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

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**Abstract.** Glauber dynamics of the Sherrington–Kirkpatrick spin-glass model in the hightemperature phase is studied using theory and computer simulations. The theoretical approach follows the spirit of Mori's continuous fraction expansion. Its predictions agree very well with the computer simulation results.

## 1. Introduction

The dynamical properties of the Sherrington–Kirkpatrick (SK) spin-glass model [1] have been a subject of continuous interest in recent years [2, 3]. Most of the theoretical studies considered Langevin dynamics of the soft-spin version of the SK model [4–6]. The softspin version, while showing very interesting dynamical properties [6], lacks the original motivation of the SK model: neither its statics nor its dynamics is exactly solvable. The results are obtained perturbatively with respect to the four-spin coupling constant u. To recover the Ising limit one has to let u approach infinity. In practice, this procedure allows one to analyse the long-time asymptotic behaviour of the spin correlations. It is not well suited to study the time dependence for all times (even for  $T \ge T_c$ ) or to calculate the so-called absolute frequency scale.

Glauber dynamics of the hard-spin version of the SK model has been analysed in the original SK paper [1] and in other early spin-glass publications [7]. These works used an *ad hoc* method to introduce a dynamical version of the Onsager reaction field term into the equations of motion. A more systematic approach was started by Sommers [8]. However, his method was criticized by Łusakowski [9] and its validity is uncertain. Recently a novel approach to Glauber dynamics of spin glasses has been proposed by Coolen, Sherrington *et al* [10, 11]. The simple version of their theory [10] describes very well the order parameter *flow direction* above the de Almeida–Thouless (AT) [12] line but misses the *slowing down* which sets in when the former line is approached from above. The more advanced version [11] agrees well with the simulation data for short times but it remains to be seen whether it predicts divergent relaxation times at and below the AT line. In another interesting recent study Nishimori and Yamana [13] analysed Glauber dynamics of the SK model via a high-temperature expansion. Their method has an obvious virtue of a systematic expansion in a small parameter. However, it cannot be applied near or below the spin-glass transition.

The original motivation for the work presented here was to improve upon the simple CS theory [10]. Briefly, we have noticed that the simple CS theory is quite similar in spirit to the Enskog kinetic theory of hard sphere fluids [14]. We expected that by using kinetic theory techniques we might be able to incorporate divergence of the relaxation times

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into the CS theory. It turned out that a more efficient way to proceed was to depart from one of the ingredients of the CS theory: while CS derive equations of motion for sampleaveraged quantities we postpone sample averaging until after the equations of motion are solved. It should be emphasized that in all other respects our zeroth-order approximation follows the spirit of the Enskog theory (and that of the simple CS theory). In the first-order approximation we include terms that would be analogous to ring and repeated ring terms in the kinetic theory.

Because we are dealing with sample-dependent quantities the structure of our theory is more complicated than that of the CS theory. Therefore we restrict ourselves to studying time-dependent spin correlations *in equilibrium*.

Elsewhere we have presented a derivation that parallels closely the kinetic theory analysis [15]. This approach seems feasible only in the high-temperature regime. In order to analyse the low-temperature dynamics we have reformulated the theory in the spirit of Mori's [16] continuous fraction expansion. Here we present a derivation of the basic equations and an application to the high-temperature phase. In the following paper [17] we analyse dynamics in the low-temperature phase.

# 2. Theory

## 2.1. Definitions

The hard-spin 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  $P(J_{ij}) \sim \exp(-J_{ij}^2/(2J^2/N))$ .

The time-dependent spin-spin correlations can be written in the following form:

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

Here  $\delta \sigma_i$  is the fluctuation of the value of the *i*th local spin,  $\delta \sigma_i = \sigma_i - \langle \sigma_i \rangle_{eq}$  and  $\langle \cdots \rangle_{eq}$  denotes the equilibrium ensemble average with the Boltzmann distribution,

$$\langle \cdots \rangle_{\text{eq}} \equiv \sum_{\sigma_1, \sigma_2, \dots} \dots P_{\text{eq}} \qquad P_{\text{eq}} \sim \exp(-\beta H).$$
 (3)

Finally,  $\Omega$  is the evolution operator

$$\Omega = -\sum_{i} (1 - S_i) w_i \tag{4}$$

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

$$w_i = (1 - \sigma_i \tanh(\beta h_i))/2 \tag{5}$$

where  $h_i$  is a local magnetic field acting on the *i*th spin

$$h_i = \sum_{j \neq i} J_{ij} \sigma_j. \tag{6}$$

Note that in equation (2) the equilibrium probability distribution  $P_{eq}$  stands to the right of the quantity being averaged and the evolution operator  $exp(\Omega t)$  acts on everything to its right (including the probability distribution).

