Nature of Ordering in Spin-Glasses

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A new equilibrium characterization of the spin-glass—paramagnet transition is presented. It is based on the size dependence of the sensitivity of the free energy to the boundary conditions. Results of numerical studies of a three-dimensional Heisenberg spin-glass at $T=0$ are consistent with an algebraic decay of this sensitivity and suggest a zero-temperature phase transition.

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The theoretical characterization of the nature of ordering in spin-glasses still remains a challenging problem. The presence of random and conflicting exchange interactions in a spin-glass leads to no discernible long-range spatial ordering of the spins. In a pioneering paper, Edwards and Anderson (EA)[1] suggested that, even though snapshots of the spin-glass and paramagnetic states look identical, the spin-glass state, unlike the paramagnet, is characterized by the spins being frozen in time. The employment of the EA order parameter[1] leads to instabilities[2] in the phase diagram for the Sherrington-Kirkpatrick[3] model of a spin-glass. Suggestions for removing this difficulty have been made by Parisi[4] and more recently by Sompolinsky.[5] It remains unclear, however, whether there is a well-defined equilibrium phase transition between the spin-glass and paramagnetic phases or whether the freezing into a spin-glass state is a nonequilibrium glass-transition-like phenomenon.[6]

In this Letter we describe a new equilibrium characterization of spin-glasses. Our approach is in the spirit of Thouless and co-workers' ideas on electron localization.[7] We propose that the size dependence of the sensitivity of the free energy to the boundary conditions is a signature of the nature of ordering. We present numerical results for a three-dimensional classical Heisenberg spin system with random nearest-neighbor interactions and at zero temperature. Our results suggest a $T=0$ phase transition in this case.

Consider a system of N spins in a cylindrical domain of length L and cross-sectional area A. We denote the free energies of the system with periodic and antiperiodic boundary conditions, applied across the ends of the cylinder, by $F_{\rm P}$ and $F_{\rm AP}$, respectively. We define

$$\Delta f = (F_{\rm AP} - F_{\rm P})/N, \tag{1}$$

$$\gamma_m = \langle \Delta f\rangle_c, \tag{2}$$

and

$$\gamma_w = \{\langle(\Delta f - \langle\Delta f\rangle_c)^2\rangle_c\}^{1/2}, \tag{3}$$

where $\langle\dots\rangle_c$ denotes a configurational average over the distribution of the exchange constants. In the case of ferromagnets or antiferromagnets the characteristic free-energy scale of the sensitivity of the system to a change in the boundary conditions is measured by the quantity γ_m.

In spin-glasses the periodic boundary conditions do not necessarily yield a lower free energy than the antiperiodic ones and γ_m should average out to zero. This leaves γ_w as the fundamental free-energy scale in the problem. We propose that in the equilibrium spin-glass phase, if such a phase indeed exists, γ_w for large L and A is an algebraic function of A and L:

$$\gamma_w = \sigma/A^r L^p. \tag{4}$$

The parameter σ and the exponents p and r are quantities which in general depend on the specifics of the system, including the dimensionality d and the temperature T. The algebraic law, Eq. (4), is in marked contrast to the behavior of the system at temperatures greater than the spin-glass freezing temperature, $T_{\rm sg}$, where γ_w, for a large constant A, decays exponentially with L. Thus σ, given by

$$\sigma = \lim_{L\to\infty} L^p \lim_{A\to\infty} A^r\gamma_w, \tag{5}$$

is nonzero in the spin-glass phase and vanishes above $T_{\rm sg}$. The parameter σ, which is the analog of the conductivity in the localization problem[8] and is a generalization of the helicity modulus or superfluid density,[9] is a quantitative measure distinguishing between the spin-glass and paramagnetic phases.

The spin-glass may be visualized as being made up of many statistically similar blocks of length L and area A. The strength of the coupling between neighboring blocks is related to the characteristic scale of the *total* free-energy sensitivity to the boundary conditions, δF, of a single block. From Eq. (4), δF is proportional to $A^{1-r}L^{1-p} \sim L^{d(1-r)+r-p}$. Following Anderson and Pond,[10] we may identify the lower critical dimensionality (lcd) of the spin-glass with $d_c = (p-r)/(1-r)$, since for $d < d_c$ the coupling energy decreases indefinitely with the scale. It should be noted that the true ground states for two different boundary conditions are not necessarily adiabatically accessible to each other. This would seem, however, to be only relevant for studying nonequilibrium dynamical effects.

