

Dynamical replica theory for disordered spin systems

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We present a method to solve the dynamics of disordered spin systems on finite time scales. It involves a closed driven diffusion equation for the joint spin-field distribution, with time-dependent coefficients described by a dynamical replica theory which, in the case of detailed balance, incorporates equilibrium replica theory as a stationary state. The theory is exact in various limits. We apply our theory to both the symmetric and the nonsymmetric Sherrington-Kirkpatrick spin glass, and show that it describes the (numerical) experiments very well.

Recently it has become clear¹ that even mean-field models exhibit the ageing phenomena, familiar from experiments on real spin glass,² that were hitherto assumed to be typical for short-range systems. This has led to a renewed interest in dynamical studies of mean-field spin-glass models and to valuable new insights into spin-glass dynamics away from equilibrium, see, e.g., Ref. 3. In this paper we present an approach to analyzing the dynamics of spin-glass models on finite time scales, leading to a dynamical replica theory, which, in the case of detailed balance, incorporates equilibrium replica theory as a stationary state (including replica symmetry breaking, if it occurs). The formalism is built on a closure procedure with which we obtain a closed diffusion equation for the joint spin-field distribution. It builds on and extends earlier studies.⁴⁻⁶ Our theory is proven to be exact for short times and in equilibrium. For intermediate times we can prove that it is exact if in the thermodynamic limit the joint spin-field distribution indeed obeys a closed dynamic equation. Here we discuss only the underlying physical ideas and the results of applying our theory to both the symmetric⁷ and the nonsymmetric⁸ Sherrington-Kirkpatrick spin glass. Full mathematical details will be published elsewhere.⁹ We believe the agreement between theory and (simulation) experiment to be quite convincing.

The generalized (asymmetric) version of the Sherrington-Kirkpatrick (SK) model,⁷ introduced in Ref. 8, consists of N Ising spins $\sigma_i \in \{-1, 1\}$ with infinite-range interactions J_{ij} :

$$J_{ij} = J_0/N + (J/\sqrt{N})[\cos(\frac{1}{2}\omega)x_{ij} + \sin(\frac{1}{2}\omega)y_{ij}]$$

$$x_{ij} = x_{ji}, \quad y_{ij} = -y_{ji}. \quad (1)$$

For $i < j$ each of the random quantities x_{ij} and y_{ij} , representing quenched disorder, are drawn independently from a Gaussian distribution with zero mean and unit variance. The evolution in time of the microscopic probability distribution $p_t(\sigma)$ is given by the master equation

$$\frac{d}{dt} p_t(\sigma) = \sum_{k=1}^N [p_t(F_k\sigma)w_k(F_k\sigma) - p_t(\sigma)w_k(\sigma)], \quad (2)$$

in which F_k is a spin-flip operator $F_k\Phi(\sigma) \equiv \Phi(\sigma_1, \dots, -\sigma_k, \dots, \sigma_N)$ and the transition rates $w_k(\sigma)$ and the local alignment fields $h_i(\sigma)$ are

$$w_k(\sigma) = \frac{1}{2} \{1 - \sigma_k \tanh[\beta h_k(\sigma)]\}, \quad h_i(\sigma) = \sum_{j \neq i} J_{ij} \sigma_j + \theta, \quad (3)$$

where $\beta = 1/T$ is the inverse temperature. The mixing angle $\omega \in [0, \pi]$ controls the degree of symmetry of the interactions (1). For $\omega = 0$ we recover the original SK spin-glass model.⁷ Now the interactions are symmetric, the dynamics obey detailed balance, and (2) reduces to a Glauber dynamics, leading asymptotically to the Boltzmann equilibrium distribution $p_\infty(\sigma) \sim \exp[-\beta H(\sigma)]$ with the conventional Hamiltonian

$$H(\sigma) = - \sum_{i < j} \sigma_i J_{ij} \sigma_j - \theta \sum_i \sigma_i. \quad (4)$$

For $\omega > 0$, however, detailed balance is violated and equilibrium statistical mechanics no longer applies. For $\omega = \pi$ the interaction matrix is fully antisymmetric.

