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Chaos in spin glasses: A renormalization-group study

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The Migdal-Kadanoff renormalization-group scheme is used to investigate chaotic behavior in the ordered phase of a three-dimensional Ising spin glass. The spin order is sensitive to a temperature change δT at length scales $L^* \sim (\gamma/\sigma \delta T)^{1/\zeta}$, where Y and σ are temperature-dependent amplitudes associated with the interfacial free energy and entropy, respectively, $\zeta = d_S/2 - y$ is the Lyapunov exponent characterizing the chaotic behavior, d_S is the fractal dimension of the interface, and $-y$ is the scaling dimension of the temperature at the zero-temperature fixed point.

Phenomenological scaling¹⁻⁴ has proved to be a simple, yet powerful, tool for the investigation of the nature of ordering in Ising spin glasses with short-range interactions. The basic idea is that for all $T < T_C$ the behavior of the system at large length scales is controlled by a zerotemperature fixed point. The zero-temperature scaling approach leads to many novel predictions. One of the most striking concerns the "chaotic" character of the ordered phase in an Ising spin glass, in which the relative orientations of spins is increasingly sensitive, as the spin separation is increased, to small perturbations in externally controlled variables, such as the temperature.

In this Rapid Communication we investigate this phenomenon within the context of a simple, explicit renormalization-group transformation-the Kadanoff renormalization-group scheme (MKRG).⁶ Here we can explicitly follow, numerically, the evolution of the bond probability distribution. We find that, at $T=0$, two neighboring bond pools, initially differing infinitesimally, diverge exponentially under iteration. Exponential divergence of neighboring trajectories is characteristic of chaotic behavior, and the rate of divergence enables us to identify the corresponding "Lyapunov exponent." In a second study, we follow the parallel evolution of two identical bond pools started at slightly different temperatures in the ordered phase. After initial transients, associated with the flow to the zerotemperature fixed point, have died away we again find exponential divergence of the pools with the same Lyapunov exponent as before. In both cases, after sufficiently many iterations (the number required depending on the initial separation of the pools) the two pools become completely uncorrelated, although they correspond to the same distribution with (essentially) the same scale width.

Before discussing the MKRG results in detail, it is useful to review the general arguments for chaotic behavior.⁵ We first consider the effect on the ground state of adding a small random perturbation, of relative strength ϵ , to each bond. If J is a measure of the width of the unperturbed bond distribution, then the energy cost, in the absence of the perturbation, of an excitation (i.e., overturned region of spins, or "droplet") of linear dimension L (measured in units of the lattice spacing), is of order JL^y . The exponent y characterizes the scaling behavior of the bond distribution at the zero-temperature fixed point; in

enormalization-group language, $-y$ is the scaling dimension of the temperature. $2-4$ In the presence of the perturbation, the excitation which originally cost energy may now be energetically *favorable*, since there is an additional contribution of order $\pm \epsilon J L^{d_S/2}$ from the perturbation where L^{a_S} is the surface area of the excitation and d_S is the "fractal dimension of the interface." 4.5 Since, on general grounds,^{4,5} $\zeta \equiv d_S/2 - y > 0$, the ground state is unstable against the perturbation on length scales $L > L^* \sim 1/\epsilon^{1/\zeta}$. The reader will recognize the above as essentially an Imry-Ma argument.⁷ The chaotic response to temperature changes follows immediately from the chaotic response to bond perturbations at $T=0$: Two identical bond pools at slightly different temperatures iterate (in the ordered phase) to two zero-temperature pools with slightly different bonds. Under subsequent iteration these pools diverge as discussed above.

The MKRG recursion relation for $d = 3$ is⁶

$$
K' = \sum_{i=1}^{4} \tanh^{-1}(\tanh K_{1i} \tanh K_{2i}) \tag{1}
$$

corresponding to the decimation process shown in Fig. l. In Eq. (1), $K_{1i} = J_{1i}/T$, etc., and J_{1i} , J_{2i} are the two bonds on the ith of the four "parallel paths" in Fig. 1. (We have specialized to dimension $d=3$ and length-scale factor $b = 2$. For general d and b the number of parallel paths is b^{d-1} .) We have chosen to use the "series-then-parallel" MKRG. The alternative "parallel-then-series" MKRG is expected to give similar results.⁶

