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Influence of boundary conditions on random unfrustrated magnetic systems

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The size dependence of the sensitivity of the free energy to a change in the boundary conditions is investigated for disordered unfrustrated systems. Characteristically different dependencies are found in the high- and low-temperature phases and an estimate of the lower critical dimensionality of the system may be obtained from the low-temperature behavior. Results of studies of random Heisenberg and Ising ferromagnets with periodic and antiperiodic boundary conditions and with random boundary conditions are presented.

I. INTRODUCTION

In a recent paper Banavar and Cieplak[1] investigated the influence of the boundary conditions on the free energy of a spin-glass and suggested an equilibrium characterization of the spin-glass phase. It is clear that the novel properties of spin-glasses arise from frustration effects due to random competing exchange interactions. Nevertheless, it would be useful to carry out similar investigations for random unfrustrated magnetic systems with a view of testing some of the concepts in Ref. 1.

Consider a system of N spins in a rectangular box of length L and cross-sectional area A. Following Ref. 1 we denote the free energies of the system with periodic and antiperiodic boundary conditions, applied across the ends of the box, by F_{P} and F_{AP}, respectively. We define

$$\Delta f=\frac{F_{\mathrm{AP}}-F_{\mathrm{P}}}{N}\ , \tag{1}$$

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

and

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

where $\langle\ \rangle_c$ denotes a configurational average over the distribution of the exchange constants.

It was noted in Ref. 1 that, for a spin-glass, γ_m averages out to zero, leaving γ_w as a characteristic free-energy scale of the sensitivity of the system to a change of boundary conditions. It was further suggested that in the spin-glass phase the length dependence of γ_w, for a fixed large A, followed an algebraic law and was markedly different from an exponential decay of γ_w found in paramagnets. It was argued that, knowing the length and area dependencies of γ_w, one could obtain the lower critical dimensionality (LCD) of the spin-glass.

In this paper we study γ_m and γ_w of several random unfrustrated magnetic systems. In the sytems we discuss, γ_m does not average out to zero and in fact provides the characteristic free-energy scale that determines the nature of the ordered phase. In Sec. II results of calculations on a classical Heisenberg chain are presented. Evidence is given for a zero-temperature phase transition and the LCD is found to be 2. Section III contains results of similar calculations on an Ising (quantum) chain.

Section IV deals with a three-dimensional classical Heisenberg system with random ferromagnetic interactions at $T=0$. Approximate analytical calculations yield results in excellent agreement with those obtained by studying the size dependence of γ_w and γ_m numerically. The numerical data on this simpler system serve as a reference for the analogous data on spin-glasses presented in Ref. 1.

It may be argued that the application of periodic and antiperiodic boundary conditions to spin-glasses is somewhat analogous to the application of random boundary conditions to a ferromagnet. In Sec. V we discuss this problem and show both for two-dimensional Ising and Heisenberg systems that the imposition of a conjugate pair of boundary conditions gives the correct size dependence for γ_m.

II. HEISENBERG CHAIN WITH RANDOM EXCHANGE COUPLINGS

Consider a one-dimensional Heisenberg system with the Hamiltonian

$$H=-\sum_{i=1}^{L-1} J_{i,i+1}\vec{S}_i\cdot\vec{S}_{i+1}+H_B \tag{4}$$

with

$$H_B=-J_{L,1}\vec{S}_L\cdot\vec{S}_1\eta \ , \tag{5}$$

where $\eta=\pm 1$ for periodic (P) and antiperiodic (AP) boundary conditions, respectively. We assume that the probability distribution of the exchange couplings $J_{i,i+1}$ is bond independent and not singular. The spins $\vec{S}_i$ are classical unit vectors. The exchange couplings are either all positive or all negative. In the latter case L is taken to be even so as to preserve the sublattice symmetry.

