1/2}. \tag{14}$$

Here the constant α is determined by the low-λ behaviour of the spectrum of the eigenvalues,

$$\rho(\lambda) \approx \alpha \lambda^{1/2} \tag{15}$$

and, according to Bray and Moore's [18] analysis,

$$\alpha = (1/\pi)(\beta J)^{-3} \overline{(1-m^2)^3}^{-1/2}. \tag{16}$$

In equation (16) the overline denotes 'spatial' averaging,

$$\overline{(1-m^2)^3} = N^{-1} \sum_i (1 - m_i^2)^3. \tag{17}$$

Finally, in equation (14) t_0^i denotes the eigenvector corresponding to the zeroth eigenvalue of the Hessian matrix,

$$\sum_j \left\{ -\beta J_{ij} + \delta_{ij} \left(\sum_k (\beta J_{ik})^2 (1 - m_k^2) + \frac{1}{1 - m_i^2} \right) \right\} t_0^j = 0. \tag{18}$$

Our second assumption concerns the eigenvector t_0. We assume that in solving equation (18) we can use the following *ansatz*,

$$t_0^i = c_i + \sum_j \beta J_{ij} d_j \tag{19}$$

where, implicitly, c_i and d_i have nonzero spatial averages. Substituting (19) into equation (18) we obtain

$$c_i \left((\beta J)^2 (1-q) + \frac{1}{1-m_i^2} \right) - d_i (\beta J)^2 + \sum_j \beta J_{ij} \left\{ \left((\beta J)^2 (1-q) + \frac{1}{1-m_i^2} \right) d_j - c_j \right\} - \sum_{j,l \neq i} \beta^2 J_{ij} J_{jl} d_l = 0. \tag{20}$$

Note that in writing equation (20) we follow Bray and Moore [18] and approximate $\sum_k (\beta J_{ik})^2 (1 - m_k^2)$ by $(\beta J)^2 (1 - q)$ where $q = \overline{m^2}$.

We now assume that the 'off-diagonal' terms in equation (20) (i.e. the last two sums) average out to 0. In this way we obtain the following *approximate* expression for the *un*normalized zeroth eigenvector

$$t_0^i = \frac{(\beta J)^2}{((\beta J)^2 (1-q) + \frac{1}{1-m_i^2})} + \sum_j \beta J_{ij}. \tag{21}$$

Finally, normalizing (21), substituting the result into equation (14), and using (16) we obtain an explicit expression for the long-time asymptotics of the spin–spin correlations. After spatial averaging the result reads

$$\overline{\langle \delta\sigma_i(t)\delta\sigma_i\rangle_{\rm eq}} \approx \frac{1}{\sqrt{\pi}}\frac{1}{(\beta J)^3\overline{(1-m^2)^3}^{1/2}} \times\left[\frac{1+(\beta J)^2\overline{\frac{(1-m^2)^2}{((\beta J)^2(1-q)(1-m^2)+1)^2}}}{(1-\langle\sigma_i\tanh(\beta h_i)\rangle_{\rm eq})(1+(\beta J)^2\overline{\frac{(1-m^2)^2}{((\beta J)^2(1-q)(1-m^2)+1)^2}})}\right]^{1/2} t^{-1/2}. \tag{22}$$

It is worth noticing at this point that if we had assumed the eigenvectors of the Hessian to be uncorrelated with $\langle\sigma_i\tanh(\beta h_i)\rangle_{\rm eq}$ (as we did when we analysed the high-temperature phase dynamics) we would have obtained the following result,

$$\overline{\langle \delta\sigma_i(t)\delta\sigma_i\rangle_{\rm eq}} \approx \frac{1}{\sqrt{\pi}}\frac{1}{(\beta J)^3\overline{(1-m^2)^3}^{1/2}}\frac{1}{1-\langle\sigma_i\tanh(\beta h_i)\rangle_{\rm eq}^{1/2}} t^{-1/2}. \tag{23}$$

As we shall show in section 4, Glauber dynamics simulation results seem to agree with equation (22) rather than with equation (23).