For any given set of l macroscopic observables $\Omega(\sigma) = [\Omega_1(\sigma), \dots, \Omega_l(\sigma)]$ we can derive a macroscopic stochastic equation in the form of a Kramers-Moyal expansion. For deterministically evolving observables (in the thermodynamic limit) on finite time scales only the first (Liouville) term in this expansion will survive, leading to the deterministic flow equation

$$\frac{d}{dt} \Omega_t$$

$$= \lim_{N \rightarrow \infty} \frac{\sum_{\sigma} p_t(\sigma) \delta[\Omega_t - \Omega(\sigma)] \sum_i w_i(\sigma) [\Omega(F_i\sigma) - \Omega(\sigma)]}{\sum_{\sigma} p_t(\sigma) \delta[\Omega_t - \Omega(\sigma)]}. \quad (5)$$

There are two *natural* ways for (5) to close. Firstly, by the argument of the subshell average in (5) depending on σ only through $\Omega(\sigma)$ [now $p_t(\sigma)$ will drop out], and secondly by the microscopic dynamics (2) allowing for equipartitioning solutions [where $p_t(\sigma)$ depends on σ only through $\Omega(\sigma)$]. In both cases the correct equations are obtained upon simply eliminating $p_t(\sigma)$ from (5). We now make two assumptions: (i) the observables $\Omega(\sigma)$ are self-averaging with respect to the microscopic realization of the disorder $\{x_{ij}, y_{ij}\}$, at any time, and (ii) in evaluating the subshell average we assume equipartitioning of probability within the Ω subshell of the ensemble. As a result the macroscopic equation (5) is replaced by a closed one, from which the unpleasant fraction can be removed with a replica identity (see, e.g., Ref. 10):

$$\frac{d}{dt} \mathbf{\Omega}_t = \lim_{N \rightarrow \infty} \lim_{n \rightarrow 0} \sum_{\sigma^1} \cdots \sum_{\sigma^n} \sum_i \left\langle w_i(\sigma^1) [\mathbf{\Omega}(F_i \sigma^1) - \mathbf{\Omega}(\sigma^1)] \prod_{\alpha=1}^n \delta[\mathbf{\Omega}_t - \mathbf{\Omega}(\sigma^\alpha)] \right\rangle_{\{x,y\}}. \quad (6)$$

For observables truly governed by a closed equation our closure procedure reduces to the natural one (in the sense discussed above), so we know by construction: if a closed self-averaging equation for $\mathbf{\Omega}_t(\sigma)$ exists, it must indeed be (6). For the set of observables $\mathbf{\Omega}(\sigma)$ we now choose the (infinite dimensional) joint spin-field distribution:

$$D(\zeta, h; \sigma) = (1/N) \sum_i \delta_{\zeta, \sigma_i} \delta[h - h_i(\sigma)] \quad (7)$$

with the local fields (3). Since both the magnetization $m = (1/N) \sum_i \sigma_i$ and the energy (4) can be written as integrals over $D(\zeta, h; \sigma)$, the theory will automatically be exact (i) in the limit $J \rightarrow 0$, (ii) for $t \rightarrow 0$ (upon choosing appropriate initial conditions), and (iii) in the limit $t \rightarrow \infty$ (for systems evolving towards equilibrium). To circumvent technical subtleties we assume that the distribution (7) is sufficiently well behaved: we evaluate $D_t(\zeta, h)$ in a number l of field arguments and take the limit $l \rightarrow \infty$ after the limit $N \rightarrow \infty$. A closed diffusion equation for $D_t(\zeta, h)$ was also derived in Ref. 11. Although similar in spirit to ours, the latter study employed a different closure procedure, lacking the properties of the present one of built-in exactness in various limits.

