Evidence Against Spin-Glass Order in the Two-Dimensional Random-Bond Ising Model

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By recursive methods, numerically exact free energies are calculated for $L \times L$ Ising lattices with bonds of randomly chosen sign, with $6 \leq L \leq 18$. Ground states of these systems are identified, and the response to ordering fields is studied. By performing Monte Carlo simulations for precisely the same systems we are able to unambiguously distinguish nonequilibrium phenomena from equilibrium properties. The L dependence of our results suggests that there is no nonzero spin-glass order parameter for $L \to \infty$.

It is currently debated whether the freeze-in of spin-glasses is a nonequilibrium phenomenon or a phase transition.[1-9] Experimental evidence on this question is still ambiguous.[8,9] Although theories along the lines of Edwards and Anderson[10] implied a phase transition, and results from computer simulations were taken as evidence for it,[11,12] later serious doubts arose: High-temperature series for a nearest-neighbor Ising system with random exchange $\pm J$ suggested the lower critical dimensionality $d_c = 4$, implying that there is no transition at nonzero temperature for $d < d_c$. While some theories[6] support this result, real-space renormalization methods yielded[2,3] $2 \leq d_c < 3$. The anomalous slow decay of the Edwards-Anderson order parameter

$$q(t) = \sum_{i=1}^{N} [\int_0^t dt' \sigma_i(t')/t]^2 N$$

with observation time t seen in simulations[7,11,12] was also taken as evidence against a transition; on the other hand, it was shown that such a decay can result from finite-size effects or very slow approach to thermal equilibrium[4] and a qualitatively similar decay is found[5] for all $2 \leq d \leq 5$.

In this Letter we apply a new technique to obtain the partition function of finite $d = 2$ Ising lattices with exchange constants distributed according to $P(J_{ij}) = c\delta(J_{ij} - J) + (1 - c)\delta(J_{ij} + J)$,[13,14] presenting results for $c = \frac{1}{2}$. Although we can treat fairly small systems (linear dimension $L \leq 18$) only, we note that Monte Carlo results for comparable systems have shown all characteristics of spin-glasses.[5,11] Computing the free energy per spin, $F = -k_B T \langle \ln Z_{\{J_{ij}\}} \rangle / L^2$, we obtain numerically exact $Z_{\{J_{ij}\}}$, while the average $\langle \cdots \rangle$ over the disorder is done approximately (taking the arithmetic average over about 30 realizations $\{J_{ij}\}$ yields sufficient accuracy). Our method starts by writing Z as follows (σ_{ij} denotes the spin in the ith row and jth column; $\tilde{J} \equiv J/k_B T$):

$$Z = \sum_{\{\sigma_{1j}\}} \sum_{\{\sigma_{2j}\}} \cdots \sum_{\{\sigma_{Lj}\}} [\prod_j \exp(\tilde{J}_{1j,1(j+1)} \sigma_{1j} \sigma_{1(j+1)}) \exp(\tilde{J}_{1j,2j} \sigma_{1j} \sigma_{2j})]$$
$$\times [\prod_j \exp(J_{2j,2(j+1)} \sigma_{2j} \sigma_{2(j+1)}) \exp(\tilde{J}_{2j,3j} \sigma_{2j} \sigma_{3j})] \times \cdots \times [\prod_j \exp(\tilde{J}_{Lj,L(j+1)} \sigma_{Lj} \sigma_{J(j+1)}]. \quad (1)$$

Here we use periodic boundaries $\sigma_{i(L+1)} = \sigma_{i1}$ in horizontal direction only, while in vertical direction Eq. (1) implies free boundaries. We compute Eq. (1) recursively. The first step is to compute the "horizontal" factor $\Pi_j \exp(J_{1j,1(j+1)} \times \sigma_{1j} \sigma_{1(j+1)})$ for all 2^L states of the $\{\sigma_{1j}\}$.[15] Then we compute the first "vertical" factor $\exp(J_{11,21} \times \sigma_{11} \sigma_{21})$ for the two possible choices of σ_{21}. Since for our choice of boundary conditions we have then taken into account all interactions of σ_{11}, we now perform the trace over σ_{11}, keeping terms for all states of $\{\sigma_{1j}\}$ ($j \geq 2$), σ_{21}. Then the second "vertical" factor $\exp(J_{12,22} \sigma_{12} \sigma_{22})$ is considered for the two states of σ_{22}, and the trace over σ_{12} is performed, etc. After completion of the second row the trace over all $\{\sigma_{1j}\}$ is completed, and we may compute now the "horizontal" factor for the second row, start the third one, etc. Thus we obtain $Z_{\{J_{ij}\}}$ numerically for arbitrary T, and computing $\ln Z_{\{J_{ij}\}}$ for a set of neighboring T's we get internal energy per spin, U, and specific heat per spin, C, with very good accuracy. The extension of the method to include arbitrary fields is straightforward.