2.3. First-order approximation

In the zeroth-order approximation we neglected the memory matrix entirely. In the next step (first-order approximation) we include it approximately. To this end we repeat the analysis of [1, section 2.3] and arrive at the following set of equations

$$\int_0^t \sum_j (\delta_{ij}\delta(t-t') + M^{\rm irr}_{ij}(t-t')\langle 1-\sigma_j\tanh(\beta h_j)\rangle_{\rm eq}^{-1})\partial_{t'}\langle\delta\sigma_j(t')\delta\sigma_k\rangle_{\rm eq} = -\langle 1-\sigma_i\tanh(\beta h_i)\rangle_{\rm eq}\sum_l A_{il}\langle\delta\sigma_l(t)\delta\sigma_j\rangle_{\rm eq}. \tag{24}$$

$$\partial_t M^{\rm irr}_{ij}(t) = \sum_{kl}\langle D_i\mathcal{Q}_0\Omega^{\rm irr}\mathcal{Q}_0 D_k\rangle_{\rm eq} C_{kl} M^{\rm irr}_{kj}(t). \tag{25}$$

Here $M^{\rm irr}$ is the *irreducible* [19] memory matrix.

In the preceding paper we invoked a high-temperature-expansion argument in order to simplify (24). Here we cannot resort to the same argument and therefore we have to replace it with two *assumptions*. Both of these assumptions concern *equilibrium* averages.

First, we assume that the off-diagonal equilibrium correlations between *irreducible* quantities (i.e. quantities that have spin correlations subtracted out) are higher order in $N^{-1/2}$ than the spin–spin correlations. For example, we assume that the $\langle D_j D_k\rangle_{\rm eq}$ for $j\neq k$ are higher order in $N^{-1/2}$ than $\langle\delta\sigma_i\delta\sigma_j\rangle_{\rm eq}$. The argument is that the former needs at least *two* independent 'connections' between i and j, each of them being of the order of spin correlations. This of course does not hold for the diagonal part: both $\langle D_i D_i\rangle_{\rm eq}$ and $\langle\delta\sigma_i\delta\sigma_i\rangle_{\rm eq}$ are finite (of the order of N^0).

Second, we assume that we can keep only the diagonal part of the memory matrix evolution operator $\langle D_i\mathcal{Q}_0\Omega^{\rm irr}\mathcal{Q}_0 D_j\rangle_{\rm eq}$,

$$\langle D_i\mathcal{Q}_0\Omega^{\rm irr}\mathcal{Q}_0 D_i\rangle_{\rm eq} = -(\beta J)^2\overline{\langle 1-\tanh^2(\beta h)\rangle_{\rm eq}}(\langle\tanh^4(\beta h_i)\rangle_{\rm eq} - \langle\tanh^2(\beta h_i)\rangle_{\rm eq}^2). \tag{26}$$

The second assumption is based on the explicit form of the off-diagonal part,

$$\langle D_i\mathcal{Q}_0\Omega^{\rm irr}\mathcal{Q}_0 D_j\rangle_{\rm eq} \sim \sum_{l\neq i, l\neq j}(\mathcal{A}_{ilj} - \mathcal{B}_{il}\mathcal{B}_{jl})J_{il}J_{jl} \qquad i\neq j \tag{27}$$

where $\mathcal{A}$ and $\mathcal{B}$ denote equilibrium averages. If the averages in $\mathcal{A}$ and $\mathcal{B}$ that involve different sites are decoupled, the term in parenthesis at the right-hand side of equation (27) vanishes. Hence, a simple power-counting argument suggests that the off-diagonal part is of higher order in $N^{-1/2}$ than the spin–spin correlations and, therefore, can be neglected.

The above assumptions allow us to reduce (24). Now, as in [1], only the diagonal elements of the memory matrix contribute and their time evolution is given by

$$\partial_t M^{\mathrm{irr}}_{ii}(t) = \langle D_i \mathcal{Q}_0 \Omega^{\mathrm{irr}} \mathcal{Q}_0 D_i \rangle_{\mathrm{eq}} C_{ii} M^{\mathrm{irr}}_{ii}(t) \tag{28}$$

where

$$M^{\mathrm{irr}}_{ii}(t=0) = C^{-1}_{ii} = \langle 1 - \tanh^2(\beta h_i)\rangle_{\mathrm{eq}} (1 - A_{ii}\langle 1 - \tanh^2(\beta h_i)\rangle_{\mathrm{eq}}). \tag{29}$$

Equations (24) and (28) with (26) and (29) constitute our first-order approximation. The only assumptions/approximations made up to this point (apart from neglecting higher-order memory functions) are the two approximations concerning *equilibrium* correlation functions: we assumed that the off-diagonal irreducible correlation functions and off-diagonal terms of the approximate evolution operator for the memory matrix can be neglected.

