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Kinetic theory approach to the SK spin glass model with Glauber dynamics

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Abstract. A new method to analyse Glauber dynamics of the Sherrington–Kirkpatrick (SK) spin glass model is presented. The method is based on ideas used in the classical kinetic theory of fluids. It is applied to study spin correlations in the high-temperature phase ($T \geqslant T_c$) of the SK model at zero external field. The zeroth-order theory is equivalent to a disorder-dependent local equilibrium approximation. Its predictions agree well with computer simulation results. The first-order theory involves coupled evolution equations for the spin correlations and the dynamic (excess) parts of the local field distributions. It qualitatively accounts for the error made in the zeroth approximation.

The dynamical properties of the Sherrington–Kirkpatrick (SK) spin glass model [1] have been a subject of continuous interest [2]. However, almost all the theoretical studies considered Langevin dynamics of the soft-spin version of the SK model [3–5]. The soft-spin version, while showing very interesting dynamical properties [5], lacks the original motivation of the SK model: neither its statics nor its dynamics is exactly solvable†. The Glauber dynamics of the SK model was studied by Sommers [6]. He recovered the results found previously for the Langevin dynamics. Sommers' method was criticized by Łusakowski [7] and its validity is uncertain‡. Recently a novel approach to Glauber dynamics of spin glasses has been proposed by Coolen, Sherrington, and coworkers (CS) [9, 10]. The simple version of their theory [9] describes very well the order parameter *flow direction* above the de Almeida–Thouless (AT) [11] line but misses the *slowing down* which sets in when the former line is approached from above. The more advanced version [10] 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.

Here we reconsider the Glauber dynamics of the SK model. The original motivation for this work was to improve the simple CS theory [9]. However, the resulting method is very different from that of CS.

CS tried to derive a general description of the SK spin glass dynamics. The theory presented here is more restricted: one studies time-dependent spin correlations *in equilibrium*

† The results are obtained perturbatively with respect to the four spin coupling 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 $T \geqslant T_c$) or to calculate the so-called absolute frequency scale.

‡ Note that in a so-called spherical SK model the Langevin and Monte Carlo dynamics lead to *different* results [8].

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in the high-temperature phase ($T \geqslant T_c$) at zero external field. The main motivation is simplicity: it is possible to derive explicit results for these correlations, and it is easy to perform accurate computer simulations that allow one to test the theoretical predictions.

Following an approach used in the kinetic theory [12], we express the correlation functions in terms of a distribution that satisfies the master equation and a specific initial condition. Next, we propose a series of approximations for this distribution that are motivated by the approximations used in the kinetic theory [13]. Successive approximations gradually include *dynamic* many-spin correlations. The static correlations are retained at every step.

The approximations are formulated for a given sample of the coupling constants. The averaging over the samples is postponed until after the resulting evolution equations are solved.

The simplest (zeroth order) approximation is equivalent to a *disorder-dependent* version of the local equilibrium approximation [14]. It leads to very simple equations of motion for the spin correlations: the relaxation matrix is a product of a relaxation rate (kinetic coefficient), τ^{-1}, that is finite at the transition temperature, T_c, and an inverse matrix of equilibrium spin correlations, A_{ij}, or the Hessian of the Thouless–Anderson–Palmer (TAP) [15] free energy. The Hessian acquires zero eigenvalues at T_c [16]. This results in a mean-field-like critical slowing down of the time-dependent correlations when T_c is approached from above and an algebraic decay $\sim t^{-1/2}$ at T_c. A comparison with the simulation data shows that the zeroth-order approximation is surprisingly accurate.

The first-order approximation takes into account *dynamic* correlations between spins and the distributions of the local fields acting on these spins: it includes time-delayed Onsager reaction fields.

The first-order approximation accounts qualitatively for the error made in the zeroth order: the predicted *difference* between the full correlations and the zeroth-order approximation is about 40% of the simulation result.