To use Eq. (1) in practice, we construct a pool of N bonds, $\{J_i^{(0)}\}$, where typically N is between 10⁴ and 10⁵, drawn from some initial distribution characteristic of spin-glass behavior (we used $N=4\times 10^4$, and a Gaussian distribution of zero mean and unit variance), and thence a lood $\{K_i^{(0)}\}$, with $K_i^{(0)} = J_i^{(0)}/T$, of dimensionless couplings. Eight members of the latter pool are selected at

FIG. 1. MKRG transformation for $d=3$ corresponding to length scale factor $b = 2$.

random and combined, according to Eq. (1), to give one member of a new pool. The process is repeated until a new pool $\{K_i^{(1)}\} = \{J_i^{(1)}/T\}$ of N couplings is produced. This corresponds to one iteration of Eq. (1). For $T > T_c$, all couplings flow to zero under repeated iteration, i.e., the probability distribution $P(K)$ approaches $\delta(K)$ for $n \rightarrow \infty$, where *n* is the iteration number. For $T < T_c$, the couplings flow to infinity: $P(K)$ approaches, for $n \rightarrow \infty$, a fixed shape, but with a width which increases by a factor 2^y at each iteration, with $y \approx 0.25$. (Equivalently, one can say that the temperature T scales to zero under iteration, asymptotically decreasing by a factor 2^y at each iteration.)

To illustrate the chaotic ordered phase, we consider first the MKRG equations at $T=0$. These are obtained via the replacement

$$
\tanh^{-1}(\tanh K_1 \tanh K_2) \rightarrow \operatorname{sgn}(K_1 K_2) \min(|K_1|, |K_2|)
$$

in Eq. (1). We take two pools $\{J_i\}, \{J_i'\},$ where $J_i' = J_i$ $+\epsilon x_i$, with $\epsilon = 10^{-6}$ and J_i, x_i independent Gaussian random variables with zero mean and unit variance, and follow the evolution of the quantity

$$
d_{(n)}^2 = \sum_i (J_i^{(n)} - J_i^{(n)})^2 / \sum_i [(J_i^{(n)})^2 + (J_i^{(n)})^2], \quad (2)
$$

with increasing iteration number n . (It is important to note that when eight members of the pool $\{J_i^{(n)}\}$ are chosen at random to compute one member of the pool $\{J_i^{(n+1)}\}$, the *corresponding* eight members of the pool $\{J_i^{(n)}\}$ are selected to compute the *corresponding* member \mathcal{O}_i is are selected to compute the *corresponding* member
of the pool $\{J_i^{(n+1)}\}$.) The result is shown in Fig. 2. Note that if the pools are regarded as points in an N dimensional space, the numerator in Eq. (4) is the square

FIG. 2. Square of the normalized distance between bond pools d_n^2 [Eq. (2)] as a function of MKRG iteration number *n*. +, $T = 0$; \triangle , $T = 0.25$; \Box , $T = 0.5$; \Box , $T = 0.8333$. The $T = 0$ results show the growth under iteration of an initially small difference (of relative size 10^{-6}) between the pools; the $T>0$ results are for initially identical pools at temperatures T , $T + \delta T$
with $\delta T/T = 10^{-6}$.
 $\frac{1}{2}$ $[(F_a - F_p)^2$

of the Euclidean distance between the pools after n iterations. The denominator normalizes $d_{(n)}^2$ to unity when the pools are completely uncorrelated.

From Fig. 2 one sees that the growth of $d_{(n)}^2$ is initially exponential, corresponding to a power-law dependence of $d_{(n)}^2$ on length scale $L = 2^n$, $d_{(n)}^2 \approx (\epsilon^2/2)L^{2\zeta}$, with $\zeta \approx 0.75$. The result for ζ is consistent with the prediction of the Imry-Ma argument given above, $\zeta = d_S/2 - y$, since $d_S = d - 1 = 2$ for the MKRG, and $y = 0.25$. The result for d_S follows from recognizing that any minimal energy nterface drawn through the basic unit of Fig. 1 will cut exactly four bonds (2^{d-1}) bonds for general d) and identifying this number with 2^{d_s} .