## 2.2. Zeroth-order approximation

To calculate the time-dependent spin–spin correlation function we follow the spirit of Mori's [16] continuous fraction expansion. In the zeroth-order approximation we restrict ourselves to the subspace spanned by the spin fluctuations. We define a projection operator on this subspace

$$\mathcal{P}_0 f(\sigma_1, \sigma_2, \ldots) = \sum_{ij} \delta \sigma_i A_{ij} \langle \delta \sigma_j f(\sigma_1, \sigma_2, \ldots) \rangle_{\text{eq}}.$$
(7)

Here the matrix A is the inverse matrix of spin correlations that is defined by the following equation:

$$\sum_{j} A_{ij} \langle \delta \sigma_j \delta \sigma_k \rangle_{\text{eq}} = \delta_{ik}.$$
(8)

Note that A is equal to the Hessian of the TAP [18] free energy. At and above  $T_c$  A is known explicitly [19, 2]:

$$A_{ij} = -\beta J_{ij} + \delta_{ij} (1 + (\beta J)^2).$$
(9)

We start by writing down a formal expression for the time derivative of the spin-spin correlations

$$\partial_t \langle \delta \sigma_i(t) \delta \sigma_j \rangle_{\text{eq}} = \langle \delta \sigma_i \Omega \exp(\Omega t) \delta \sigma_j \rangle_{\text{eq}}.$$
(10)

Next, we insert into it the identity operator written as a sum of the projection  $\mathcal{P}_0$  and the orthogonal projection  $\mathcal{Q}_0 = \mathcal{I} - \mathcal{P}_0$ 

$$\left\langle \delta \sigma_i \Omega \exp(\Omega t) \delta \sigma_j \right\rangle_{\text{eq}} = \left\langle \delta \sigma_i \Omega \left( \mathcal{P}_0 + \mathcal{Q}_0 \right) \exp(\Omega t) \delta \sigma_j \right\rangle_{\text{eq}}.$$
(11)

In the zeroth-order approximation we neglect the contribution involving  $Q_0$ . Then, using the definition of the projection operator  $\mathcal{P}_0$  we get

$$\partial_t \langle \delta \sigma_i(t) \delta \sigma_j \rangle_{\rm eq} = \sum_{kl} \langle \delta \sigma_i \Omega \delta \sigma_k \rangle_{\rm eq} A_{kl} \langle \delta \sigma_l(t) \delta \sigma_j \rangle_{\rm eq}.$$
(12)

Finally, using the explicit form of the evolution operator we rewrite the above result in the following way:

$$\partial_t \langle \delta \sigma_i(t) \delta \sigma_j \rangle_{\text{eq}} = -(1 - \langle \sigma_i \tanh(\beta h_i) \rangle_{\text{eq}}) \sum_l A_{il} \langle \delta \sigma_l(t) \delta \sigma_j \rangle_{\text{eq}}.$$
 (13)

This equation is equivalent to a disorder-dependent version of the local equilibrium approximation of Kawasaki [20]. It is identical to the evolution equation obtained from the zeroth-order kinetic theory [15].

One sees immediately that the evolution equation (12) with the Hessian (9) is almost identical to that derived in the original SK paper [1]. It should be emphasized, however, that a dynamical version of the Onsager reaction field term has been naturally included in the matrix A.

Straightforward calculation shows that the sample-averaged solution of (12) has the same form as the sample-averaged solution of the SK equation if the timescale of SK is rescaled by a factor

$$\tau = 1/(1 - \overline{\langle \tanh(\beta h)\sigma\rangle_{eq}}).$$
(14)

Here the overline denotes the 'spatial average':  $\overline{f} = (1/N) \sum_{i} f_{i}$ . Explicitly, we find

$$[\langle \delta\sigma_i(t)\delta\sigma_i(0)\rangle_{\rm eq}] = \frac{2}{\pi} \int_{-1}^1 dx \, \frac{(1-x^2)^{1/2}}{1+(\beta J)^2 - 2\beta Jx} \exp\left(-(1+(\beta J)^2 - 2\beta Jx)\frac{t}{\tau}\right).$$
(15)

Here [...] denotes sample averaging over the probability distribution  $P(J_{ij})$ . Note that in order to get the above result we have used the usual approximation that the eigenvectors of the Hessian are uncorrelated.