Following Blume, Heller, and Lurie[2] we write the partition function for the system as

$$Z_{\mathrm{P,AP}}=\frac{1}{(4\pi)^L}\int d\vec{S}_1\cdots\int d\vec{S}_L A(\vec{S}_1,\vec{S}_2)A(\vec{S}_2,\vec{S}_3)\cdots A(\vec{S}_L,\pm\vec{S}_1) \ , \tag{6}$$

where

$$A(\vec{S}_i,\vec{S}_{i+1})=\exp(\beta J_{i,i+1}\vec{S}_i\cdot\vec{S}_{i+1}) \ , \tag{7}$$

$\beta=1/k_BT$, and $d\vec{S}_i$ represents an element of solid angle of the ith spin. We are interested in the free-energy difference per spin, which is given by

$$\Delta f=\frac{k_BT}{L}\ln\left[\frac{Z_{\mathrm{P}}}{Z_{\mathrm{AP}}}\right] . \tag{8}$$

We can calculate Δf by considering the integral eigenvalue problem

$$\int\frac{d\vec{S}_{i+1}}{4\pi}A(\vec{S}_i,\vec{S}_{i+1})\psi_n(\vec{S}_{i+1}) =\lambda_n(\beta J_{i,i+1})\psi_n(\vec{S}_i) \ . \tag{9}$$

It has been shown by Blume *et al.*[2] that for isotropic exchange couplings the eigenfunctions ψ_n are the spherical harmonics $Y_l^m(\vec{S}_i)$ and the corresponding eigenvalues are $\lambda_n=i_l(\beta J_{i,i+1})$. Here the functions $i_l(x)$ are spherical Bessel functions of imaginary argument and the eigenvalues do not depend on m. Since the eigenfunctions $\psi_n(\vec{S})$ form a complete set, the kernel of the integral equation (9) can be written as

$$A(\vec{S}_i,\vec{S}_{i+1})=4\pi\sum_{l,m} i_l(\beta J_{i,i+1}) \times Y_l^{m*}(\vec{S}_i)Y_l^m(\vec{S}_{i+1}) \ . \tag{10}$$

By substituting (10) into (6) and by making use of the orthogonality of the eigenfunctions we get

$$\begin{aligned} Z_{\mathrm{P,AP}}&=\sum_{l,m}\prod_{i=1}^{L} i_l(\beta J_{i,i+1})\int d\vec{S}_1 Y_l^{m*}(\vec{S}_1)Y_l^m(\pm\vec{S}_1)\\ &=\sum_{l=0}^{\infty}(2l+1)(\pm1)^l\prod_{i=1}^{L} i_l(\beta J_{i,i+1})=\prod_{i=1}^{L} i_0(\beta J_{i,i+1})\left[1\pm3\prod_{i=1}^{L}\frac{i_1(\beta J_{i,i+1})}{i_0(\beta J_{i,i+1})}+\cdots\right] . \end{aligned} \tag{11}$$

The result for the bulk partition function [the first term of Eq. (11)] is in agreement with that obtained by Fisher[3] and Tomita and Mashiyama[4] when there is no disorder in the exchange couplings.

The expansion employed in Eq. (11) does not hold at $T=0$ as, at $T=0$, all eigenvalues become equal. For $T\neq0$, we have

$$\lambda_{l+1}(\beta J_{i,i+1})<\lambda_l(\beta J_{i,i+1}) \ ,$$

and then

$$\Delta f\approx\frac{6k_BT}{L}\prod_{i=1}^{L}\frac{i_1(\beta J_{i,i+1})}{(\beta J_{i,i+1})} \ . \tag{12}$$

The expansion (12) for Δf is exact as $T\to\infty$ and can be considered as the leading term in a $1/T$ expansion. On performing the configurational average we get

$$\gamma_m=6k_BT\frac{a^L}{L} \tag{13}$$

and

$$\gamma_w=6k_BT\frac{1}{L}(b^{2L}-a^{2L})^{1/2} \ , \tag{14a}$$

which for $L\gg1$ becomes

$$\gamma_w\approx6k_BT\frac{b^L}{L} \ . \tag{14b}$$

Here

$$a=\left\langle \frac{i_1(\beta J_{1,2})}{i_0(\beta J_{1,2})} \right\rangle_c$$
$$=\left\langle \coth(\beta J_{1,2})-\frac{1}{\beta J_{1,2}} \right\rangle_c \tag{15}$$

and

$$b=\left\langle \left[\frac{i_1(\beta J_{1,2})}{i_0(\beta J_{1,2})} \right]^2 \right\rangle_c^{1/2} .$$

