

Dynamical Probability Distribution Function of the SK Model at High Temperatures

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The microscopic probability distribution function of the Sherrington-Kirkpatrick (SK) model of spin glasses is calculated explicitly as a function of time by a high-temperature expansion. The resulting formula to the third order of the inverse temperature shows that an assumption made by Coolen, Laughton and Sherrington in their recent theory of dynamics is violated. Deviations of their theory from exact results are estimated quantitatively. Our formula also yields explicit expressions of the time dependence of various macroscopic physical quantities when the temperature is suddenly changed within the high-temperature region.

KEYWORDS: SK model, dynamics, high-temperature expansion, probability distribution function, equipartitioning

The dynamics of the Sherrington-Kirkpatrick (SK) model of spin glasses¹⁾ has been discussed for many years.²⁾ However, no explicit exact expressions of evolution equations have been given for macroscopic physical quantities such as the magnetization or susceptibility.

For a closely related problem, the dynamics of the Hopfield model of neural networks,³⁾ the situation is somewhat different. For a finite number of embedded patterns p , it is possible to write down a set of evolution equations of macroscopic order parameters explicitly.⁴⁻⁶⁾ If, on the other hand, the number of patterns p is proportional to the system size N , the problem is quite non-trivial and there has been no exact theory describing the time dependence of physical quantities.

Coolen and Sherrington (CS)^{7,8)} claimed to have derived the exact solution of this latter problem (in which p is proportional to N) using physical assumptions on the microscopic probability distribution function. They assumed that the microscopic probability distribution function is a constant within a subspace in which a limited number of macroscopic order parameters take fixed values. They called this property equipartitioning. In the equilibrium limit the equipartitioning holds trivially because the Boltzmann factor is a constant for a given value of the energy. In general non-equilibrium situations, however, it is not clear whether or not equipartitioning is a valid assumption. Ozeki and Nishimori⁹⁾ showed by Monte Carlo simulations that numerical data for the noise distribution function, in terms of which the time evolution of macroscopic quantities is determined, deviate from the predictions of CS. Thus the method of CS yields approximations, not exact results, for the dynamics of the Hopfield model. CS then applied the same idea to the SK model,¹⁰⁾ and discussed the dynamics in terms of approximate closed-form evolution equations of a few macroscopic order parameters.

The most recent development along this line is due to Coolen, Laughton and Sherrington (CLS).^{11,12)} This recent work is a sophistication of their previous method, using a continuous function instead of a few order param-

eters to describe the dynamics of the macroscopic state of the system. The basic assumption of equipartitioning of the microscopic probability distribution function remains essentially intact. More precisely, they assumed that the microscopic probability distribution function $p_t(\sigma)$ is a constant (i.e., it does not depend on the spin configuration σ) once the value of the single-site spin-field distribution function

$$D(\zeta, h) = \frac{1}{N} \sum_i \delta_{\zeta, \sigma_i} \delta(h - h_i) \quad (1)$$

is given, where the local field is

$$h_i(\sigma) = \sum_{j(\neq i)} J_{ij} \sigma_j. \quad (2)$$

They conjectured, based partly on comparison with numerical data, that this sophisticated version is either exact or a very good approximation.

In the present letter we solve the master equation of the SK model explicitly by a high-temperature expansion. The resulting formula for the microscopic probability distribution function shows that the assumption of equipartitioning is violated. Thus the CLS theory is not exact even in its sophisticated form. We derive quantitative estimations of deviations of their theory from exact results. We also show that our formula is useful for predicting the behavior of physical quantities after a sudden change of temperature within the high-temperature region.

The SK model is described by N Ising spins interacting with each other via random infinite-range interactions J_{ij} :

$$H(\sigma) = - \sum_{i < j} J_{ij} \sigma_i \sigma_j. \quad (3)$$

The J_{ij} represents quenched disorder the values of which are obtained independently from a Gaussian distribution with mean J_0/N and variance J^2/N . The microscopic probability distribution function $p_t(\sigma)$ obeys the master equation

$$\begin{aligned} & \frac{1}{p_t(\boldsymbol{\sigma})} \frac{d}{dt} p_t(\boldsymbol{\sigma}) \\ &= \frac{1}{p_t(\boldsymbol{\sigma})} \sum_k p_t(F_k \boldsymbol{\sigma}) w_k(F_k \boldsymbol{\sigma}) - \sum_k w_k(\boldsymbol{\sigma}). \end{aligned} \quad (4)$$

Here F_k is a single spin flip operator

$$F_k \Phi(\boldsymbol{\sigma}) \equiv \Phi(\sigma_1, \dots, -\sigma_k, \dots, \sigma_N)$$

and the transition rate is defined by

$$w_k(\boldsymbol{\sigma}) = \frac{1}{2} \{1 - \sigma_k \tanh \beta h_k(\boldsymbol{\sigma})\}. \quad (5)$$

The inverse temperature is denoted as β .

