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Equivalence of statistical-mechanical and dynamic descriptions of the infinite-range Ising spin-glass

C. Dasgupta
Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138
*and School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455**

H. Sompolinsky
Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138
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We prove the equivalence between the dynamic mean-field theory of the Ising spin-glass and the statistical-mechanical theory of Thouless, Anderson, and Palmer (TAP). Individual low-free-energy TAP solutions describe short-time properties, whereas thermodynamic equilibrium corresponds to averaging over all such solutions. The square of the staggered magnetization associated with the largest eigenvalue of the interaction matrix scales as $N^{5/6}$ (N is the number of spins). Results are confirmed by Monte Carlo simulation and numerical solution of the TAP equations.

A recent theory[1] of the dynamics of the Sherrington-Kirkpatrick (SK) model[2] of the infinite-range Ising spin-glass (SG) showed that the time evolution in the SG phase involves a hierarchy of macroscopically long relaxation times. This has raised an important question, namely, whether the usually accepted ergodic hypothesis about the equivalence between statistical-mechanical averages and long-time properties breaks down in SG's and perhaps in other amorphous systems. Closely related issues concern the nature of the metastable SG states and the properties of the corresponding free-energy barriers which give rise to the long relaxation times. The mean-field theory of Thouless, Anderson, and Palmer (TAP),[3] in which the random site magnetizations $\{m_i\}$ are used to describe the SG state, provides a natural framework for studying these issues. Unfortunately, despite considerable effort,[4,5] many questions about the TAP equations remain unanswered. It is not known whether the TAP approach is consistent with dynamic and replica[6] theories. It has been shown[4] that the TAP equations have a very large number of solutions; but it is not clear whether these solutions describe short-time or equilibrium properties. Also, the basic nature of the random SG ordering remains controversial. The natural order parameters in the TAP framework are the staggered magnetizations associated with the eigenvectors of the random interaction matrix $\underline{J}$. Originally, TAP assumed that the staggered magnetization associated with the largest eigenvalue is macroscopic, i.e., $O(\sqrt{N})$, where N is the number of spins, whereas in a more recent work,[5] it was argued that all the staggered magnetizations are of $O(1)$.

In this paper, we first show analytically that the statistical-mechanical description of TAP is completely consistent with the dynamic theory. Individual low-free-energy TAP solutions describe the short-time properties of the system, whereas averaging the random magnetizations over TAP solutions lying within a certain range in phase space is equivalent to relaxation in a certain time scale. We also show that the distribution of staggered magnetizations is sharply peaked at the largest eigenvalues of $\underline{J}$ for all $T < T_c$. The square of the staggered magnetization associated with the largest eigenvalue scales as $N^{5/6}$. We then present results of a Monte Carlo (MC) simulation and numerical solution of the TAP equations, which confirm these predictions.

The SK Hamiltonian for a system of N Ising spins $\sigma_i (= \pm 1)$ is

$$H = -\frac{1}{2} \sum_{i \neq j} J_{ij} \sigma_i \sigma_j \ , \tag{1}$$

where the J_{ij}'s are independent Gaussian random variables with variance $\tilde{J}/\sqrt{N}$. When written in terms of the staggered magnetizations $M_\lambda \equiv \sum_i m_i \langle i|\lambda\rangle$, where $\langle i|\lambda\rangle$ is the ith element of the eigenvector of $\underline{J}$ with eigenvalue J_λ, the TAP equations take the form

$$M_\lambda = \sum_i \langle i|\lambda\rangle \tanh\left(\sum_\nu [A(J_\nu) M_\nu + \beta h_\nu] \langle i|\nu\rangle \right), \tag{2}$$

where $A(J_\lambda) = \beta J_\lambda - \beta^2 \tilde{J}^2 (1 - q_{\rm EA})$, $q_{\rm EA}$ is the Edwards-Anderson[7] order parameter, and h_λ's are staggered fields. For $N \to \infty$, the eigenvalue density obeys the semicircular law

$$\rho(J_\lambda) = \frac{1}{2\pi \tilde{J}^2} (4\tilde{J}^2 - J_\lambda^2)^{1/2}, \quad |J_\lambda| \leq 2\tilde{J} \ . \tag{3}$$