We now sketch the derivation of the results. We consider the Glauber dynamics for the SK model of a spin glass. The time evolution is given by the master equation for the spin probability distribution $P(\boldsymbol{\sigma}; t)$,

$$\partial P(\boldsymbol{\sigma}; t)/\partial t = -\sum_i (1 - S_i) w_i(\boldsymbol{\sigma}) P(\boldsymbol{\sigma}; t). \tag{1}$$

Here $\boldsymbol{\sigma} \equiv \{\sigma_1, \ldots, \sigma_N\}$ denotes the spin configuration, S_i is the spin-flip operator, $S_i \sigma_i = -\sigma_i$, and $w_i(\boldsymbol{\sigma})$ is the transition rate, $w_i(\boldsymbol{\sigma}) = (1 - \sigma_i \tanh(\beta h_i))/2$, with h_i being a local magnetic field acting on the ith spin, $h_i = \sum_{j \neq i} J_{ij} \sigma_j$. The J_{ij} are the exchange coupling constants that 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 correlations of the total magnetization in equilibrium, $(1/N)[\langle m(t) m(0) \rangle_{\mathrm{eq}}]$. Here $m(t) = \sum_i \sigma_i(t)$ is the fluctuation of the magnetization (for $T \geqslant T_c$ at zero external field $\langle \sigma_i \rangle_{\mathrm{eq}} \equiv 0$), the angular brackets $\langle \ldots \rangle_{\mathrm{eq}}$ denote the equilibrium ensemble average, and the square brackets $[\ldots]$ denote the sample averaging over the distribution of J_{ij}'s.

The sample averaging will be performed as the last stage of the analysis. Therefore, for the most part we deal with sample-dependent quantities such as $\langle \sigma_i(t) m(0) \rangle_{\mathrm{eq}}$. This is analogous to the TAP [15] analysis of the equilibrium SK model and early work [1, 17] on the Glauber dynamics of the SK model. It is different from the CS approach and also from most of the other approaches to both Langevin [3–5] and Glauber [6] dynamics.

The correlations $\langle \sigma_i(t) m(0) \rangle_{\mathrm{eq}}$ are defined in terms of a conditional distribution $P(\boldsymbol{\sigma}; t | \boldsymbol{\sigma}')$ and the equilibrium distribution $P_{\mathrm{eq}}(\boldsymbol{\sigma})$ [18]. We define a distribution $P_m(\boldsymbol{\sigma}; t)$

as

$$P_m(\boldsymbol{\sigma};t) \equiv \sum_{\boldsymbol{\sigma}'} P(\boldsymbol{\sigma};t|\boldsymbol{\sigma}')\left(\sum_j \sigma_j'\right) P_{\rm eq}(\boldsymbol{\sigma}'). \tag{2}$$

The distribution P_m satisfies the master equation (1) and the initial condition $P_m(\boldsymbol{\sigma};t=0) = P_{\rm eq}(\boldsymbol{\sigma})\sum_i \sigma_i$†.

The time-dependent spin correlations in equilibrium $\langle\sigma_i(t)m(0)\rangle_{\rm eq}$ can be calculated as averages over P_m,

$$\langle\sigma_i(t)m(0)\rangle_{\rm eq} = \sum_{\boldsymbol{\sigma}} \sigma_i P_m(\boldsymbol{\sigma};t) = \langle\sigma_i\rangle(t). \tag{3}$$

Hereafter $\langle\ldots\rangle(t)$ denotes the average over the time-dependent distribution P_m. In the following a series of approximations for this distribution is proposed.

In the zeroth approximation, we assume that $P_m(t)$ can be expressed in terms of the single-spin averages, $\langle\sigma_i\rangle(t)$. More precisely, we assume that P_m has the same form as an equilibrium distribution for the system in an external field with the field chosen in such a way that the single-spin averages have correct values. Explicitly,

$$P_m(\boldsymbol{\sigma};t) \approx P_{\rm eq}(\boldsymbol{\sigma}) \sum_i \sigma_i b_i(t) \tag{4}$$

where fields $b_i(t)$, $i = 1,\ldots$ satisfy the following equations,

$$\langle\sigma_i\rangle(t) = \sum_k \langle\sigma_i\sigma_k\rangle_{\rm eq} b_k(t). \tag{5}$$

Solving equation (5) for the $b_k(t)$ gives

$$P_m(\boldsymbol{\sigma};t) \approx P_{\rm eq}(\boldsymbol{\sigma}) \sum_{ij} \sigma_i A_{ij} \langle\sigma_j\rangle(t). \tag{6}$$

Here the matrix A_{ij} is the inverse of the matrix of the equilibrium spin correlations, $\sum_j A_{ij}\langle\delta\sigma_j\delta\sigma_k\rangle_{\rm eq} = \delta_{ik}$. Note that A_{ij} is identical to the Hessian of the TAP free energy [15].