We can now run the familiar machinery of replica theory and evaluate (6) for the choice (7). The distribution $D_t(\zeta, h)$ can be shown to indeed evolve deterministically. Details of

this exercise, as usual involving a saddle-point problem, can be found in Ref. 9. The result is the diffusion equation

$$\begin{aligned} \frac{\partial}{\partial t} D_t(\zeta, h) = & \frac{1}{2} [1 + \zeta \tanh(\beta h)] D_t(-\zeta, h) \\ & - \frac{1}{2} [1 - \zeta \tanh(\beta h)] D_t(\zeta, h) \\ & + \frac{\partial}{\partial h} \left\{ D_t(\zeta, h) [h - \theta - J_0 \langle \tanh(\beta H) \rangle_{D_t}] \right. \\ & + \mathcal{A}[\zeta, h; D_t] \\ & \left. + J^2 [1 - \langle \sigma \tanh(\beta H) \rangle_{D_t}] \frac{\partial}{\partial h} D_t(\zeta, h) \right\} \quad (8) \end{aligned}$$

with the short hand $\langle f(\sigma, H) \rangle_D = \int d\mathbf{H} \int d\mathbf{H} D(\sigma, H) f(\sigma, H)$. We find all interesting physics to be concentrated in a single driving term \mathcal{A} :

$$\begin{aligned} \mathcal{A}[\zeta, h; D] = & - \lim_{n \rightarrow 0} \sum_{\alpha\beta} (q^{-1})_{\alpha\beta} \{ \langle \tanh(\beta H_1) \sigma_\alpha \rangle_M \\ & \times \langle \delta[h - H_1] \delta_{\zeta, \sigma_1} [H_\beta - \theta - J_0 m \\ & + iJ^2 \cos \omega(\mathbf{R}^\dagger \sigma)_\beta] \rangle_M \\ & + \cos \omega \langle \delta[h - H_1] \delta_{\zeta, \sigma_1} \sigma_\alpha \rangle_M \langle \tanh(\beta H_1) \\ & \times [H_\beta - \theta - J_0 m + iJ^2 \cos \omega(\mathbf{R}^\dagger \sigma)_\beta] \rangle_M \}. \quad (9) \end{aligned}$$

This involves an effective measure M in replica space

$$\langle f[\mathbf{H}, \sigma] \rangle_M = \frac{\int d\mathbf{H} \sum_{\sigma} M[\mathbf{H}, \sigma] f[\mathbf{H}, \sigma]}{\int d\mathbf{H} \sum_{\sigma} M[\mathbf{H}, \sigma]},$$

$$\begin{aligned} M[\mathbf{H}, \sigma] = \exp \left\{ -i \hat{\mathbf{m}} \cdot \sigma - \frac{1}{2} J^2 \sigma \cdot \mathbf{Q} \sigma - i \sum_{\alpha} \hat{D}_{\alpha}(\sigma_{\alpha}, H_{\alpha}) \right. \\ \left. - \frac{1}{2J^2} [\mathbf{H} - \theta - J_0 \mathbf{m} + iJ^2 \cos \omega \mathbf{R}^\dagger \sigma] \cdot \mathbf{q}^{-1} [\mathbf{H} - \theta - J_0 \mathbf{m} + iJ^2 \cos \omega \mathbf{R}^\dagger \sigma] \right\} \quad (10) \end{aligned}$$