As discussed by SK [1] the formula (15) leads to the algebraic  $t^{-1/2}$  decay of the spin correlations at the transition temperature  $T_c = J$ . Note that the prefactor of the  $t^{-1/2}$  term is *different* from that predicted by SK.

The factor (14) can be calculated using the probability distribution of the local fields calculated in [21]. Explicitly, we get

$$\tau^{-1} = 1 - [\langle \tanh^2(\beta h) \rangle_{eq}] = 1 - \frac{1}{J\sqrt{2\pi}} \int_{-\infty}^{\infty} dh \, \tanh^2(\beta h) \cosh(\beta h) \exp(-\beta^2 J^2/2 - h^2/2J^2).$$
(16)

Note that here we have implicitly used the usual approximation of replacing the spatial average by the sample average.

We will compare the theoretical prediction (15) with the simulations in section 4. Here we only note that at  $T = T_c$  numerical integration gives  $\tau \approx 2.2242$  which roughly corresponds to the discrepancy between the original SK result (equation (15) with  $\tau = 1$  or equation (5.27) of [1]) and the simulation data they presented (figure 13(c) of [1]).

Finally, it should be noticed here that the zeroth-order approximation is exact at short times. More precisely, equation (13) reproduces exactly the first time-derivative of the spin correlations at t = 0. This is of course analogous to the simple CS theory being exact at short times.

#### 2.3. First-order approximation

In order to go beyond the zeroth-order theory we first use the standard projection operator manipulations [22] in order to rewrite the exact evolution equation (11) in the following way:

$$\int_{0}^{t} \sum_{j} (\delta_{ij}\delta(t-t') + M_{ij}^{irr}(t-t')\langle 1 - \sigma_{j} \tanh(\beta h_{j})\rangle_{eq}^{-1}) \partial_{t'} \langle \delta\sigma_{j}(t')\delta\sigma_{k}\rangle_{eq}$$
  
=  $-\langle 1 - \sigma_{i} \tanh(\beta h_{i})\rangle_{eq} \sum_{l} A_{il} \langle \delta\sigma_{l}(t)\delta\sigma_{j}\rangle_{eq}.$  (17)

Here  $M^{irr}$  is the *irreducible* [22] memory matrix

$$M_{ij}^{\rm irr}(t) = \langle D_i \exp(\mathcal{Q}_0 \Omega^{\rm irr} \mathcal{Q}_0 t) D_j \rangle_{\rm eq}$$
<sup>(18)</sup>

with  $D_i$  defined as

$$D_i = -\mathcal{Q}_0(\sigma_i - \tanh(\beta h_i)) \tag{19}$$

and  $\Omega^{irr}$  is the irreducible part of the evolution operator,

$$\Omega^{\rm irr} = \Omega - \sum_{ij} \Omega \delta \sigma_i \rangle_{\rm eq} [\langle \delta \sigma_i \Omega \delta \sigma_j \rangle_{\rm eq}]^{-1} \langle \delta \sigma_j \Omega.$$
<sup>(20)</sup>

 $D_i$  can be interpreted as the *part of the time derivative* of the *i*th spin fluctuation that is *orthogonal* to all the spin fluctuations. To this end we have to define a conjugate evolution operator  $\Omega^*$ 

$$\Omega^* = -\sum_i w_i (1 - S_i) \tag{21}$$

that acts on the spin variables, and then we check that the time derivative of  $\delta \sigma_i$  is given by the following expression:

$$\partial_t \delta \sigma_i = \Omega^* \delta \sigma_i = -(\sigma_i - \tanh(\beta h_i)). \tag{22}$$

It should be emphasized here that the formal manipulations leading to the evolution equation (17) have a simple physical interpretation [22]: the irreducible memory matrix renormalizes the *inverse rate* of spin flips.