After a large number of iterations n^* , such that $L^* \equiv 2^{n^*} \approx 1/\epsilon^{1/\zeta}$, $d_{(n)}^2$ saturates at unity, corresponding to completely uncorrelated pools, i.e., to an instability of the ground state to the perturbation on length scales greater than L^* . This is in complete accord with the results of the exact numerical studies of $d = 2$ systems presented in Ref. 5. In that case, however, the results were inferred from data obtained for relatively small values of $L (L \le 10)$ and large values of ϵ , such that $\epsilon L^{\zeta} = O(1)$, whereas with the MKRG we can go to effectively enormous values of L , and hence small values of ϵ , without difficulty. In addition we can study $d = 3$ and the chaotic response to a change in temperature, the latter being absent for $d = 2$ due to the absence of a phase transition at a nonzero temperature (since $y < 0$ for $d = 2$). ^{5,8}

To investigate sensitivity to temperature, we again compute $d'_{(n)}$, Eq. (2), where $\{J_i\}$, $\{J_i'\}$ are now pools of initially identical bonds at different temperatures T, $T + \delta T$. The results are shown in Fig. 2 for three different temperatures (all below T_c), with $\epsilon = \delta T/T$ equal to 10⁻⁶ in each case. After initial transients associated with the flow of the pools to zero temperature have died away, $d_{(n)}^2$ again diverges exponentially with n , with the same exponent (i.e., the same ζ) as in the zero-temperature study. After a large number of iterations, d_n^2 again saturates at unity, indicating an instability of the spin-glass order established at a temperature T to a temperature change δT , on length scales greater than $L^* \propto 1/(\delta T)^{1/\zeta}$.

This result can be expressed more precisely, and more generally, in terms of the "interface free energy" F_{int} and the "interface entropy" S_{int} . The former may be defined, for a particular sample, as the difference in free energies between periodic (p) and antiperiodic (a) boundary conditions,

$$
F_{\rm int} = F_a - F_p.
$$

Then

$$
S_{\rm int} = -dF_{\rm int}/dT = S_a - S_p
$$

For spin glasses, these quantities may have either sign, and it is convenient to consider the scale dependence of the root-mean-square values.¹ For all $T < T_c$, the largescale behavior is controlled by the zero-temperature fixed point, so that F_{int} eventually scales with linear dimension L as L^y . A "generalized stiffness coefficient" $Y(T)$ may be defined by 1,3,4

$$
\frac{1}{2} \left[(F_a - F_p)^2 \right]_{\text{av}}^{1/2} \to \Upsilon(T) L^y, \ L \to \infty , \tag{3}
$$

where \iint_{av} indicates an average over samples and the factor $\frac{1}{2}$ is for later convenience. Within the MKRG, a member of the pool $\{J_i^{(n)}\}$ plays the role of $(F_a - F_p)/2$ for a sample of linear dimension $L = 2ⁿ$. Hence, within the MKRG,

$$
\left(\frac{1}{N}\sum_{i=1}^{N}\left(J_i^{(n)}\right)^2\right)^{1/2} \to \Upsilon(T)2^{ny}, \; n \to \infty \; . \tag{4}
$$

Y has its maximum value at $T=0$, and vanishes like $(T-T_c)$ ^{vy}, where v is the correlation length exponent, for $T \rightarrow T_C$. 3,4,9

How does S_{int} scale with L for large L? Suppose S_{int} - L^x. Since F_{int} plays the role of an effective coupling at scale L, $\delta F_{\text{int}} = -S_{\text{int}}\delta T - L^x \delta T$ is the change in that coupling induced by a temperature change δT . The system will reorganize at scale L^* when the relative change
in the coupling $\delta F_{\text{int}}/F_{\text{int}} \sim L^{*(x-y)} \delta T$ is of order unity, in the coupling or $\int_0^{\pi} e^{i\theta} \, dx$.
i.e., when $\delta T \sim L^{*(y-x)}$. But the general arguments given above (and the explicit results of the MKRG) imply that such reorganization occurs when $\delta T \sim L^{* - \zeta}$. Thus $x - y = \zeta \equiv d_S/2 - y$, giving $x = d_S/2$. This result, first suggested in Ref. 4, is seen to be a consequence of the flow to the zero-temperature fixed point at large length scales.