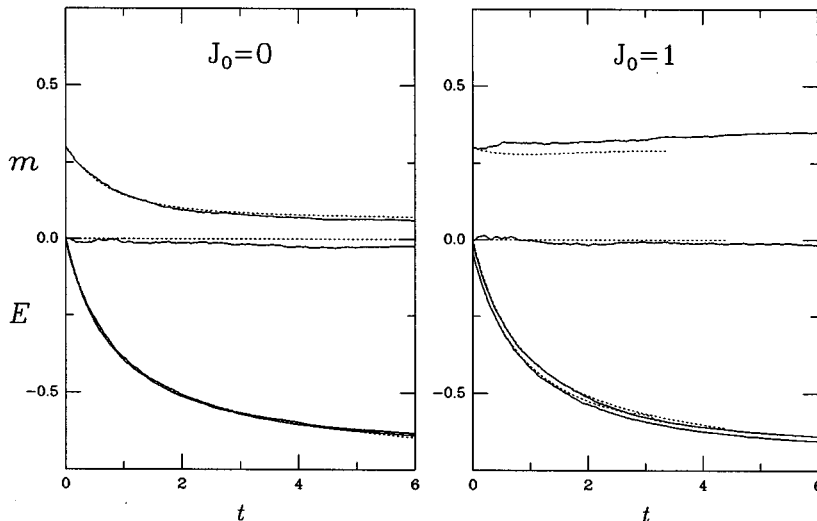


FIG. 1. Magnetization m and energy per spin E in the $J=1$ SK model at $T=0$, for $J_0=0$ (left) and $J_0=1$ (right). Solid lines: numerical simulations with $N=8000$; dotted lines: result of solving the RS diffusion equation.

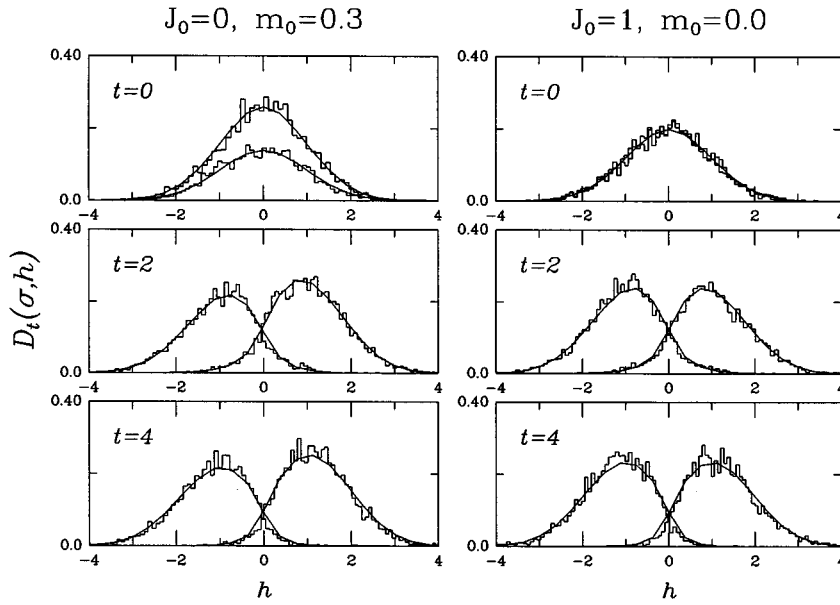


FIG. 2. Field distributions $D_t(\sigma, h)$ in the $J=1$ SK model at $T=0$, for $J_0=0$ (left) and $J_0=1$ (right). Histograms: numerical simulations with $N=8000$; lines: result of solving the RS diffusion equation.

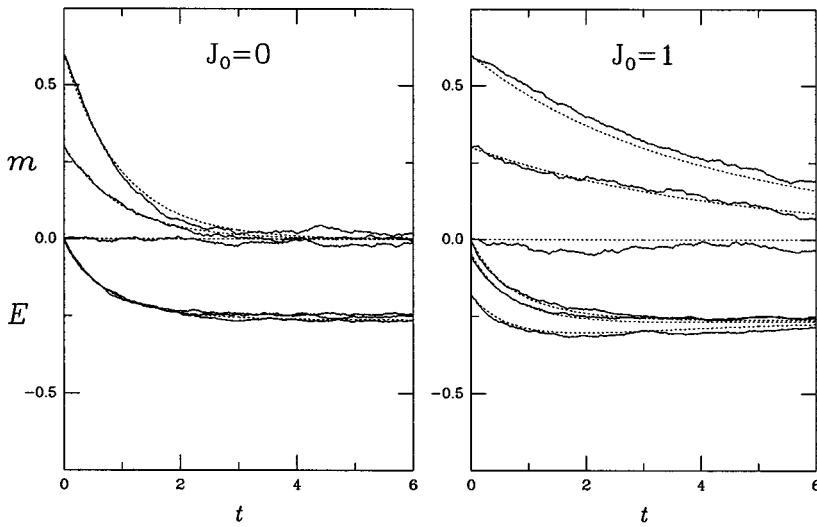


FIG. 3. Magnetization m and energy per spin E in the asymmetric $J=1$ SK model at $T=0$, for $J_0=0$ (left) and $J_0=1$ (right). Solid lines: numerical simulations with $N=5600$; dotted lines: result of solving the RS diffusion equation.