The ansatz (6) is similar to the local equilibrium approximation introduced by Kawasaki [14]. The new element of this work is to use the local equilibrium approximation for the *disorder-dependent* distribution P_m.

To derive the equations of motion for the spin averages, we start from the exact evolution equations,

$$\partial\langle\sigma_i\rangle(t)/\partial t = -\langle\sigma_i\rangle(t) + \langle\tanh(\beta h_i)\rangle(t). \tag{7}$$

Then we use ansatz (6) to calculate the averages on the right-hand side of equations (7) and obtain

$$\frac{\partial\langle\sigma_i\rangle(t)}{\partial t} = (-1 + \langle\tanh(\beta h_i)\sigma_i\rangle_{\rm eq}) \sum_j A_{ij}\langle\sigma_j\rangle(t). \tag{8}$$

According to equations (8), the dynamics of the spin correlations follows a van Hove mean-field-like picture: the relaxation matrix is a product of the relaxation rate, $\tau^{-1} = 1 - \langle\tanh(\beta h_i)\sigma_i\rangle_{\rm eq}$, and the inverse matrix of the spin correlations (Hessian), A_{ij}. Each of equations (8) contains an Onsager correction term [1] that has been introduced phenomenologically in early works [1, 17]. Within the zeroth-order theory the correction term is *instantaneous*: the reaction field at a given time depends on the value of the spin average at the same time.

† Note that $P_m(t)$ is normalized to zero and therefore, strictly speaking, is not a *probability* distribution.

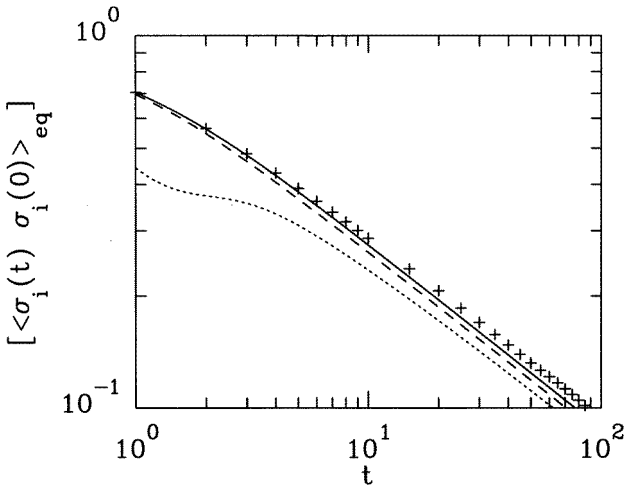

Figure 1. Spin correlation function at the transition temperature T_c. Crosses: Glauber dynamics simulation data; broken curve: the zeroth-order theory (local equilibrium approximation); full curve: the first-order approximation; dotted curve: the second-order Sommers' theory.

The relaxation rate can be calculated with the help of the equilibrium probability distribution of the local fields, $P_{\rm eq}(h)$ [19]. A numerical evaluation shows that at T_c the relaxation rate is finite. On the other hand, the Hessian, A_{ij}, acquires zero eigenvalues at the transition temperature [16] and this fact leads to a mean-field-like critical slowing down as T_c is approached from above. Moreover, at T_c one obtains asymptotically $[\langle\sigma_i\rangle(t)] \sim t^{-1/2}$.

In the high-temperature phase at zero external field, the Hessian is known explicitly:

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

It follows that the evolution equations (8) are almost identical to those derived in the original SK paper [1]. The solution has the same form as the solution of the SK equations if the timescale of SK is rescaled by factor τ.

Figure 1 compares the predictions of the zeroth-order theory with numerical simulations of the SK model at the transition temperature. 10 samples of $N = 10\,000$ spins each have been simulated using the algorithm of Mackenzie and Young [20]. A very long equilibration time of 10 000 Monte Carlo steps (MCS) per spin was used. Subsequently the data for the time-dependent correlation function $(1/N)\sum_i \langle\sigma_i(t)\sigma_i(0)\rangle_{\rm eq}$ were collected† and averaged over different time origins [21]. The figure indicates that the zeroth-order theory is quite accurate: its predictions differ from the simulation data by less than 11%. Figure 1 also plots the predictions of the second-order Sommers theory. They were obtained by solving explicitly equation (18) of [6], using the fluctuation-dissipation theorem to get the Laplace transform of the correlation function, and finally inverting the Laplace transform numerically [22].