From Eqs. (13) and (14), it is clear that both γ_m and γ_w are exponential functions of L. It is interesting to note that in this model, at nonzero temperatures, the correlation between two spins decays exponentially as the separation between them increases.[4]

In the limit of high temperatures

$$a=\tfrac{1}{3}\beta\langle J_{1,2}\rangle_c \tag{16}$$

and

$$b=\tfrac{1}{3}\beta\langle J_{1,2}^2\rangle_c^{1/2} . \tag{17}$$

At $T=0$ the system orders ferromagnetically or antiferromagnetically, depending on the sign of the exchange couplings. Antiperiodic boundary conditions impose a twist in the ground-state configuration. The relative angle between neighboring spins becomes modified by an amount proportional to π/L. Thus

$$\Delta f=\frac{1}{L}\sum_{i=1}^{L} |J_{i,i+1}|[1-\cos(\pi\alpha_{i,i+1}L)] , \tag{18a}$$

which in the $L \gg 1$ limit becomes

$$\Delta f=\frac{\pi^2}{2L^3}\sum_{i=1}^{L} |J_{i,i+1}|\alpha_{i,i+1}^2 , \tag{18b}$$

where $\alpha_{i,i+1}$ is a coefficient of proportionality such that $\sum_i^L \alpha_{i,i+1}=L$. The requirement of minimal energy imposes the condition

$$J_{i,i+1}\alpha_{i,i+1}=\mathscr{J} \quad (L \gg 1) , \tag{19}$$

where $\mathscr{J}$ denotes a constant. This constant is equal to $L(\sum_i^L J_{i,i+1}^{-1})^{-1}$. We have assumed that none of the exchange constants $J_{i,i+1}$ is zero. If this is not the case, the one-dimensional system splits up into two different subsystems and the usual thermodynamical limit cannot be taken.

In sharp contrast to the situation at $T\neq 0$, the $T=0$ values of γ_m and γ_w are algebraic functions of L for sufficiently large L. We find

$$\gamma_m=\frac{1}{2L^2}\pi^2\langle\, |J_{1,2}|\,\alpha_{1,2}^2\rangle_c$$
$$=\frac{1}{2L^2}\pi^2\left\langle \frac{\mathscr{J}^2}{|J_{1,2}|} \right\rangle_c \tag{20}$$

and

$$\gamma_w=\frac{1}{2L^{5/2}}\pi^2(\langle J_{1,2}^2\alpha_{1,2}^4\rangle_c-\langle J_{1,2}\alpha_{1,2}^2\rangle_c^2)^{1/2}$$
$$=\frac{1}{2L^{5/2}}\pi^2\left[\left\langle \frac{\mathscr{J}^4}{J_{1,2}^2}\right\rangle_c-\left\langle \frac{\mathscr{J}^2}{J_{1,2}}\right\rangle_c^2\right]^{1/2} . \tag{21}$$

The quantity γ_m is identified as the characteristic free-energy scale for the sensitivity of the system to a change in the boundary conditions. The power-law dependence of γ_m on L at $T=0$, taken together with the exponential dependence at nonzero temperatures, confirms a zero-temperature phase transition. Furthermore, the L^{-2} dependence of γ_m, which as shown in Sec. IV, holds also in higher dimensions, confirms that the LCD of the Heisenberg spin system[5,6] is 2. It is interesting to note that the $L^{-5/2}$ law for γ_w is in accord with the central limit theorem and shows that the distribution of the free energies around the mean value narrows more rapidly than the rate at which the mean value approaches zero. It is possible to rewrite Eq. (20) as

$$\gamma_m=\frac{1}{2}\Upsilon\frac{\pi^2}{L^2} \tag{22}$$

where $\Upsilon=\langle\, |J_{1,2}|\,\alpha_{1,2}^2\rangle_c$ is a generalization of the helicity modulus[7] to random systems.