We have carried out numerical calculations of γ_w in a simple model system at $T=0$. We consider classical Heisenberg spins on a simple cubic lattice ($d=3$) coupled by nearest-neighbor exchange interactions. The distribution of exchange couplings was Gaussian characterized by unit variance and zero mean value. In order to determine the length dependence of γ_w we investigated systems with $A = 12\times 12$ and L equal to 4, 6, and 8. Periodic boundary conditions are applied in the transverse directions (across the ends of the 12×12 planes). In the longitudinal directions either periodic or antiperiodic boundary conditions could be applied.

Following Walker and Walstedt,[11] "ground states" of our systems were determined by starting from a random configuration of spins and aligning them sequentially in the direction of their instantaneous local fields. We define one iteration as N such spin alignments. The number of different starting configurations was 30 for $L=4$ and 50 for $L=6$ and 8. About a quarter of the systems were investigated for 20–50 additional initial configurations. We found that nearly complete equilibrium was achieved after about 800 iterations, at which stage the lowest-energy state was picked as the true ground state. Usually, duplicates of the ground state were obtained. The ground state was then fully equilibrated by up to 1000 additional iterations. While it is, in general, impossible to be sure that one has indeed found the true ground state, our analysis leads us to believe that the total error made is not significant. On the other hand, a meaningful investigation of systems with $L=12$ could not be carried out with only 50 initial configurations. This is due to a rapid increase of the number of "ground states" as a function of the size of the system.

For each size, Δf was determined for 23 different samples. Assuming that $\gamma_m = 0$, we calculated γ_w. Figure 1 shows a plot of $\ln\gamma_w(L)$ vs $\ln L$.[12] Our results are consistent with an algebraic decay [Eq. (4)] with $p=3$. The straight line shows this asymptotic law. Taking into account actual nonzero values of γ_m (due to finite sampling) or using $\langle|\Delta f|\rangle_c$ as the characteristic free-energy scale leads to virtually the same power law in L. Systematic deviations from the asymptotic behavior are found for smaller-sized systems. It is interesting to note that for the spin-glass samples in which all of the exchange constants have been replaced by their absolute values (ferromagnetic), the asymptotic length dependence for both γ_m and γ_w is found even for

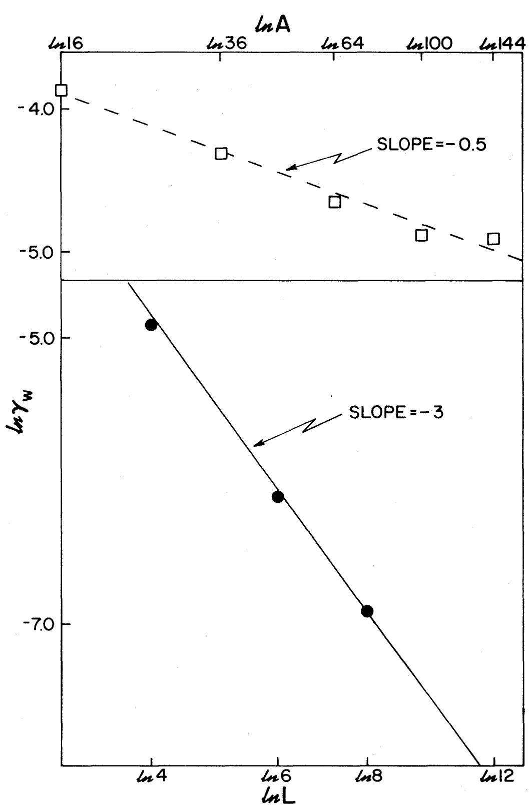

FIG. 1. Plot of $\ln\gamma_w$ vs $\ln L$ (circles) and vs $\ln A$ (squares). The length dependence is for $A=12\times 12$, whereas the area dependence is for $L=4$.

$L=6$.

With the data in Fig. 1 the possibility of an exponential decay cannot be ruled out completely. Our preliminary data for $L=12$ samples give $\gamma_w(12)\sim\gamma_w(8)$. It seems unlikely that detailed studies, leading to identification of the true ground states, would lower $\gamma_w(12)$ sufficiently to be consistent with an exponential law. Because of the existence of finite barriers the EA order parameter is 1 at $T=0$ in our model system. It would not be surprising, therefore, to have the free-energy sensitivity to the boundary conditions be an algebraic function of L. The main requirement of such a dependence is that the applied boundary conditions couple to the spin-glass ordering and our data suggest that this may indeed be the case.