Figure 2 plots the difference between the simulation data and the predictions of the zeroth-order theory. It is clear that the zeroth-order approximation is not exact. This fact can also be seen from an analysis of the short-time behaviour of the spin correlations: the zeroth-order theory exactly reproduces the first time derivative at $t = 0$ but *not* the second- and higher-order derivatives.

† To improve the statistics, we use the identity $(1/N)[\langle m(t)m(0)\rangle_{\rm eq}] = [\langle\sigma_i(t)\sigma_i(0)\rangle_{\rm eq}]$.

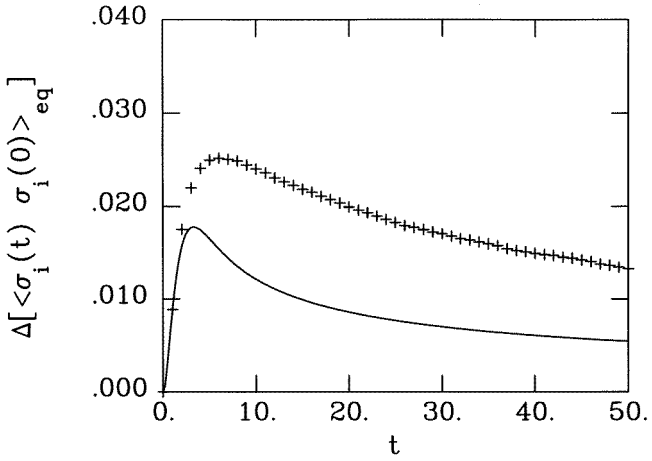

Figure 2. The difference between the full spin correlation function and the local equilibrium approximation at the transition temperature T_c. Crosses: Glauber dynamics simulation data; full curve: the first-order approximation.

To improve upon the zeroth-order theory it is necessary to go beyond the local equilibrium approximation and include *dynamic* correlations [13, 23]. It follows from the physics of the SK model and from the analysis of the short time expansion of the time-dependent spin correlations that the first additional set of variables to be included are the dynamic (excess) parts of the local field distributions, $\delta P_i(h;t)$†. They are defined as the differences between the true distributions and their values in the local equilibrium ensemble (6),

$$\delta P_i(h;t) = \langle \delta(h-h_i)\rangle(t) - \sum_{jk}\langle \delta(h-h_i)\sigma_j\rangle_{\rm eq} A_{jk}\langle\sigma_k\rangle(t). \tag{10}$$

At $t=0$ the excess parts vanish, $\delta P_i(h;t=0)=0$.

To derive equations of motion for the spin averages and the excess parts of the local field distributions we need an approximate expression for the distribution P_m in terms of $\langle\sigma_i\rangle(t)$ and $\delta P_i(h;t)$. We assume that P_m has the following form:

$$P_m(\boldsymbol{\sigma};t) \approx P_{\rm eq}(\boldsymbol{\sigma})\left(\sum_{ij}\sigma_i A_{ij}\langle\sigma_j\rangle(t) + \sum_{ij}\int {\rm d}h\,\delta^e(h-h_i)\int {\rm d}q\, C_{ij}(h,q)\delta P_j(q;t)\right). \tag{11}$$

Here $\delta^e(h-h_i)$ is the microscopic expression for the excess part of the local field distribution,

$$\delta^e(h-h_i) = \delta(h-h_i) - \sum_{jk}\langle\delta(h-h_i)\sigma_j\rangle_{\rm eq} A_{jk}\sigma_k \tag{12}$$

and $C_{ij}(h,q)$ is the inverse 'matrix' of the correlations of the excess local field distributions, $\sum_j \int {\rm d}q\, C_{ij}(h,q)\langle\delta^e(q-h_j)\delta^e(p-h_k)\rangle_{\rm eq} = \delta_{ik}\delta(h-p)$.