Within these two assumptions it is possible to go further and consider higher-order approximations. The structure of the theory will remain the same: at a higher-order level a new (diagonal) memory matrix appears.

It should be noted here that the first-order memory function is regular in the low-temperature phase. Therefore it will not change the long-time asymptotic result of the zeroth-order theory: spin–spin correlations decay as $t^{-1/2}$. In the absence of any reason to the contrary we shall assume that all the higher-order memory functions are regular.

In order to get explicit results at the first-order level one has to solve equations (24) and (28). Again, to calculate spin–spin correlations for all times we need the whole spectrum of the eigenvalues and eigenvectors of the Hessian (and other equilibrium correlations). On the other hand the calculation of the amplitude of the $t^{-1/2}$ tail is easier. To get the explicit expression for the tail amplitude we use approximations described in the previous section. First, we decompose the matrix of the spin correlations, then we neglect the off-diagonal term in the equations of motion for the amplitudes, and finally we use approximate expressions for the zeroth eigenvector.

3. Computer simulations

We performed a series of Glauber dynamics simulations of the SK model at temperatures T_c, $0.5T_c$ and $0.1T_c$ using the algorithm of Mackenzie and Young [10]. We used different equilibration times and sample sizes as described below.

We monitored the time-dependent spin–spin correlation function,

$$[\langle \sigma_i(t)\sigma_i(0)\rangle_{\mathrm{eq}}] = (1/N)\sum_i \langle \sigma_i(t)\sigma_i(0)\rangle_{\mathrm{eq}} \tag{30}$$

and its time derivative,

$$\frac{\mathrm{d}}{\mathrm{d}t}[\langle \sigma_i(t)\sigma_i(0)\rangle_{\mathrm{eq}}] = (1/N)\sum_i \langle (\tanh(\beta h_i(t)) - \sigma_i(t))\sigma_i(0)\rangle_{\mathrm{eq}}. \tag{31}$$

We monitored the derivative independently because, in contrast to the spin–spin correlation function, the derivative does decay to zero in the low-temperature phase. Thus it is easier to get a dynamic exponent out of the derivative.

There are two delicate issues in simulating low-temperature dynamics of spin glasses. The first concerns the size of the simulated system (i.e. finite sample size effects). The

second is whether the system has been well equilibrated. Of course these two issues are coupled together.

For a finite size sample there are transitions between different 'pure' [3] states that are absent in the thermodynamic limit. In particular, for an SK spin glass it was found [10] that there is a spectrum of relaxation times associated with transitions between different pure states that diverge like $\exp(cN^{1/4})$ where N is the number of spins. In addition, at zero external field there is an additional relaxation timescale proportional to $\exp(dN^{1/2})$ that is associated with reversal of all the spins.

It follows that, for a given sample size, the results of finite size simulations are representative of the thermodynamic limit results only for times much shorter than the above-mentioned relaxation times. Here we are presenting data for the correlation functions for times up to 100 Monte Carlo steps per spin (MCS). A comparison of this timescale, 100 MCS, with the finite-sample relaxation times obtained in [10] shows that our results should be representative of the thermodynamic limit results. In particular, we believe that, for our sample sizes and on the timescale of 100 MCS, we cannot see fluctuations associated with transitions between different states.

One should realize that, in addition to the finite size effects mentioned above there are other, more conventional, finite size effects. For example we found that the $t = 0$ value of the time derivative of the spin–spin correlation function at $T = 0.1$ decreases by about 10% as N increases between 3000 and 10 000.

The second issue deals with equilibration. This problem has been treated by a brute force method. We were most concerned with the lowest temperature ($T = 0.1T_c$) and performed detailed studies in this case. The approach was as follows: to establish the required equilibration time, $\tau_{\rm eq}$, we monitored the time derivative for a number of different equilibration times. We started with the largest sample size we could simulate ($N = 10\,000$) and used large numbers of samples ($n_{\rm sample} = 50$). We used equilibration times of 100, 1000, 10 000 and 100 000 MCS. The last one was the longest equilibration time we could achieve for this sample size. Next, we collected the data for the time derivative (31). For each case the data were collected (after equilibration) over time intervals of 500 MCS. It was clear from the resulting plot that there was a systematic difference between the results obtained with the two longest equilibration times. In addition, the difference was an increasing function of time. This was, of course, a clear signature of *aging* [6].