Somewhat more involved is the identification of ground states. We start by storing the n ($n \approx 10^2$) states of the first row having the lowest energies. We combine these states with all states of the second row, and keep again the n states which now have the lowest energy, etc. After completion of this procedure we compare the total en-

ergy $U(k)$ for each of the remaining n states $\{k\}$ with $L^2U(T=0)$: If $U_{\rm tot}(k)=L^2U(T=0)$, then k is a ground state. If no ground state is found, n has to be increased and the procedure repeated. An alternative is a standard Monte Carlo run for our set $\{J_{ij}\}$ and slowly cooling the temperature down to $T=0$, starting at $T=2J$ from a random spin configuration and recording the internal energy. A comparison with $U(T=0)$ as obtained above shows that for $L=12$ the cooling time t_c must be 5×10^3 to 10^4 Monte Carlo steps (MCS)/spin, while for $L=16$ t_c must be 10^4 to 2×10^4, and for $L=18$ t_c must be 3×10^4 to 6×10^4. Correcting for the effects of our two free boundaries, we also find the ground-state energy of larger systems reliably. For $L=32$ a time $t_c=2\times10^5$ was necessary to actually reach this extrapolated ground-state energy. Since in previous simulations[7,11,12] much smaller t_c's were used, we conclude that true thermal equilibrium was not reached there at low temperatures. Hence much of the anomalous slow dynamics of this model, as well as the irreversible behavior, are due to the fact that the system is locked in low-lying metastable states, and one has to cross fairly large energy barriers by overturning clusters of spins to reach still lower "valleys" in configuration space. This result confirms recent suggestions of Dasgupta, Ma, and Hu.[16]

These nonequilibrium effects, however, do not invalidate all Monte Carlo data. Figure 1 shows the specific heat of a 16×16 system obtained from our exact method. Monte Carlo results with a total observation time $t_{\rm obs}=2\times10^4$ are included, where the system was started either from a ground state or a disordered state ($t_c=2\times10^3$ only). These data agree with each other as well as with the exact results and with the $L=80$ data of Kirkpatrick.[12] Figure 2(a) shows Monte Carlo results for $q(t)$ for the same runs. These data again agree with each other at least roughly, and imply a freeze-in transition at $k_BT/J\approx1.3\pm0.1$, in agreement with Ref. 12. Because of the finiteness of our systems, there is of course no symmetry breaking in an exact calculation, and $q\equiv\sum_i\langle\sigma_i\rangle^2/N=0$ for all $N<\infty$. For studying the ordering it is hence more convenient to use the order parameter ψ measuring the alignment to ground-state spin configurations.[4,5,11] For a finite system this order parameter is related to the associate susceptibility χ_ψ by[17,18] [$N\equiv L^2$ in our case]

$$\psi^2=k_BT\chi_\psi/N=\sum_{i,j}\langle\sigma_i\sigma_j\rangle_0\langle\sigma_i\sigma_j\rangle_T/N^2. \qquad (2)$$