The form of distribution (11) is motivated by approximations used in the kinetic theory [13, 23]. Briefly, to obtain (11) we assume that $P_m(t)$ has the same form as an equilibrium distribution for the system in the presence of external perturbations that are chosen in such a way that, at a given time, the single-spin averages and the excess parts of the local field

† A similar additional variable was used in the more advanced version of the CS theory [10]. They, however, used disorder averaged quantities throughout.

distributions are $\langle\sigma_i\rangle(t)$ and $\delta P_i(h;t)$, respectively. Now we will show that with the help of (11) one can describe qualitatively the difference between the predictions of the local equilibrium approximation and the simulation data.

First, we derive the equations of motion for the spin averages. We start from the exact equations (7), use (11) to calculate averages, and obtain the following equations of motion,

$$\frac{\partial\langle\sigma_i\rangle(t)}{\partial t} = -\frac{1}{\tau}\sum_j A_{ij}\langle\sigma_j\rangle(t) + \int \mathrm{d}h\ \tanh(\beta h)\delta P_i(h;t). \tag{13}$$

Next, derive equations of motion for the excess parts of the local field distributions. To this end, start from exact evolution equations,

$$\frac{\partial\delta P_i(h;t)}{\partial t} = \left\langle\left[\sum_i w_i(\boldsymbol{\sigma})(1-S_i)\delta^e(h-h_i)\right]\right\rangle(t) \tag{14}$$

use distribution (11), and obtain

$$\begin{aligned}\frac{\partial\delta P_i(h;t)}{\partial t} &= -[(\beta J)^2\tanh(\beta h) - \beta h]P_{\mathrm{eq}}(h)\frac{\partial}{\partial t}\langle\sigma_i\rangle(t)\\ &\quad + \frac{(\beta J)^2}{\tau}\frac{\partial}{\partial\beta h}\int \mathrm{d}q\,[P_{\mathrm{eq}}(h)\delta(h-q) - P_{\mathrm{eq}}(h)P_{\mathrm{eq}}(q)]\\ &\quad \times\frac{\partial}{\partial\beta q}\int \mathrm{d}q'\,C_{ii}(q,q')\delta P_i(q';t)\end{aligned} \tag{15}$$

where $P_{\mathrm{eq}}(h)$ is the equilibrium local field distribution. To derive (15) we keep two-point equilibrium correlations, e.g. $\langle\sigma_i\sigma_j\rangle_{\mathrm{eq}}$, but neglect *higher-order connected* correlations involving *different* lattice sites, e.g. $\langle\delta^e(h-h_i)\delta^e(q-h_j)\rangle_{\mathrm{eq}}$ for $i\neq j$†.

According to equations (13), the reaction field consists of two parts: an instantaneous reaction, proportional to the spin average at the same time, and a time-delayed reaction. It follows from (15) that the delayed reaction field acting on the ith spin at a given time depends on the values of this spin at earlier times.

Solving formally equations (15) and substituting the result into equations (13) we obtain a set of effective equations of motion that involve only the single-spin averages. These equations have the same *structure* as the memory function equation derived recently by Kawasaki [24] for dissipative stochastic systems: the inverse frequency, τ, gets renormalized by inclusion of the dynamic correlations.

To derive explicit results for the time-dependent correlations, we solve the integro-differential equation (15) approximating $\delta P_i(h;t)$ by a finite sum of basic functions.

In figure 2 the theoretical predictions for the difference between the full spin correlations and the local equilibrium result are compared with the simulation data. The agreement is quantitative for short times (the first-order theory reproduces exactly first two time derivatives of the spin correlations at $t=0$) and qualitative at long times.

It is evident from figure 2, and it can be shown theoretically, that the first-order theory is not exact. Glauber dynamics of the SK model is more complicated than statics: in addition to (possibly time-delayed) Onsager reaction fields other *dynamic* correlations have to be included.

In summary, it has been shown that the ideas of the classical kinetic theory of fluids can be used to analyse Glauber dynamics of the SK spin glass model. The very simple disorder-dependent local equilibrium approximation leads to quantitatively accurate predictions for the spin correlations, at least in the high-temperature phase of the SK model. This fact

† It can be argued that the neglected correlations do not contribute in the thermodynamic limit.

suggests that *a* disorder-dependent approximation might be a good starting point in the search for a general theory of the SK model dynamics. Secondly, the error made in the zeroth approximation can be accounted for by including time-delayed Onsager reaction fields. The resulting theory can be improved further by incorporating more complicated dynamic correlations. Finally, the method presented here can be generalized to dynamics of neural networks and other Ising-like systems.

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