We should emphasize at this point that, strictly speaking, we are simulating off-equilibrium spin–spin correlations $\langle \delta\sigma(t_{\rm eq}+t)\delta\sigma(t_{\rm eq})\rangle$. In order to be able to compare our simulations with the theoretical predictions that result in time-dependent spin–spin correlations *in equilibrium* we have to make sure that the equilibration time $t_{\rm eq}$ is sufficiently large. Specifically, as discussed in [6, 14], only in the regime $0 \leqslant t \ll t_{\rm eq}$ is time-translational invariance (approximately) satisfied. Our operational criterion is that $\langle \delta\sigma(t_{\rm eq}+t)\delta\sigma(t_{\rm eq})\rangle$ should be independent of $t_{\rm eq}$.

Furthermore, we would like to point out that because of aging we cannot monitor equilibration by looking for a saturation of the total energy as a function of the equilibration time (the same comment applies to any single-time quantity).

Since we could not increase the equilibration time we switched to smaller samples. We used $N = 4000$ and $n_{\rm sample} = 100$. At this size we could extend the equilibration time up to 500 000 MCS. The results of the two runs ($\tau_{\rm eq} = 100\,000$ and $\tau_{\rm eq} = 500\,000$) are shown in figure 1. It seems now that the results are independent of the equilibration time up to $t \approx 40$. We believe that the difference between the two runs seen at the longest times ($50 \leqslant t \leqslant 100$) is associated with enormous sample-to-sample fluctuations rather than with too-short equilibration time.

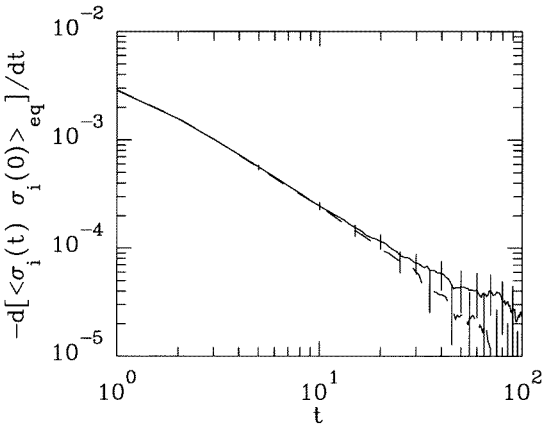

Figure 1. Time derivative of spin–spin correlation function at $T = 0.1T_c$. Sample size $N = 4000$, number of samples in each case, $n_{\text{sample}} = 100$. Broken curve: equilibration time, $\tau_{\text{eq}} = 100\,000$; full curve: $\tau_{\text{eq}} = 500\,000$. Error bars are plus/minus three standard deviations.

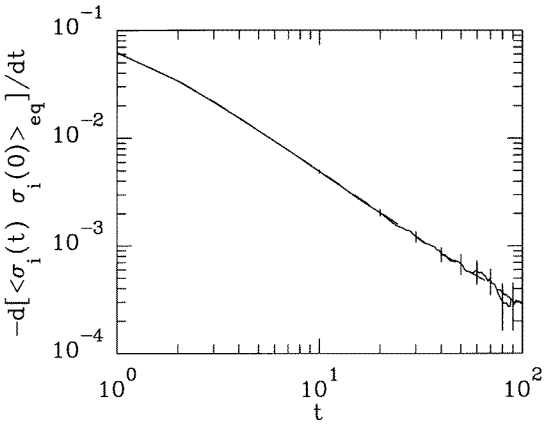

Figure 2. Time derivative of spin–spin correlation function at $T = 0.5T_c$. Broken curve: sample size $N = 3000$, number of samples, $n_{\text{sample}} = 200$, equilibration time, $\tau_{\text{eq}} = 10\,000$. Full curve: $N = 3000$, $n_{\text{sample}} = 30$, $\tau_{\text{eq}} = 50\,000$. Error bars are plus/minus three standard deviations.

We also studied time dependence of correlation functions at $T = 0.5T_c$. We used slightly smaller samples, $N = 3000$ larger number of samples, $n_{\text{sample}} = 200$, and an order of magnitude shorter equilibration time, $\tau_{\text{eq}} = 10\,000$. We also run $n_{\text{sample}} = 30$ samples of the same size with $\tau_{\text{eq}} = 50\,000$. The results were virtually identical, see figure 2. Thus we concluded that the $N = 3000$, $\tau_{\text{eq}} = 10\,000$ samples were well equilibrated.

Finally, for a comparison we also show the data for $T = T_c$. At this temperature we used $N = 3000$, $n_{\text{sample}} = 100$ and $\tau_{\text{eq}} = 10\,000$ MCS.