In a previous work,[5] it was shown that in the $N \to \infty$

limit, the right-hand side of Eq. (2) can be written as

$$M_\lambda = m_\lambda + \chi_0[A(J_\lambda)M_\lambda + \beta h_\lambda] \ , \tag{4}$$

where m_λ, the contribution to M_λ from all other magnetizations, depends on λ only through $\langle i|\lambda\rangle$ and, in particular, the configuration average $\langle m_\lambda^2\rangle \equiv Q$ is independent of λ. The coefficient χ_0 is equal to $(1-q_{\rm EA})$ if linear-response theory holds (i.e., in the SK solution). Allowing for $\chi_0-(1-q_{\rm EA}) \equiv \Delta_0 \neq 0$ yields[5] the Sommers's solution.[8] In this work, we show that the introduction of a nonzero Δ_0 leads to other solutions as well.

To see this, we note that the TAP equations are expected to have many solutions.[4] Thus the M_λ's in Eq. (2) refer, strictly speaking, to the magnetizations in a *particular solution.* In any particular stable solution, linear-response theory must hold. Therefore Δ_0 is associated with transitions between different solutions. This implies that for $\Delta_0 \neq 0$, Eq. (4) is ill defined since Δ_0 is *not* a property of a particular solution, whereas M_λ is. Instead, Δ_0 should couple to the magnetization averaged over the solutions which are involved in the transitions giving rise to a finite Δ_0. The result of this averaging clearly depends upon the correlations between different solutions. In the thermodynamic limit, only the solutions with the lowest free energy per spin are relevant. In order to describe the correlations among these solutions, we make, in analogy with the dynamic theory,[1] the following ansatz: The correlations between different solutions are characterized by a suitably defined "distance" in phase space separating them. It is reasonable to assume that in a large system, there is a broad distribution of distances. We order the different scales of distance by a parameter $x \in [0,1]$. The end $x=1$ corresponds to solutions which are highly correlated, so that averaging over these solutions does not modify the properties of a single solution. On the other hand, $x=0$ corresponds to solutions which are farthest apart from each other, and therefore, least correlated.[9] We denote by $m_i(x)$ and $M_\lambda(x)$ the values of the local or staggered magnetization calculated by averaging over all solutions which are *within* distance x. Similarly, $\chi_0(x) = 1-q_{\rm EA}+\Delta_0(x)$ is the "susceptibility" which includes contributions from transitions among solutions within distance x. Accordingly, $-\Delta_0'(x) \equiv -d\Delta_0(x)/dx$ represents the contribution to Δ_0 from transitions between solutions which are at a distance x from one another. We can then write Eq. (4) in the following modified form:

$$M_\lambda(1) = m_\lambda(1) + (1-q_{\rm EA})A(J_\lambda)M_\lambda(1) - A(J_\lambda)\int_0^1 \Delta_0'(u)M_\lambda(u)\,du \ . \tag{5}$$

Here, we have put $h_\lambda = 0$, and assumed that $q_{\rm EA} = 1/N\sum_i m_i^2(1)$ is the same in all solutions of interest. Averaging Eq. (5) over all solutions within distance x [upon averaging, $m_\lambda(1) \to m_\lambda(x)$, $M_\lambda(1) \to M_\lambda(x)$, $M_\lambda(u) \to M_\lambda(x)$ for $u \geq x$, and $M_\lambda(u)$, $u < x$ remains unchanged], and using the results[1] $\Delta_0(1)=0$ and $M_\lambda(0)=0$, we obtain

$$M_\lambda(x) = m_\lambda(x) + A(J_\lambda)\int_0^x \chi_0(u)M_\lambda'(u)\,du \ . \tag{6}$$

Differentiating Eq. (6) with respect to x, we get

$$M_\lambda'(x) = \frac{m_\lambda'(x)}{1-\chi_0(x)A(J_\lambda)} \ . \tag{7}$$

Defining

$$q_\lambda'(x) \equiv \langle [M_\lambda'(x)]^2\rangle = \frac{d}{dx}\langle [M_\lambda(x)]^2\rangle$$

(Ref. 10) and using Eq. (7), we get

$$q_\lambda'(x) = Q'(x)/[1-\chi_0(x)A(J_\lambda)]^2 \ ,$$
$$Q'(x) \equiv \langle [m_\lambda'(x)]^2\rangle \ . \tag{8}$$