In the zeroth-order approximation we neglected the renormalization of the inverse rate completely. In the next step (first-order approximation) we include it approximately. To this end we first define a projection operator on the subspace spanned by  $D_i$ 

$$\mathcal{P}_1 f(\sigma_1, \sigma_2, \ldots) = \sum_{ij} D_i C_{ij} \langle D_j f(\sigma_1, \sigma_2, \ldots) \rangle_{\text{eq}}.$$
(23)

Here C is the inverse matrix of the correlations of the projected time derivatives

$$\sum_{j} C_{ij} \langle D_j D_k \rangle_{\text{eq}} = \delta_{ik}.$$
(24)

Next, we write down a formal expression for the time derivative of the memory function and insert into it the identity operator written as a sum of the projection  $\mathcal{P}_1$  and the orthogonal projection  $\mathcal{Q}_1 = \mathcal{I} - \mathcal{P}_1$ 

$$\partial_t M_{ij}^{\text{irr}}(t) = \langle D_i \mathcal{Q}_0 \Omega^{\text{irr}} \mathcal{Q}_0 \exp(\mathcal{Q}_0 \Omega^{\text{irr}} \mathcal{Q}_0 t) D_j \rangle_{\text{eq}} = \langle D_i \mathcal{Q}_0 \Omega^{\text{irr}} \mathcal{Q}_0 (\mathcal{P}_1 + \mathcal{Q}_1) \exp(\mathcal{Q}_0 \Omega^{\text{irr}} \mathcal{Q}_0 t) D_j \rangle_{\text{eq}}.$$
(25)

In the first-order approximation we neglect the contribution involving  $Q_1$ 

$$\partial_t M_{ij}^{\rm irr}(t) \approx \langle D_i \mathcal{Q}_0 \Omega^{\rm irr} \mathcal{Q}_0 \mathcal{P}_1 \exp(\mathcal{Q}_0 \Omega^{\rm irr} \mathcal{Q}_0 t) D_j \rangle_{\rm eq}.$$
(26)

Then, using the definition of the projection operator  $\mathcal{P}_1$ , we get

$$\partial_t M_{ij}^{\rm irr}(t) = \sum_{kl} \langle D_i Q_0 \Omega^{\rm irr} Q_0 D_k \rangle_{\rm eq} C_{kl} M_{kj}^{\rm irr}(t).$$
<sup>(27)</sup>

At this point we note that in the high-temperature limit the off-diagonal equilibrium correlations between *irreducible* quantities (i.e. quantities that have spin correlations subtracted out) are of higher order in  $N^{-1/2}$  than the spin–spin correlations. This can be easily shown by a high-temperature expansion.

Moreover, it can also be shown that the off-diagonal part of the memory matrix evolution operator  $\langle D_i Q_0 \Omega^{irr} Q_0 D_j \rangle_{eq}$ ,  $i \neq j$ , can be neglected in the thermodynamic limit. Hence, only the diagonal part

$$\langle D_i \mathcal{Q}_0 \Omega^{\mathrm{irr}} \mathcal{Q}_0 D_i \rangle_{\mathrm{eq}} = -(\beta J)^2 \overline{\langle 1 - \tanh^2(\beta h) \rangle_{\mathrm{eq}}} (\langle \tanh^4(\beta h_i) \rangle_{\mathrm{eq}} - \langle \tanh^2(\beta h_i) \rangle_{\mathrm{eq}}^2)$$
(28)

is relevant.

Finally we see that in the first-order approximation only the diagonal elements of the memory matrix contribute and, moreover, that their time evolution is given by

$$\partial_t M_{ii}^{\rm irr}(t) = \langle D_i \mathcal{Q}_0 \Omega^{\rm irr} \mathcal{Q}_0 D_i \rangle_{\rm eq} C_{ii} M_{ii}^{\rm irr}(t)$$
<sup>(29)</sup>

where

$$M_{ii}^{\rm irr}(t=0) = C_{ii}^{-1} = \langle 1 - \tanh^2(\beta h_i) \rangle_{\rm eq} (1 - A_{ii} \langle 1 - \tanh^2(\beta h_i) \rangle_{\rm eq}).$$
(30)

Equations (17) and (29) with (28) and (30) constitute our first-order approximation. In the high-temperature regime it is actually possible to go beyond the first-order approximation. The structure of the theory remains the same: at any higher order level a new (diagonal) irreducible memory matrix appears.

It should be noted here that one should not expect any divergence of the memory function relaxation time at the transition temperature:  $\langle D_i Q_0 \Omega^{irr} Q_0 D_i \rangle_{eq}$  stays positive and  $C_{ii}$  does not approach 0 as  $T \to T_c$ .