We should add that during some of the simulation runs we also collected the data for the equilibrium correlations that enter into the theoretical expression for the amplitude of the algebraic tail of the correlation function. The equilibrium data were collected (after equilibration) over time intervals of 500 or 1000 MCS.

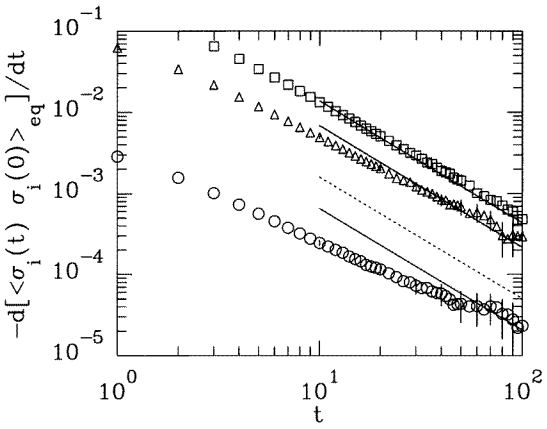

Figure 3. Time derivative of spin–spin correlation function at and below the transition temperature T_c. Symbols: Glauber dynamics simulation data; squares: $T = T_c$ (100 samples of 4000 spins each, $\tau_{eq} = 10\,000$); triangles: $T = 0.5T_c$ (30 samples of 4000 spins each, $\tau_{eq} = 50\,000$); circles: $T = 0.1T_c$ (100 samples of 4000 spins each, $\tau_{eq} = 500\,000$); full lines: long-time asymptotic decays predicted by the first-order approximation; dotted lines: first-order approximation predictions obtained by *neglecting* the correlations between the zeroth eigenvector of the Hessian and other equilibrium quantities. Error bars are plus/minus three standard deviations. Note that for the time derivative the present theory predicts $\sim t^{-3/2}$ decay.

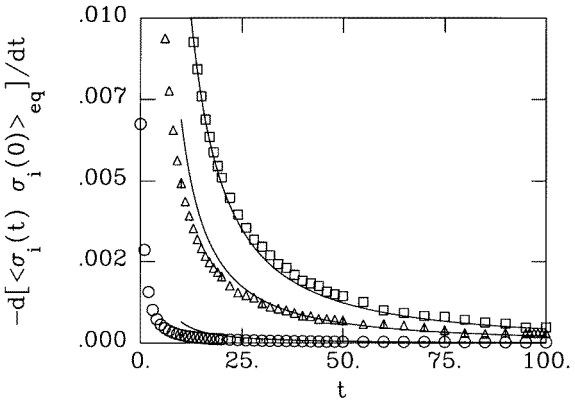

Figure 4. Linear–linear plot of the data of figure 5.

4. Comparison: theory versus simulations

In figures 3 and 4 we compare predictions of the first-order approximation with the results of the computer simulations. The theory describes correctly the temperature dependence of the amplitude of the long-time part of the time derivative of the spin correlations. The simulation results are consistent with a $t^{-3/2}$ tail in the derivative (and a $t^{-1/2}$ tail in the spin–spin correlations) at all three temperatures. However, considerable sample-to-sample fluctuations do not allow us to rule out a nonuniversal dynamic exponent.

Parenthetically, we would like to remark that had we assumed the eigenvectors of the Hessian to be uncorrelated we would have obtained equation (23) (and its generalization in the first-order approximation) for the long-time behaviour of the correlation function. As

shown in figure 3 (dotted line), at $T = 0.1T_c$ the amplitude of the derivative that results from neglecting these correlations exceeds the simulation data by a factor of about 2.5.

It should be noticed here that the simulation data *can* be fitted to power law decays with temperature-dependent exponents. For example, from $T = 0.1T_c$ data we obtain a $t^{-1.2}$ decay (of the time derivative of spin–spin correlations) for t between 4 and 20. However, it seems to us that in this time region one should not see the asymptotic exponent yet. Indeed, a power law fit to $T = T_c$ data in the same time region gives a $t^{-1.4}$ decay whereas the asymptotic exponent is equal to 1.5. Moreover, a full analytical calculation suggests that at $T = T_c$ the asymptotic behaviour is reached after about 30 MCS. We believe that at lower temperatures the asymptotic behaviour is reached even later.