III. ISING CHAIN WITH RANDOM EXCHANGE COUPLINGS

In analogy with the discussion in Sec. II we now treat an Ising chain[8] with the Hamiltonian given by

$$H=-\sum_{i=1}^{L-1} J_{i,i+1}\sigma_i^z\sigma_{i+1}^z+H_B \tag{23}$$

with

$$H_B=-J_{L,1}\sigma_L^z\sigma_1^z\eta , \tag{24}$$

where again $\eta=\pm 1$ for periodic and antiperiodic boundary conditions, respectively. Here σ_i^z denotes the z-component Pauli matrix at the ith site. If σ_i stands for one of the two eigenvalues of σ_i^z, then the partition functions for the two kinds of boundary conditions read

$$Z_{\mathrm{P,AP}}=\sum_{\sigma_1}\cdots\sum_{\sigma_L}\langle\sigma_1|\mathrm{P}_{1,2}|\sigma_2\rangle\cdots\times\langle\sigma_L|\mathrm{P}_{L,1}|\pm\sigma_1\rangle$$

$$=\sum_{\sigma_1}\langle\sigma_1|\prod_{i=1}^{L}\mathrm{P}_{i,i+1}|\pm\sigma_1\rangle\ , \tag{25}$$

where

$$\mathrm{P}_{i,i+1}=e^{\beta J_{i,i+1}\sigma_i^z\sigma_{i+1}^z}=\begin{bmatrix} e^{\beta J_{i,i+1}}, & e^{-\beta J_{i,i+1}} \\ e^{-\beta J_{i,i+1}}, & e^{\beta J_{i,i+1}} \end{bmatrix}\ . \tag{26}$$

The eigenvalues of $\mathrm{P}_{i,i+1}$ are

$$\lambda_{\pm}(\beta J_{i,i+1})=e^{\beta J_{i,i+1}}\pm e^{-\beta J_{i,i+1}}\ . \tag{27}$$

It is straightforward to show that

$$Z_{\mathrm{P,AP}}=\prod_{i=1}^{L}\lambda_+(\beta J_{i,i+1})\pm\prod_{i-1}^{L}\lambda_-(\beta J_{i,i+1})\ . \tag{28}$$

For nonzero temperatures

$$\lambda_-(\beta J_{i,i+1})<\lambda_+(\beta J_{i,i+1})$$

and

$$\Delta f\simeq\frac{2k_BT}{L}\prod_{i=1}^{L}\frac{\lambda_-(\beta J_{i,i+1})}{\lambda_+(\beta J_{i,i+1})}\ . \tag{29}$$

It follows that γ_m and γ_w decay exponentially on increasing L and are given by

$$\gamma_m=2k_BT\frac{\tilde{a}^L}{L} \tag{30}$$

and

$$\gamma_w=2k_BT\frac{\tilde{b}^L}{L}\quad(L\gg1)\ , \tag{31}$$

where

$$\tilde{a}=\langle\tanh^2(\beta J_{1,2})\rangle_c\ , \tag{32}$$

$$\tilde{b}=\langle\tanh^2(\beta J_{1,2})\rangle_c^{1/2}\ . \tag{33}$$

At high temperatures $\tilde{a}=\beta\langle J_{1,2}\rangle_c$ and $\tilde{b}=\beta\langle J_{1,2}^2\rangle_c^{1/2}$.