Let us solve the master equation (4) by a high-temperature expansion in the form

$$p_t(\boldsymbol{\sigma}) = \exp \{ \beta f_t(\boldsymbol{\sigma}) + \beta^2 g_t(\boldsymbol{\sigma}) + \beta^3 u_t(\boldsymbol{\sigma}) + \dots \} \quad (6)$$

under the initial condition

$$p_{t=0}(\boldsymbol{\sigma}) = \exp \{ -\beta_0 H(\boldsymbol{\sigma}) \}. \quad (7)$$

Normalization of the distribution function (6) is irrelevant for the following argument. Inserting eq. (6) into the master equation (4) and expanding the result in powers of β , we obtain the right-hand side of the master equation as

$$\begin{aligned} & \frac{1}{p_t(\boldsymbol{\sigma})} \sum_k p_t(F_k \boldsymbol{\sigma}) w_k(F_k \boldsymbol{\sigma}) - \sum_k w_k(\boldsymbol{\sigma}) \\ & \sim \sum_k \left\{ 1 + \beta \Delta_k f_t + \beta^2 \left(\frac{1}{2} (\Delta_k f_t)^2 + \Delta_k g_t \right) \right. \\ & \quad \left. + \beta^3 \left(\frac{1}{6} (\Delta_k f_t)^3 + \Delta_k f_t \Delta_k g_t + \Delta_k u_t \right) + \dots \right\} \\ & \quad \times \frac{1}{2} \left(1 + \beta \sigma_k h_k - \frac{1}{3} \beta^3 \sigma_k h_k^3 + \dots \right) \\ & \quad - \frac{1}{2} \sum_k \left(1 - \beta \sigma_k h_k + \frac{1}{3} \beta^3 \sigma_k h_k^3 - \dots \right) \end{aligned} \quad (8)$$

where $\Delta_k f_t \equiv f_t(F_k \boldsymbol{\sigma}) - f_t(\boldsymbol{\sigma})$, and similarly for $\Delta_k g_t$ and $\Delta_k u_t$.

To evaluate the first-order term $f_t(\boldsymbol{\sigma})$ in eq. (6), we retain only the terms proportional to β in eq. (8) and compare these with the left-hand side of eq. (4). The result is

$$\frac{df_t}{dt} = \frac{1}{2} \sum_k \Delta_k f_t - 2H(\boldsymbol{\sigma}). \quad (9)$$

The following form is a possible solution of this equation:

$$f_t(\boldsymbol{\sigma}) = a(t) H(\boldsymbol{\sigma}). \quad (10)$$

Inserting eq. (10) into eq. (9), we find

$$\dot{a}(t) = -2a(t) - 2.$$

This equation is easily solved under the initial condition $a(t=0) = -\beta_0/\beta$, which corresponds to eq. (7), as

$$a(t) = \left(1 - \frac{\beta_0}{\beta} \right) e^{-2t} - 1. \quad (11)$$

Since eq. (9) is a first-order differential equation, the

above expression (10) with eq. (11) represents the unique solution. The first-order contribution has thus been obtained as

$$p_t(\boldsymbol{\sigma}) = \exp \left[\{ (\beta - \beta_0) e^{-2t} - \beta \} H(\boldsymbol{\sigma}) \right]. \quad (12)$$

It is noted here that β_0 should be at most of the same order as β because $a(t)$ in eq. (10) has implicitly been assumed to be of order unity.

Similarly, from the second-order term of β in eq. (8), we have

$$\frac{dg_t}{dt} = \frac{1}{2} \sum_k \Delta_k g_t + (\alpha^2 e^{-4t} - \alpha e^{-2t}) \sum_k h_k^2, \quad (13)$$

where $\alpha \equiv 1 - \beta_0/\beta$. This equation suggests a solution of the following form:

$$g_t(\boldsymbol{\sigma}) = b_1(t) \sum_i h_i^2 + b_2(t). \quad (14)$$

Inserting eq. (14) into eq. (13) and using the relation

$$\Delta_k (h_i)^2 = -4h_i J_{ik} \sigma_k + 4J_{ik}^2,$$

we find

$$\dot{b}_1(t) = -2b_1(t) + \alpha^2 e^{-4t} - \alpha e^{-2t}. \quad (15)$$

Since the $b_2(t)$ -term in eq. (14) does not depend on the spin configuration and affects only the overall normalization of the probability distribution function (6), we do not write down the evolution equation for $b_2(t)$ here. The solution of eq. (15) is

$$b_1(t) = -\frac{\alpha^2}{2} e^{-4t} - \left(\alpha t - \frac{\alpha^2}{2} \right) e^{-2t}. \quad (16)$$

The initial condition is $b_1(t=0) = 0$ because the first-order contribution, eq. (12), already satisfies the initial condition (7).