The staggered susceptibility $\chi_\lambda(x)$, which describes the response of $M_\lambda(x)$ to a staggered field that couples to transitions among solutions within distance x, can be calculated by including such a field in Eq. (6). We find

$$\chi_\lambda(x) = \beta/[\chi_0^{-1}(x) - A(J_\lambda)] \ . \tag{9}$$

Defining

$$q'(x) \equiv \int q_\lambda'(x)\rho(J_\lambda)\,dJ_\lambda$$

and

$$\chi(x) \equiv \int \chi_\lambda(x)\rho(J_\lambda)\,dJ_\lambda \ ,$$

and using the probability distribution $\rho(J_\lambda)$ given in Eq. (3), we obtain

$$\chi_\lambda(x) = [r(x)+E_\lambda]^{-1}, \quad E_\lambda = 2\tilde{J} - J_\lambda \ ,$$
$$r(x) = \chi^{-1}(x)[1-\tilde{J}\chi(x)]^2 \ , \tag{10}$$

and

$$q_\lambda'(x) = q'(x)\chi_\lambda^2(x)[\chi^{-2}(x) - \tilde{J}^2] \ . \tag{11}$$

Extending previous calculations of q and χ [Eqs. (11)–(15) of Ref. 5] by defining a local noise as a sum over x Gaussian variables, it is straightforward to derive the self-consistent equations for $q(x)$ and $\chi(x)$, which are identical to those found in the dynamic theory.[1] This proves the equivalence of the TAP approach with the dynamic theory.

Using the result[1] that $\chi(0) = \tilde{J}^{-1}$ for all $T < T_c = \tilde{J}$, we note that $r(x) \propto [\chi(0)-\chi(x)]^2$ and, in particular, $r(0)=0$ at all $T < T_c$. Thus the smaller x is, the sharper $q_\lambda'(x)$ is peaked at the band edge $E_\lambda = 0$ $(J_\lambda = 2\tilde{J})$. In particular, the infinitesimally small q which remains after averaging over almost all of the solutions [i.e., $q_\lambda'(0)$] is, according to Eq. (11), completely concentrated at the edge:

$$q_\lambda'(0) \propto \delta(E_\lambda) \ . \tag{12}$$

As x is increased, more and more states are occupied. Using the relation[1] $\chi(0)-\chi(x) \propto q^2(x)$, which is valid for small $q(x)$, we have

$$q_\lambda(x) \sim \int_0^{q(x)} dq \frac{q^2}{(E_\lambda+\alpha q^4)^2} \ , \tag{13}$$

where $\alpha \sim$ const as $q \to 0$. This means that for all $x>0$ and, in particular, for $x=1$ (i.e., for individual solutions), the distribution of magnetizations diverges at the edge as $E_\lambda^{-5/4}$. This result implies that $\langle [M_{2\tilde{J}}(1)]^2 \rangle$ is *not* of order unity, but scales as some power of N. To determine this power, we note that $q'_{2\tilde{J}}(0) \propto [r_N(0)]^{-3/2}$, where $r_N(0)$ is the small but finite value of $r(x=0)$ in a finite system of N spins. Equation (12) implies that $q'_{2\tilde{J}}(0)$ is of order N. Thus we have $r_N(0) \propto N^{-2/3}$, from which it follows that

$$q_{2\tilde{J}}(x) \propto [r_N(0)]^{-5/4} \propto N^{5/6}, \quad x>0 \ . \tag{14}$$

The N dependence of $r_N(0)$ also implies that at $T=T_c$, the staggered susceptibility at the band edge diverges as

$$\chi_{2\tilde{J}} \propto N^{2/3} \ . \tag{15}$$

In order to check the prediction of this theory, we have carried out a MC simulation of the SK model. For temperatures close to T_c, we found that the spin averages go to zero within the measuring time (typically, 2000–4000 MC steps per spin), due to the turning over of all the spins in the system. For this reason, the spin averages were measured at temperatures less than $0.8\tilde{J}$. In all cases, we found that the distribution of the staggered magnetization is sharply peaked at $J_\lambda = J_0$, the largest eigenvalue of the interaction matrix $\underline{J}$. A typical distribution of $q_\lambda = \langle M_\lambda^2 \rangle$ for $N=100$ at $T=0.5\tilde{J}$ is shown in Fig. 1.