To get explicit results from the first-order approximation we have to solve a system of equations (17) and (29). In the high-temperature phase we *pre-average* equation (29) to get

$$\partial_t \overline{M^{\text{irr}}}(t) = \overline{\langle DQ_0 \Omega^{\text{irr}} Q_0 D \rangle_{\text{eq}}} \overline{C} \overline{M^{\text{irr}}}(t)$$
 (31)

with

$$\overline{M^{\rm irr}}(t=0) = \overline{\langle 1 - \tanh^2(\beta h) \rangle_{\rm eq}} (1 - (1 + (\beta J)^2) \overline{\langle 1 - \tanh^2(\beta h) \rangle_{\rm eq}})$$
(32)

and then we use the pre-averaged irreducible memory function in equation (17). The main argument for the pre-averaging is analytical simplicity. However, we expect that in the high-temperature phase pre-averaging should be justifiable.

Equations (17) and (31) can be easily solved. We find that the first-order approximation results in a minute correction of the zeroth-order one. This fact could have been anticipated: numerical integration using the local field distribution of [21] shows that at the transition temperature  $\overline{M^{\text{irr}}}(t=0) \approx 0.045$ .

# 3. Computer simulations

We performed a series of Glauber dynamics simulations of the SK model at temperatures  $2T_c$ ,  $1.5T_c$ ,  $1.25T_c$ , and  $T_c$  using the algorithm of Mackenzie and Young [23]. Above the transition temperature we used equilibration times varying between 100 Monte Carlo steps per spin (MCS) at  $2T_c$  and 200 MCS at  $1.25T_c$ . At the transition temperature we used very long equilibration time of 10000 MCS. We used sample sizes of N = 3000: at each temperature we simulated 100 samples.

After equilibrating the system we collected the data for the time-dependent spin-spin correlation function

$$[\langle \sigma_i(t)\sigma_i(0)\rangle_{\rm eq}] = (1/N)\sum_i \langle \sigma_i(t)\sigma_i(0)\rangle_{\rm eq}$$
(33)

and for its time derivative, i.e. for the following correlation function:

$$\frac{\mathrm{d}}{\mathrm{d}t}[\langle \sigma_i(t)\sigma_i(0)\rangle_{\mathrm{eq}}] = (1/N)\sum_i \langle (\tanh(\beta h_i(t)) - \sigma_i(t))\sigma_i(0)\rangle_{\mathrm{eq}}.$$
(34)

We monitored the derivative independently having in mind the low-temperature phase: in contrast to the correlation function the derivative decays to zero even in the low-temperature phase.

### 4. Results and discussion

In figure 1 we compare time-dependent spin correlations calculated from the first-order theory with the results of the computer simulations. On the scale of the figure the predictions of the zeroth-order theory are indistinguishable from those of the first order.

In figure 2 we compare the time derivative of the spin correlations calculated from the first-order theory with the results of the computer simulations. Again, on the scale of the figure the predictions of the zeroth-order theory are indistinguishable from those of the first order.



**Figure 1.** Time-dependent spin–spin correlation function as a function of time. Symbols: Glauber dynamics simulation data; squares:  $T = 2T_c$ ; circles:  $T = 1.5T_c$ ; triangles:  $T = 1.25T_c$ ; crosses:  $T = T_c$ . Solid lines: predictions of the first-order theory.



**Figure 2.** Time derivative of the spin–spin correlation function. Symbols: Glauber dynamics simulation data; squares:  $T = 2T_c$ ; circles:  $T = 1.5T_c$ ; triangles:  $T = 1.25T_c$ ; crosses:  $T = T_c$ . Solid lines: predictions of the first-order theory.

Qualitatively *and* quantitatively there is perfect agreement between the theory and simulations. It should be emphasized here that it is the first time such an agreement has been achieved for the time-dependent spin correlations, even in the high-temperature phase.

It should also be realized that in spite of this quantitative agreement the first-order theory is *not* exact. There is an infinite number of higher-order irreducible memory functions and we do not have any argument that would allow us to neglect them. In this regard it seems that, even in the high-temperature phase, dynamics of the SK model is much more complicated than its equilibrium properties.

Finally, we would like to comment on the relation between our theory and the simple

CS approach [10]. CS, in effect, use a *local in time* closure hypothesis in the evolution equations for the sample-averaged quantities. If we were to derive an equation of motion for the sample averaged spin–spin correlation function from the zeroth-order approximation (equation (13)), our closure approximation would be *non-local* in time. Hence, we do not disagree with the main CS assumption that (certain) dynamic quantities are self-averaging and therefore it should be possible to derive equations of motion that would involve sample-averaged quantities only. On the other hand, we suspect that these equations of motion might be non-local in time. One should note at this point that the equations of motion for the time-dependent correlations that are derived in the soft-spin approach are, in fact, non-local in time.

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