Consider now the situation at $T=0$. On imposition of antiperiodic boundary conditions the system flips at its weakest bond $J_{\min}$. Therefore,

$$\Delta f=\frac{2|J_{\min}|}{L} \tag{34}$$

and

$$\gamma_m=\frac{1}{L}2\langle|J_{\min}|\rangle_c\ , \tag{35}$$

$$\gamma_w=\frac{2}{L}(\langle J_{\min}^2\rangle_c-\langle J_{\min}\rangle_c^2)^{1/2}\ . \tag{36}$$

It is clear that the Ising chain undergoes a zero-temperature phase transition and, in contrast to the Heisenberg system, has a LCD of 1. (We have assumed that $\langle|J_{\min}|\rangle_c$ is independent of length. If, in fact, due to the nature of the probability distribution, $\langle|J_{\min}|\rangle_c$ has a length dependence, it seems that in higher dimensions and for reasonable probability distributions, this spurious length dependence disappears, restoring the result that the LCD is 1.)

IV. THREE-DIMENSIONAL DISORDERED HEISENBERG FERROMAGNET

Consider now the three-dimensional Heisenberg system given by the Hamiltonian

$$\begin{aligned}H=&-\sum_{i=1}^{L-1}\sum_{k=1}^{\sqrt{A}}\sum_{l=1}^{\sqrt{A}}J_{i,i+1}^{k,l}\vec{\mathrm{S}}_{i,kl}\cdot\vec{\mathrm{S}}_{i+1,k,l}\\&-\sum_{i=1}^{L}\sum_{k=1}^{\sqrt{A}-1}\sum_{l=1}^{\sqrt{A}}J_{k,k+1}^{i,l}\vec{\mathrm{S}}_{i,k,l}\cdot\vec{\mathrm{S}}_{i,k+1,l}\\&-\sum_{i=1}^{L}\sum_{k=1}^{\sqrt{A}}\sum_{l=1}^{\sqrt{A}-1}J_{l,l+1}^{i,k}\vec{\mathrm{S}}_{i,k,l}\cdot\vec{\mathrm{S}}_{i,k,l+1}+H_B\ ,\end{aligned} \tag{37}$$

with

$$\begin{aligned}H_B=&-\eta\sum_{k=1}^{\sqrt{A}}\sum_{l=1}^{\sqrt{A}}J_{L,1}^{k,l}\vec{\mathrm{S}}_{L,k,l}\cdot\vec{\mathrm{S}}_{1,k,l}\\&-\sum_{i=1}^{L}\sum_{l=1}^{\sqrt{A}}J_{\sqrt{A},1}^{i,l}\vec{\mathrm{S}}_{i,\sqrt{A},l}\cdot\vec{\mathrm{S}}_{i,1,l}\\&-\sum_{i=1}^{L}\sum_{k=1}^{\sqrt{A}}J_{\sqrt{A},1}^{i,k}\vec{\mathrm{S}}_{i,k,\sqrt{A}}\cdot\vec{\mathrm{S}}_{i,k,1}\ ,\end{aligned} \tag{38}$$

and η takes on the values ±1 for periodic and antiperiodic boundary conditions, respectively. Periodic boundary conditions are imposed across the planes of area A. The exchange interactions are assumed to be all positive (ferromagnetic) and for convenience they have been divided into couplings within the planes of area A ($J_{k,k+1}^{i,l}$ and $J_{l,l+1}^{i,k}$) and the interplanar ones ($J_{i,i+1}^{k,l}$).

At high temperatures, in the paramagnetic phase, correlations between spins decay exponentially as their separation increases. Thus, for large L, the dominant length dependence of Δf, and therefore also of γ_m and γ_w, is expected to follow an exponential law, similar to the explicit results for the one-dimensional systems studied in Secs. II and III.