The third-order term of β in eq. (8) yields

$$\begin{aligned} \frac{du_t}{dt} &= \frac{1}{2} \sum_k \Delta_k u_t \\ & \quad - 4J^2 (2\alpha e^{-2t} - 1) b_1(t) H(\boldsymbol{\sigma}) \\ & \quad + \left(\frac{2}{3} \alpha^3 e^{-6t} - \alpha^2 e^{-4t} \right) \sum_k \sigma_k h_k^3 \\ & \quad - 2(2\alpha e^{-2t} - 1) b_1(t) \sum_{k,l} J_{kl} h_k h_l. \end{aligned} \quad (17)$$

The following form seems an appropriate solution of this equation:

$$u_t(\boldsymbol{\sigma}) = c_1(t) H(\boldsymbol{\sigma}) + c_2(t) \sum_i \sigma_i h_i^3 + c_3(t) \sum_{i,j} J_{ij} h_i h_j. \quad (18)$$

The first term of the right-hand side of eq. (17) is calculated under the assumption (18) as

$$\begin{aligned} & \frac{1}{2} \sum_k \Delta_k u_t = c_1(t) \{ -2H(\boldsymbol{\sigma}) \} \\ & \quad + c_2(t) \left\{ -4 \sum_k \sigma_k h_k^3 - 12J^2 H(\boldsymbol{\sigma}) - 4 \sum_{k,l} J_{kl}^3 \sigma_k \sigma_l \right\} \end{aligned}$$

$$+ c_3(t) \left\{ -2 \sum_{k,l} J_{kl} h_k h_l + 2 \sum_{k,l,m} J_{kl} J_{km} J_{lm} \right\}. \quad (19)$$

The expressions including J_{kl}^3 or $J_{kl}J_{km}J_{lm}$ do not appear in eq. (18). Thus eq. (18) may at first sight appear inappropriate as the solution of eq. (17). However, a simple order estimate using the relation

$$J_{kl} = \frac{J_0}{N} + \frac{Jz_{kl}}{\sqrt{N}},$$

where z_{kl} is a Gaussian variable with vanishing mean and unit variance, reveals that these J^3 -terms are at most of order \sqrt{N} . Therefore these J^3 -contributions can be ignored compared to the other terms which are all of order N . In this way, we find that eq. (18) gives a consistent solution of eq. (17) with coefficients satisfying

$$\begin{aligned} \dot{c}_1(t) &= -2c_1(t) - 12J^2c_2(t) \\ &\quad - 4J^2b_1(t)(2\alpha e^{-2t} - 1) \\ \dot{c}_2(t) &= -4c_2(t) + \frac{2}{3}\alpha^3 e^{-6t} - \alpha^2 e^{-4t} \\ \dot{c}_3(t) &= -2c_3(t) - 2b_1(t)(2\alpha e^{-2t} - 1). \end{aligned}$$

These differential equations are solved as

$$c_1(t) = J^2 \left\{ -2\alpha^3 e^{-6t} + (4\alpha^3 - 4\alpha^2 - 10\alpha^2 t) e^{-4t} + (2\alpha^2 t - 2\alpha t^2 + 4\alpha^2 - 2\alpha^3) e^{-2t} \right\} \quad (20a)$$

$$c_2(t) = -\frac{1}{3}\alpha^3 (e^{-6t} - e^{-4t}) - \alpha^2 t e^{-4t} \quad (20b)$$

$$c_3(t) = -\frac{1}{2}\alpha^3 e^{-6t} + \left(\alpha^3 - \frac{1}{2}\alpha^2 - 2\alpha^2 t \right) e^{-4t} + \left(\alpha^2 t - \alpha t^2 - \frac{1}{2}\alpha^3 + \frac{1}{2}\alpha^2 \right) e^{-2t} \quad (20c)$$

under the initial condition $c_1 = c_2 = c_3 = 0$.

We have obtained the probability distribution function of the SK model at high temperature as

$$\begin{aligned} p_t(\sigma) = \exp \left[\beta a(t) H(\sigma) + \beta^2 b_1(t) \sum_i h_i^2 \right. \\ \left. + \beta^3 \left\{ c_1(t) H(\sigma) + c_2(t) \sum_i \sigma_i h_i^3 \right. \right. \\ \left. \left. + c_3(t) \sum_{i,j} J_{ij} h_i h_j \right\} + \dots \right], \quad (21) \end{aligned}$$

where $a(t), b_1(t), c_1(t), c_2(t)$ and $c_3(t)$ are given in eqs. (11), (16) and (20a) – (20c). The result (21) shows that there exists a term proportional to $\sum_{i,j} J_{ij} h_i h_j$ representing correlations of internal fields at different sites.