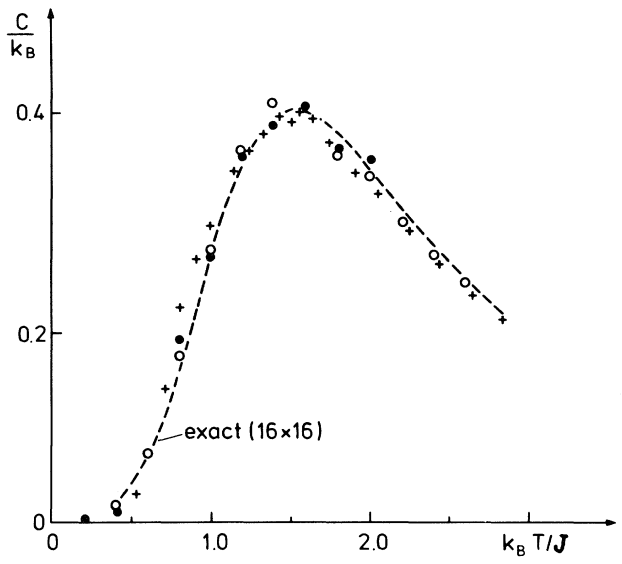

FIG. 1. Specific heat per spin plotted vs temperature for a particular realization of the $\pm J$ spin-glass for $L=16$. Monte Carlo results for precisely the same system are included for runs starting either with a random spin configuration (full circles) or with a ground-state configuration (open circles). Plusses denote Monte Carlo results for $L=80$ of Ref. 12.

We obtain ψ^2 from Monte Carlo simulations by starting in the lth ground state $\{\sigma_i^{(l)}\}$ and calculating the time average of $\psi_l^2(t)=[\sum_i\sigma_i^{(l)}\sigma_i(t)/N]^2$. This quantity has to be averaged over all ground states, but it turns out that an average over only several of them yields sufficient accuracy. In the exact calculation we obtain $\psi_l^2=k_BT\,\chi_\psi^{ll}/N$ from applying a field $H_\psi^{(l)}$, whose direction at each site i is given by $\{\sigma_i^{(l)}\}$, and with use of $\chi_\psi^{ll}=\partial^2F/\partial(H_\psi^{(l)})^2$. From Fig. 2(b) we note that the simulation greatly overestimates ψ^2 at low T. Obviously, by far too large correlations $\langle\sigma_i\sigma_j\rangle_T$ at large distances $\vec{r}_i-\vec{r}_j$ are predicted because the system stays in an energetically favorable valley in configuration space [close to the particular ground state $\{\sigma_i^{(l)}\}$] for a long time. Hence Monte Carlo results for both ψ^2 and $q(t)$ cannot be expected to closely approximate the *equilibrium* behavior of an infinite system.

In a Mattis spin-glass or equivalent Ising ferromagnet, ψ^2 as defined in Eq. (2) quickly approaches the order parameter squared of the infinite system as N increases, see Fig. 3. We note that in the "frustrated" case, ψ^2 steadily decreases as N is increased. The saturation value $\psi^2(T=0)$ decreases so strongly that we suggest

$$\lim_{N\to\infty}\psi^2(T=0)=0,$$

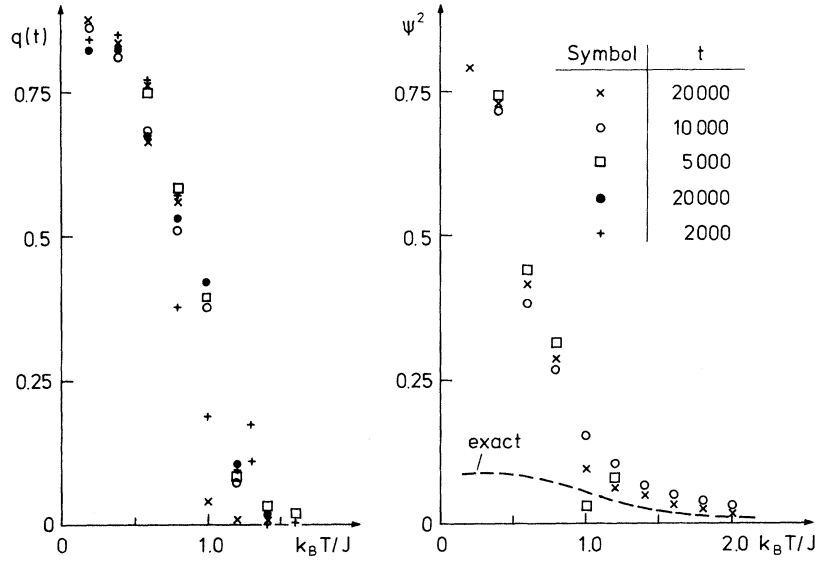

FIG. 2. Spin-glass order parameters $q(t)$ (left part) and ψ^2 (right part) plotted vs temperature, as obtained from Monte Carlo and exact calculation, with use of $L=16$ and a realization $\{J_{ij}\}$ which has particularly small ψ^2. Various observation times are shown (data for $t=2000$ are the results for $L=80$ of Ref. 12; these data and the full circles have random spin configurations as initial condition, while the others have a ground state as initial condition).