The above considerations allow us to derive a more quantitative relation between L^* and δT . By analogy with Eq. (3) we can introduce an amplitude function $\sigma(T)$ for S_{int} via

$$
\frac{1}{2}\left[(S_a - S_p)^2 \right]_{\rm av}^{1/2} \to \sigma(T) L^{d_S/2}, \ L \to \infty \ . \tag{5}
$$

Within the MKRG this becomes, in analogy with Eq. (4), using $d_S = 2$ (for $d = 3$),

$$
\left(\frac{1}{N}\sum_{i=1}^{N}\left(J_i^{(n)}-J_i^{(n)}\right)^2\right)^{1/2}\to\sigma(T)2^n\delta T,\ \ n\to\infty\ ,\qquad(6)
$$

provided $\delta T \ll 2^{n\zeta}$. With this insight one recognizes, from Eq. (2), that $d_{(n)}^2/(\delta T)^2$ is simply the ratio of the meansquare interface entropy to the mean-square interface free energy. Determining the length L^* by setting $[(\delta F_{int})^2]_{av}^{7/2}$ equal to $[F_{int}^2]_{av}^{1/2}$ is equivalent to setting $d_{(n)}^2$ of order unity $(\frac{1}{2}, \text{ to be precise})$ in the MKRG and gives $L^* = (\gamma/\sigma \delta T)^{1/\zeta}$. The function $\sigma(T)$ should vanish

^{&#}x27;J. R. Banavar and M. Cieplak, Phys. Rev. Lett. 48, 832 (1982).

- 2W. L. McMillan, J. Phys. C 17, 3189 (1984).
- $3A$. J. Bray and M. A. Moore, in Heidelberg Colloquium on Glassy Dynamics and Optimisation, edited by L. Van Hemmen and I. Morgenstern (Springer-Verlag, Heidelberg, 1986).
- 4D. S. Fisher and D. A. Huse, Phys. Rev. Lett. 56, 1601 (1986).
- 5A. J. Bray and M. A. Moore, Phys. Rev. Lett. 58, 57 (1987).
- 6B. W. Southern and A. P. Young, J. Phys. C 10, 2179 (1977); S. Kirkpatrick, Phys. Rev. B 15, 1533 (1977).

FIG. 3. Temperature dependence of a typical MKRG coupling normalized by 2^{ny} , after *n* iterations. \circ , $n = 8$; \circ , $n = 10$; \circ , $n = 12.$

inearly with T for $T \to 0, ^4$ while for $T \to T_C$ it should
vanish as $(T_C - T)^{\nu d_S/2 - 1}$ 10 Thus for $T \to 0, L^*$
 $\sim (T_C^2/T \delta T)^{1/\zeta}$, while for $T \to T_C, L^*/\zeta \sim [(T_C - T)/$ $ST]$ ^{1/ ζ}, where ξ is the correlation length, provided $\delta T \ll T_C - T$.

The striking fact that $S_{int} = -dF_{int}/dT$ scales as a higher power of the length than F_{int} implies that F_{int} must develop, as L increases, ever more structure as a function of T and become, in the thermodynamic limit, nondifferentiable everywhere in the interval $(0, T_C)$. The characteristic temperature resolution of the structure is given by $\delta T \sim (\gamma/\sigma)L^{-\zeta}$. To investigate this within the MKRG we look at the temperature dependence of a typical member of the bond pool, normalized by 2^{ny} , as a function of iteration number n . Typical results are shown in Fig. 3, for $n = 8$, 10, 12, and provide a vivid illustration of the onset of chaos with increasing n .

- 7Y. Imry and S.-K. Ma, Phys. Rev. Lett. 35, 1399 (1975).
- SA. J. Bray and M. A. Moore, J. Phys. C 17, L463 (1984); W. L. McMillan, Phys. Rev. B 29, 4026 (1984); 31, 340 (1985).
- ${}^{9}R.$ G. Caflisch, J. R. Banavar, and M. Cieplak, J. Phys. C 18, L991 (1985).
- ⁰This follows from finite-size scaling near T_C :

$$
[F_{\text{int}}^2]_{\text{av}}^{1/2} = f(L^{1/\nu}(T_C-T))
$$

implies

$$
[S_{\rm int}^2]_{\rm av}^{1/2} = L^{1/\nu} s(L^{1/\nu} (T_C - T)) \sim L^{d_S/2} (T_C - T)^{\nu d_S/2 - 1}
$$

for
$$
L^{1/\nu}(T_C-T) \gg 1
$$
.