Let us turn now to the $T=0$ situation. With periodic boundary conditions in the longitudinal (parallel to L) direction, the ground state corresponds to a configuration in which all spins are parallel. The corresponding energy is

$$F_P = -\sum_{i=1}^{L}\sum_{k=1}^{\sqrt{A}}\sum_{l=1}^{\sqrt{A}}(J_{i,i+1}^{k,l}+J_{k,k+1}^{i,l}+J_{l,l+1}^{i,k}), \tag{39}$$

provided the spins are assumed to be of unit length. Antiperiodic boundary conditions impose a twist in this configuration. Since in the A planes the boundary conditions remain periodic, the spins within each plane stay roughly parallel to each other. They would be exactly parallel if the intraplanar couplings were much stronger than the interplanar ones. In our approximation only one-third of the bonds gets twisted. The twisting angle is of the order of π/L. Thus

$$\Delta f \approx \frac{1}{AL}\sum_{i=1}^{L}\sum_{k=1}^{\sqrt{A}}\sum_{l=1}^{\sqrt{A}} J_{i,i+1}^{k,l}[1-\cos(\pi\alpha_{i,i+1}^{k,l}/L)] \tag{40}$$

where $\alpha_{i,i+1}^{k,l}$ are parameters to be chosen so as to minimize the free-energy difference. In what follows we make the simplifying approximation $\alpha_{i,i+1}^{k,l}=1$. The size dependence thus obtained is, however, independent of this approximation. We find

$$\Delta f \approx \frac{1}{LA}(1-\cos\pi/L)\sum_{i=1}^{L}\sum_{k=1}^{\sqrt{A}}\sum_{l=1}^{\sqrt{A}} J_{i,i+1}^{k,l} . \tag{41}$$

This yields

$$\gamma_m \approx (1-\cos\pi/L)\langle J_{1,2}^{1,2}\rangle_c \tag{42}$$

and

$$\gamma_w \approx \frac{1}{\sqrt{AL}}(1-\cos\pi/L)[\,\langle (J_{1,2}^{1,2})^2\rangle_c - \langle J_{1,2}^{1,2}\rangle_c^2]^{1/2} . \tag{43}$$

For $L \gg 1$ Eqs. (42) and (43) become

$$\gamma_m \approx \frac{1}{2}\frac{\pi^2}{L^2}\langle J_{1,2}^{1,1}\rangle_c \tag{44}$$

and

$$\gamma_w \approx \frac{\pi^2}{2A^{1/2}L^{5/2}}[\langle (J_{1,2}^{1,1})^2\rangle_c - \langle J_{1,2}^{1,1}\rangle_c^2]^{1/2} . \tag{45}$$

Similar results are obtained for a random Heisenberg antiferromagnet at zero temperature. Note that Eqs. (44) and (45), which were derived using the one-dimensional approximation, hold in any dimension, with the exception that at $d=1$ the $A^{-1/2}$ factor in (45) disappears.

In spin-glasses, γ_m averages out to zero, leaving γ_w as the characteristic energy scale of the sensitivity to changes in boundary conditions. In a spin-glass numerical calculations[1] of γ_w suggest that $\gamma_w \sim A^{-1/2}L^{-3}$. The higher power of L is due to frustration effects in spin-glasses which lead to a large ground-state degeneracy. This degeneracy results in the system being better able to adjust to changes in the boundary conditions than in the disordered ferromagnet.

With the use of the present approach it is straightforward to show that for spiral systems[9] without any disorder (ferromagnets and antiferromagnets may be considered as special cases of spiral systems) at $T=0$, $\gamma_m \sim L^{-2}$. This follows readily from the fact that imposition of antiperiodic boundary conditions effectively shifts the pitch of the spiral by π/L. Since the incremental free energy, by general symmetry arguments, must be even in π/L and must go to zero as π/L tends to zero, a Taylor expansion of Δf is expected to have $(\pi/L)^2$ as its leading term. The LCD of such systems is therefore equal to 2.

It is useful to test the approximate results, Eqs. (44) and (45), by carrying out numerical calculations of γ_m and γ_w for disordered ferromagnets. To obtain the length and area dependencies of γ_m and γ_w the 23 spin-glass samples, studied in Ref. 1, were investigated after replacing all of the exchange interactions by their absolute values. The probability distribution of the exchange couplings for the spin-glass samples was Gaussian, characterized by zero mean and unit variance.