In our opinion, in order to obtain reliable estimates for the dynamic exponents one would have to extend the present simulations up to at least a few hundred MCS. This would require much longer equilibration times and more sample averaging. In addition sample size dependence would have to be carefully investigated: for short and intermediate times (when the sample-to-sample fluctuations are small) we see systematic size dependence. At $T = 0.1T_c$ the derivative of the spin–spin correlations decreases by about 10% as N increases between 3000 and 10 000; the effective exponent (for $4 \leqslant t \leqslant 20$) increases by about the same amount.

At present, our computational resources do not allow us to pursue the above described simulation program. It is our hope that this work will stimulate renewed interest in long-time dynamics of the hard-spin SK model.

5. Conclusions

We have presented here a theory for Glauber dynamics of the SK model. Within our theory at the nth level of approximation the dynamics of spin–spin correlations (in equilibrium) is described by a coupled set of equations involving, in addition to the spin–spin correlations, n irreducible memory matrices (memory functions). Under rather mild assumptions concerning *equilibrium* spin correlations only the diagonal elements of the memory matrices contribute. Furthermore, both the initial values and the relaxation times for the memory matrices are finite. It thus seems that, at all levels, irreducible memory functions do not change the Glauber dynamics of hard spins qualitatively, and that the dynamic exponent is equal to that predicted by the zeroth-order approximation. This has to be contrasted with Langevin dynamics of the soft-spin SK model where, according to Sompolinski and Zippelius [5], the memory function (i.e. the self-energy) slows down the dynamics qualitatively and leads to a nonuniversal dynamic exponent.

Unlike in the high temperature phase, below T_c the zeroth-order equation of motion cannot be solved exactly. Our approximate solution leads to a universal dynamic exponent equal to $\frac{1}{2}$.

To check the theory we performed extensive Glauber dynamics simulations of the SK model. We showed that the theory predicts correctly the amplitude of the long-time decay of the spin–spin correlations (note that the theory, by construction, reproduces exactly the short-time behaviour of the spin–spin correlations). However, the simulations were not able to distinguish between a universal exponent and a temperature-dependent one.

Acknowledgments

I would like to thank Marshall Fixman for stimulating discussions. This work was partially supported by NSF grant no CHE-9624596.

References

[1] Szamel G 1998 *J. Phys. A: Math. Gen.* **31** 10 045
[2] Sherrington D and Kirkpatrick S 1975 *Phys. Rev. Lett.* **35** 1972
Kirkpatrick S and Sherrington D 1978 *Phys. Rev.* B **17** 4384
[3] Binder K and Young A P 1986 *Rev. Mod. Phys.* **58** 801
[4] Fisher K H and Hertz J A 1991 *Spin Glasses* (Cambridge: Cambridge University Press)
[5] Sompolinsky H and Zippelius A 1981 *Phys. Rev. Lett.* **47** 359
Sompolinsky H and Zippelius A 1982 *Phys. Rev.* B **25**
[6] See, e.g. Cugliandolo L F and Kurchan J 1994 *J. Phys. A: Math. Gen.* **27** 5749
[7] Kinzel W and Fisher K H 1977 *Solid State Commun.* **23** 687
[8] Fisher K H 1983 *Solid State Commun.* **46** 309
[9] Coolen A C C and Sherrington D 1993 *Phys. Rev. Lett.* **71** 3886
Coolen A C C and Sherrington D 1994 *J. Phys. A: Math. Gen.* **27** 7687
Laughton S N, Coolen A C C and Sherrington D 1996 *J. Phys. A: Math. Gen.* **29** 763
[10] Mackenzie N D and Young A P 1983 *J. Phys. C: Solid State Phys.* **16** 5321
[11] Sommers H J 1987 *Phys. Rev. Lett.* **58** 1268
[12] Łusakowski A 1991 *Phys. Rev. Lett.* **66** 2543
[13] Marinari E, Parisi G and Rossetti D *Preprint*
[14] See also Cugliandolo L F and Kurchan J 1993 *Phys. Rev. Lett.* **71** 173
[15] Mori H 1965 *Prog. Theor. Phys.* **34** 399
[16] Kawasaki K 1966 *Phys. Rev.* **145** 224
Kawasaki K 1966 *Phys. Rev.* **148** 375
[17] Thouless D J, Anderson P W and Palmer R G 1977 *Phil. Mag.* **35** 593
[18] Bray A J and Moore M A 1979 *J. Phys. C: Solid State Phys.* **12** L441
[19] Kawasaki K 1995 *Physica* A **215** 61