One of the fundamental assumptions of the CLS theory^{11,12)} is equipartitioning. That is, $p_t(\sigma)$ is assumed to be a constant in a subspace with a given value of the single-site spin-field distribution function $D(\zeta, h)$ defined in eq. (1). Our result for $p_t(\sigma)$ shows that this assumption is violated because a constant $D(\zeta, h)$ does not mean a constant value of the field-correlation term $\sum_{i,j} J_{ij} h_i h_j$. This term represents correlations of h_i at different sites and hence cannot be expressed using only the single-site

spin-field distribution function $D(\zeta, h)$. Therefore the CLS theory is not exact.

For a quantitative estimation of various terms in eq. (21), we have plotted the coefficients $a(t)$ to $c_3(t)$ in Fig. 1 for the initial condition $\beta_0 = 0$. This figure shows that the coefficient $c_3(t)$ of the field-correlation term is not necessarily small compared to the others in some time regions, particularly around $t = 2$. Nevertheless, in many cases, the effects of the field-correlation term may not be apparent in physical observables written only in terms of $D(\zeta, h)$, such as the internal energy and the magnetization. This would be one reason why the CLS theory predicts the time dependence of these physical quantities quite accurately, if not exactly, as shown numerically by CLS themselves.

An interesting feature of our formula (21) is that, for small β and β_0 , $p_t(\sigma)$ is well approximated only by the first-order contribution given explicitly in eq. (12). The first-order term has the form of a Boltzmann factor $\exp\{-\beta_{\text{eff}}(t)H(\sigma)\}$. Thus the system can be regarded as being in equilibrium with effective temperature $T_{\text{eff}}(t) = 1/\beta_{\text{eff}}(t)$ at any given t . This allows us to calculate various macroscopic physical quantities

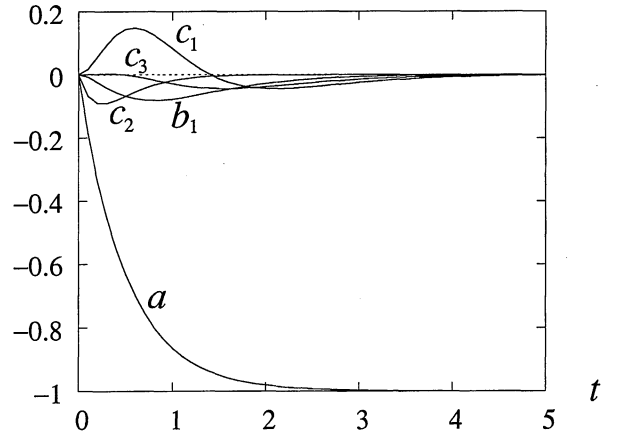


Fig. 1. Time evolution of the coefficients of the high-temperature expansion. The initial condition is $\beta_0 = 0$. We set $J = 1$.

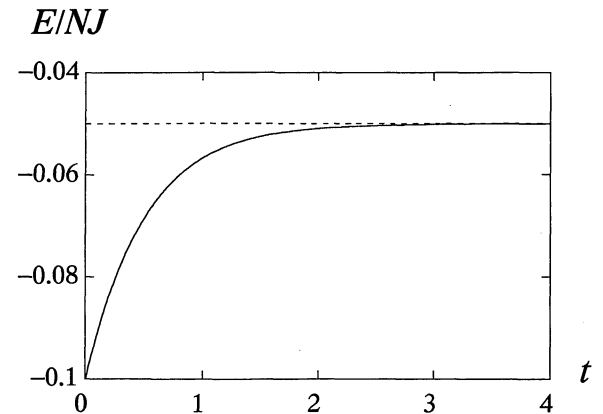


Fig. 2. Time evolution of the internal energy for the initial and final temperatures $T_0/J = 5$ and $T/J = 10$, respectively. The center of distribution of exchange interactions is $J_0 = 0$. The dotted line represents the asymptotic value of the energy, $E/NJ = -0.05$.

in non-equilibrium situations using equilibrium statistical mechanics. An example is given in Fig. 2 for the time development of the internal energy in the case with $T_0/J = 5$ and $T/J = 10$. The center of distribution of the exchange interactions is $J_0 = 0$.

Concerning the generality of the present method, although the SK model has been discussed explicitly here, it is possible to apply the same technique to any models including non-random systems and short-range models. The resulting form of the microscopic probability distribution is almost independent of details of the model. Only minor changes in coefficients are sufficient in many cases. In particular, in the case of the Hopfield model, the appearance of various complicated terms in the probability distribution (21) explains why the simple two-parameter dynamics of CS^{7,8)} is not exact as found numerically.⁹⁾

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