i.e., no order even in the ground state. On the other hand, the system differs from an ordinary paramagnet, for which $\psi^2 \equiv 1/N$. We have strong correlations in the ground state, consistent with other approaches[18,19]; the N dependence of $\psi^2(T=0)$ in Fig. 3 suggests that

$$\langle \sigma_i \sigma_j \rangle^2 \xrightarrow[|\vec{r}_i-\vec{r}_j|\to\infty]{} 1/|\vec{r}_i-\vec{r}_j|^p$$

(in the fully frustrated Ising antiferromagnet this decay also occurs with $p=1$,[20] and perhaps $p \leq 1$ in our case as well). This result would be consistent with the fact that concentration expansions for χ_ψ in diluted spin-glasses yield a strong divergence.[18] If such a power-law decay also occurs for $0<T<T_c$, it would imply a transition without order parameter just as in the $d=2$ XY model.[21] The inflection points in the curves of Fig. 3 would be an estimate of T_c. These inflection points seem to shift towards smaller T as N increases, and hence there may be $T_c=0$ for $d=2$. But the similarity of Monte Carlo results for all d, $2 \leq d \leq 5$, where $q(t)$ slowly decays with time, and ψ^2 quickly decreases with temperature,[5] could indicate that a transition of this type occurs at higher dimensionalities.

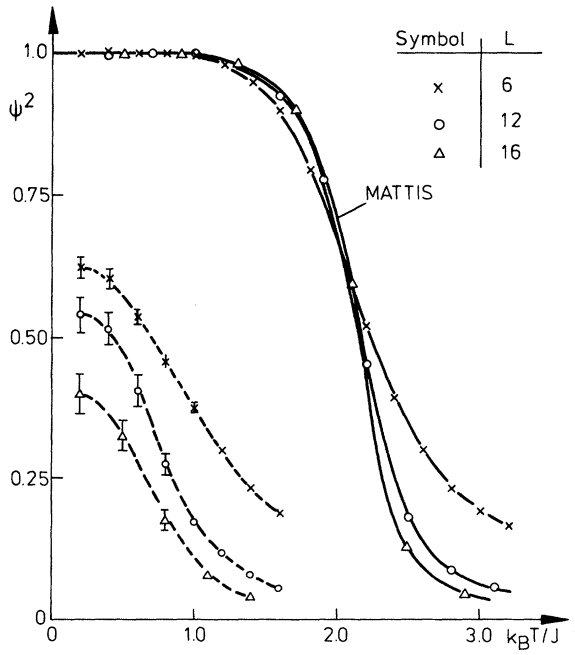

FIG. 3. Average spin-glass order parameter ψ^2 plotted vs temperature for several L. Error bars are calculated from averages over 100 realizations $\{J_{ij}\}$ for $L=6$, 40 realizations for $L=12$, and 25 realizations for $L=16$. Full curves denote exact results for $\pm J$ Mattis spin-glasses of the same size (note $k_BT_c^{\text{Mattis}}/J \cong 2.27$).

We have obtained similar results for the spin-glass with Gaussian bond distribution, too: Monte Carlo results for specific heats are reliable, but the relaxation time to reach a ground state increases exponentially with system size. There is one important difference: The order parameter of the Gaussian model approaches unity for $T \to 0$ for all L!