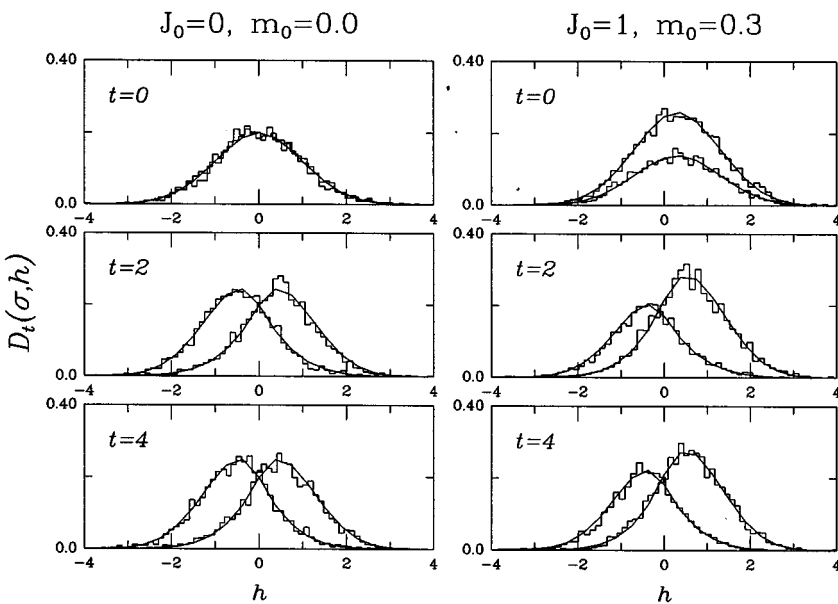


FIG. 4. Field distributions $D_t(\sigma, h)$ in the asymmetric $J=1$ SK model at $T=0$, for $J_0=0$ (left) and $J_0=1$ (right). Histograms: numerical simulations with $N=5600$; lines: result of solving the RS diffusion equation.

with $\mathbf{H}=(H_1, \dots, H_n)$ and $\boldsymbol{\sigma}=(\sigma_1, \dots, \sigma_n)$. The $n \times n$ matrices $\{\mathbf{q}, \mathbf{Q}, \mathbf{R}\}$, the n vectors $\{\hat{\mathbf{m}}, \mathbf{m}\}$, and the functions $\hat{D}_\alpha(\sigma, H)$ are obtained by extremization of the surface Ψ :

$$\begin{aligned} \Psi = & i \sum_{\alpha\sigma} \int dH D(\sigma, H) \hat{D}_\alpha(\sigma, H) + i \sum_{\alpha} m_{\alpha} \hat{m}_{\alpha} \\ & + \frac{1}{2} J^2 \sum_{\alpha\beta} [q_{\alpha\beta} Q_{\alpha\beta} + \cos\omega R_{\alpha\beta} R_{\beta\alpha}] - \frac{1}{2} \ln \det \mathbf{q} \\ & + \ln \int d\mathbf{H} \sum_{\boldsymbol{\sigma}} M[\mathbf{H}, \boldsymbol{\sigma}]. \end{aligned} \quad (11)$$

For the detailed balance case $\omega=0$ [the SK (Ref. 7) model], the equilibrium state calculated within equilibrium statistical mechanics,¹² is found to define a stationary state of (8). Here we restrict ourselves to replica-symmetric (RS) saddle points of Ψ , an analysis of (11) involving broken replica symmetry à la Parisi¹² is the subject of a future study. It is a straightforward exercise to work out the RS saddle-point equations and the corresponding expression \mathcal{A}_{RS} for the driving term (9), which, upon insertion into (8), controls the evolution of the joint spin-field distribution in RS approximation. Evaluating \mathcal{A}_{RS} requires solving the RS saddle-point equations at each instance of time. In the usual manner one can also calculate the de Almeida-Thouless instability¹³ with respect to replicon fluctuations; here involving variation of three order-parameter matrices, as opposed to one.