In order to determine whether this feature is also present in solutions of the TAP equations, we then obtained (for $N=50$ and $N=100$) self-consistent solutions of these equations for the same bond configurations as those used in the MC calculation by using the MC spin averages $\{m_i\}$ as the starting values in a numerical search procedure. We found convergence to a stable self-consistent solution in about 40% of the cases. The values of $\{m_i\}$ in each of these solutions were found to be very close to those obtained in the MC simulation. As shown in Fig. 1, the distribution of M_λ^2 averaged over the TAP solutions for $N=100$, $T=0.5\tilde{J}$ is almost identical to the MC result. We thus conclude that the MC results correspond to a *particular* solution of the TAP equations[11] and, hence, to $x=1$. The distributions shown in Fig. 1 are in good qualitative agreement with the form predicted in Eq. (13). A comparison between the distributions for $N=100$ and $N=50$ clearly shows that the peak at $J_\lambda = J_0$ becomes sharper with increasing N, as expected.

In Fig. 2, we have shown the dependence of q_{J_0} on

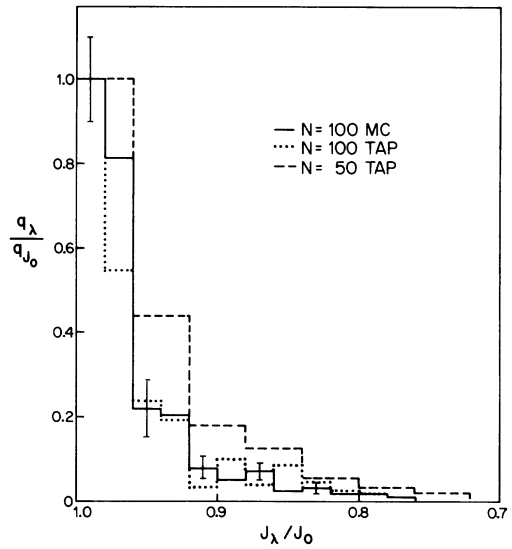

FIG. 1. Distribution of staggered magnetization at $T=0.5\tilde{J}$. Error bars, estimated from sample to sample variations, are shown for the MC results for $N=100$.

N at two different temperatures on a log-log plot. We have scaled q_{J_0} by the measured values of q in order to take into account the small variations of q with N. The data points are well represented by straight lines with slope 0.86 ± 0.10 for $T=0.7\tilde{J}$, and 0.83 ± 0.08 for $T=0.5\tilde{J}$. This is clearly consistent with a power $\frac{5}{6}$, predicted in Eq. (14). Recently, Young and Kirkpatrick[12] have obtained similar results from a study of the exact ground states of small sys-

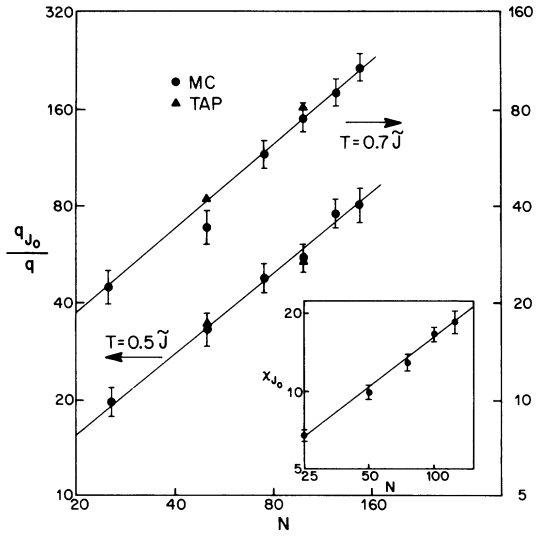

FIG. 2. Variation of q_{J_0} with N at $T=0.7\tilde{J}$ and $T=0.5\tilde{J}$. The inset shows the N dependence of the staggered susceptibility χ_{J_0} at $T=\tilde{J}$. The straight lines drawn through the data points are the best fits.

tems. In the inset of Fig. 2, we have shown the N dependence of the MC results for χ_{J_0} at $T=\tilde{J}$. The log-log plot is well described by a straight line with slope 0.65 ± 0.07, in good agreement with Eq. (15). The numerical results thus strongly support the theoretical predictions about the short-time behavior. A numerical verification of the predicted long-time behavior resulting from transitions among distant TAP solutions would require simulating large samples for which many such solutions would be present.

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*Present address.

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