In conclusion, by combining our recursive calculation of partition functions of finite disordered systems with simulations, we have separated equilibrium from nonequilibrium effects. From the size dependence we conclude that there is no nonzero order parameter for $d=2$ Ising $\pm J$ spin-glasses, although there are strong spin correlations over large distances at low temperatures. Applications of our method to $c\neq\frac{1}{2}$ and Ising systems with random fields are in progress.[22] Clearly, this method should yield useful results for a large class of models for disordered materials. In addition, investigating a possible power-law decay of correlations theoretically from the point of view of frustration and gauge invariance[12,14] would be very interesting.

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[1]R. Fisch and A. B. Harris, Phys. Rev. Lett. 38, 785 (1977).
[2]P. W. Anderson and C. M. Pond, Phys. Rev. Lett. 40, 903 (1978).
[3]W. Kinzel and K. H. Fischer, J. Phys. C 11, 2115 (1975).
[4]D. Stauffer and K. Binder, Z. Phys. B 30, 313 (1978).
[5]D. Stauffer and K. Binder, Z. Phys. B 34, 97 (1979).
[6]A. J. Bray and M. A. Moore, Phys. Rev. Lett. 41, 1068 (1978), and J. Phys. C 12, 79 (1979).
[7]A. J. Bray and M. A. Moore, J. Phys. F 7, L333 (1977), and C 11, 1187 (1978).
[8]E. D. Dahlberg, M. Hardiman, R. Orbach, and J. Souletie, Phys. Rev. Lett. 42, 401 (1979).
[9]H. v. Löhneysen, J. L. Tholence, and R. Tournier, J. Phys. (Paris), Colloq. 39, C6-992 (1978).
[10]S. F. Edwards and P. W. Anderson, J. Phys. F 5, 965 (1975).
[11]K. Binder and K. Schröder, Phys. Rev. B 14, 2142 (1976).
[12]S. Kirkpatrick, Phys. Rev. B 16, 4630 (1977).
[13]To reduce fluctuations going from one realization $\{J_{ij}\}$ to another one, we furthermore require (at $c=\frac{1}{2}$), for each individual realization, that $\Sigma_{\langle i,j\rangle}J_{ij}=0$, and that the concentration of frustrated plaquettes [G. Toulouse, Commun. Phys. 2, 115 (1977)] exactly equals $\frac{1}{2}$. These conditions follow from $P(J_{ij})$ for $N\to\infty$ but would hold only approximately for finite N. This "restricted" $P(J_{ij})$ is also a valid distribution for a spin-glass, of course.
[14]Toulouse, Ref. 13.
[15]It is the storage requirement for this factor which prevents us from studying larger L.
[16]C. Dasgupta, S.-k. Ma, and C.-k. Hu, to be published.
[17]K. Binder, Z. Phys. B 26, 339 (1977).
[18]A. Aharony and K. Binder, to be published.
[19]J. Vannimenus and L. de Sèze, unpublished.
[20]J. Stephenson, J. Math. Phys. 11, 420 (1970).
[21]J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6, 1181 (1973).
[22]I. Morgenstern and K. Binder, unpublished.

Frustration Effect in Quantum Spin Systems

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We have calculated the ground-state properties of the $s=\frac{1}{2}$ XY and Heisenberg models on finite triangular and square lattices with competing interactions which would lead to frustrated classical spin models. The evidence favors the hypothesis that quantum spin models on infinite two-dimensional lattices experience no frustration.

The concept of the *frustration* effect in spin systems with competing interactions has been elaborated especially for the $s=\frac{1}{2}$ Ising model[1,2] and for the planar model.[3] The assignment of the signs of the interactions to bonds of the lattice is such that the ground state of these classical systems is highly degenerate. A motivation for such studies is the elucidation of the nature of spin-glasses.[4] The first frustrated system studied was the Ising antiferromagnet on the triangular lattice.[5]

Frustrated spin models are usually characterized by the Hamiltonian

$$\mathcal{H}=-\tfrac{1}{2}\sum_{\langle ij\rangle}J_{ij}\sum_{\alpha=1}^{n}S_i^{\alpha}S_j^{\alpha}. \tag{1}$$

The first sum is over nearest-neighbor pairs of sites on a lattice. $n=1$, 2, and 3 correspond to the Ising, XY, and Heisenberg models, respectively. In the classical ($S=\infty$) limit, S_i^{α} is a Cartesian component of a unit vector; in the ex-

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