In order to obtain the area dependence of γ_w, we have investigated systems with $L=4$ and $A=4\times4$, 6×6, 8×8, 10×10, and 12×12. For $A=16$, 36, and 64 we took into account 70 samples to lower the statistical error related to the smaller number of spins. For $A=100$ and 144 we considered 23 samples each. Figure 1 shows a plot of $\ln\gamma_w$ vs $\ln A$. The data are consistent with $r=\frac{1}{2}$ in Eq. (4).

Our results, $p=3$ and $r=\frac{1}{2}$, lead to the characteristic scale of the total free-energy difference δF being proportional to $A^{1/2}L^{-2}\sim L^{-1}$. This suggests the absence of the spin-glass phase at any finite temperature. Further, the algebraic dependence of δF on L at $T=0$ provides evidence for a zero-temperature phase transition.

It is interesting to compare our findings with those of Anderson and Pond.[10] Using the Migdal-Kadanoff approximation they obtained an effective exchange coupling J_{eff} proportional to $A^{1/2}L^{-1}\sim L^0$ for a three-dimensional (3D) vector spin-glass, implying that the system was at its lcd. In fact it has been suggested by Anderson[13] that the properties of the spin-glass may be understood in analogy with those of the 2D x-y model. Note that J_{eff} has the same area dependence as δF. However, the Migdal-Kadanoff approximation, on scaling away the area dependence, becomes a 1D approximation and leads to an unfrustrated ferromagnetlike length dependence.

Walstedt[14] has obtained the exchange stiffness of a Ruderman-Kittel-Kasuya-Yosida (RKKY) spin-glass by starting from a "ground state" and relaxing the system to a local energy minimum in the vicinity of the original "ground state" after imposing a small twist in the boundary conditions. Such a procedure does not explore all of phase space and indicates an L^{-1} length dependence for the characteristic total free-energy difference in agreement with the prediction of Anderson and Pond[10] (Walstedt did not investigate any area dependence in his analysis).

In contrast to Walstedt's analysis, we attempt to find the true ground state for each boundary condition. The existence of multiple "ground states" in a spin-glass allows the system to adjust more easily to changes in the boundary conditions leading to a stronger length dependence than that obtained by Walstedt. In fact, for a given boundary condition, the differences between "ground-state" energies per spin are comparable, and in many instances smaller, than the energy shift (γ_w) produced by a change in the boundary conditions.

With the numerical results on the 3D system, it is not possible to obtain the lcd of the Heisenberg spin-glass since variation of the dimensionality could change the amount of frustration in the system and result in a different exponent p.

Monte Carlo computations on an RKKY spin-glass in $d=3$ by Walstedt and Walker[15] yield no cusp in the susceptibility in the absence of any anisotropy. On the other hand, introduction of a small amount of anisotropic interactions causes the cusp to appear. This is presumably due to a trapping of the system in the vicinity of a particular energy minimum over the time scale of the simulation. It is an intriguing possibility that it is this trapping that makes the system behave as though it were at its lcd and causes the spin-glass-like peak in the susceptibility.

We conclude by noting that the equilibrium characterization introduced here, based on the size dependence of the sensitivity of the free energy to the boundary conditions, may be applicable in other situations where there is no obvious long-range order but an algebraic decay of correlation is expected.

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ONSET OF DIFFUSION AND UNIVERSAL SCALING IN CHAOTIC SYSTEMS. T. Geisel and J. Nierwetberg [Phys. Rev. Lett. 48, 7 (1982)].

The arrow in Eq. (3c) should be a double arrow denoting logical implication.

MAGNETIC SPECTRA AND ELECTRON TRANSPORT OF CURRENT-CARRYING PLASMAS. Cheng Chu [Phys. Rev. Lett. 48, 246 (1982)].

The right-hand side of Eq. (1) should read (5–8) instead of (5–80).

TIME SCALE OF FISSION AT HIGH ANGULAR MOMENTUM. A. Gavron, J. R. Beene, B. Cheynis, R. L. Ferguson, F. E. Obenshain, F. Plasil, G. R. Young, G. A. Petitt, M. Jääskeläinen, D. G. Sarantites, and C. F. Maguire [Phys. Rev. Lett. 47, 1255 (1981)].

Recently we have attempted to verify the fast-