We test our theory by comparing the results of solving numerically equation (8) in RS ansatz, for the two model choices $\omega=0$ and $\omega=\pi/2$, with the results of performing numerical simulations of the discretized version of the stochastic dynamics (2,3). Since solving (8) requires a significant computational effort, even within the RS ansatz, we restrict our experiments to zero external fields and to initial configurations with spin states chosen independently at random, given a required initial magnetization. For the original SK model, obtained for $\omega=0$, the results of confronting (8) with typical simulation experiments at $T=0$ are shown in Figs. 1 and 2, for $J_0=0$ (left pictures) and $J_0=1$ (right pictures). In Fig. 1 the top graphs represent the magnetization m and the lower graphs represent the energy per spin E ; for the initial conditions $m_0=0$ and $m_0=0.3$. Figure 2 shows the corresponding distributions $D_t(\sigma, h)$ for one particular choice of initial state [$D_t(1, h)$: upper graph in $t=0$ window, right graph in $t>0$ windows; $D_t(-1, h)$: lower graph in $t=0$ win-

dow, left graph in $t>0$ windows]. For $J_0=1$ we were not able to calculate the solution of Eq. (8) up to $t=6$, due to the critical behavior of the saddle-point equations. For the fully asymmetric model, $\omega=\pi/2$, one finds much simpler equations, due to a decoupling of the spins from the fields. In this case Eq. (8) allows for solutions where $D_t(1, h) + D_t(-1, h)$ remains of a Gaussian form at all times, in accordance with Refs. 8 and 14. The results of confronting (8) with $T=0$ simulation experiments for the asymmetric $\omega=\pi/2$ SK model are shown in Figs. 3 and 4, for $J_0=0$ (left pictures) and $J_0=1$ (right pictures); for the initial conditions $m_0=0$, $m_0=0.3$, and $m_0=0.6$. Figure 4 shows the distributions $D_t(\sigma, h)$ for one particular initial state [$D_t(1, h)$: upper graph in $t=0$ window, right graph in $t>0$ windows; $D_t(-1, h)$: lower graph in $t=0$ window, left graph in $t>0$ windows].

In this paper we have shown how one can solve the dynamics of disordered spin systems on finite time scales with a dynamical generalization of equilibrium replica theory. Although we have restricted our analysis by making the replica-symmetric (RS) ansatz, on the time scales considered the agreement between theory and simulation experiment is already quite satisfactory. At this stage we need more efficient numerical procedures in order to extend the time scales for which we can solve the equations of the theory. This would enable us to compare, for instance, with data such as the ones in Ref. 15, and to investigate the possible existence of stationary states other than the one corresponding to thermal equilibrium. Our theory is by construction exact in various limits. Its full exactness depends crucially on whether the joint spin-field distribution indeed obeys a closed self-averaging dynamic equation, which is difficult to verify. We plan to investigate several approaches to this problem in the near future. Firstly, we want to apply our formalism to disordered spin systems for which the dynamics has been solved by other means, like the toy model,⁶ or the spherical spin glass.¹⁶ Secondly we want to try to derive a diffusion equation for the joint spin-field distribution, starting from the exact (but rather complicated) closed equations for the correlation function $C(t, t')$ and the response function $G(t, t')$, each with two real-valued arguments (two times). The present formalism also involves two functions $D_t(1, h)$ and $D_t(-1, h)$, with two real-valued arguments each (one time and one field). It is therefore quite imaginable that both formalisms constitute exact descriptions of the dynamics of disordered spin models.

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