Briefly, the ground-state energy of the system was determined by starting from a random configuration of spins and aligning them sequentially in the direction of their instantaneous local fields. Since the ground state of the disordered ferromagnet with given boundary conditions is unique, only one initial configuration was needed. The magnetization and staggered magnetization of the ground state was monitored during the runs.

Figures 1 and 2 show plots of the length and area dependencies of γ_m and γ_w, respectively. The

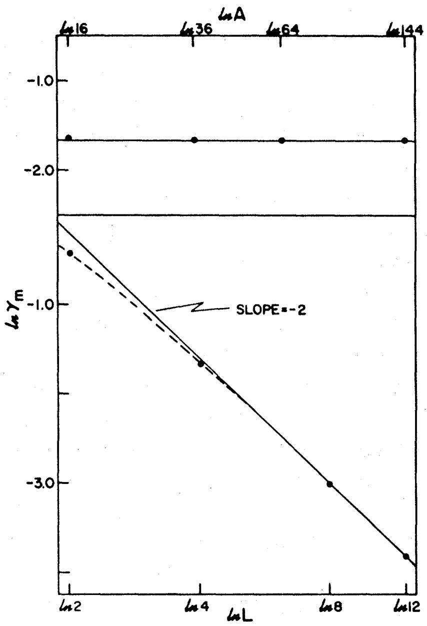

FIG. 1. Plot of $\ln\gamma_m$ vs $\ln L$ and vs $\ln A$ for a three-dimensional disordered Heisenberg ferromagnet. The length dependence is for $A=12\times 12$, whereas the area dependence is for $L=4$. The dashed curve is given by the equation $\gamma_m=\gamma_0\,(1-\cos\pi/L)$.

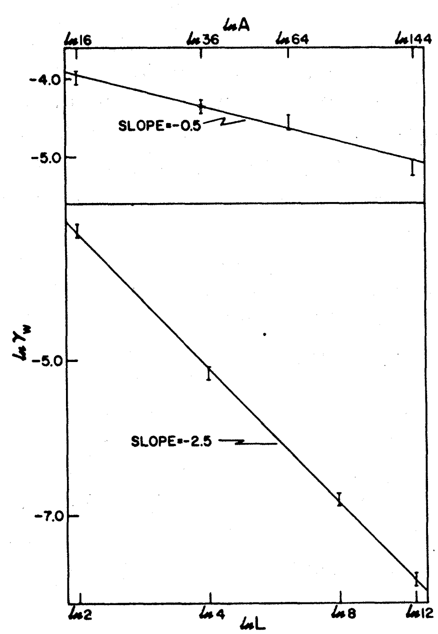

FIG. 2. Plot of $\ln\gamma_w$ vs $\ln L$ and vs $\ln A$ for a three-dimensional disordered Heisenberg ferromagnet. The length dependence is for $A=12\times 12$, whereas the area dependence is for $L=4$.

dashed curve in Fig. 1 is given by the equation

$$\gamma_m=\gamma_0(1-\cos\pi/L)\ , \tag{46}$$

as in Eq. (42), while the solid line represents the asymptotic limit of the above equation [Eq. (44)]. It is seen that the data points lie exactly on the dashed curve and the asymptotic limit is reached already for $L\approx 6$. Note that γ_m is independent of A. As seen in Fig. 2, γ_w is found to be proportional to $L^{-5/2}A^{-1/2}$, in accord with Eq. (44). The coefficients of proportionality of both γ_m and γ_w are found to agree with Eqs. (44) and (45) when $\langle\, |J_{1,2}|\,\rangle_c=\sqrt{2/\pi}$ and $\langle J_{1,2}^2\rangle_c=1$. These expectation values are characteristic of the Gaussian probability distribution considered. The agreement is within 20% and the effective exchange couplings seem to have reduced values.

The theoretical results of this section have been obtained on the assumption that all the exchange constants are nonzero. Otherwise, the problem becomes one of percolation. Studies of the sensitivity of systems near the percolation threshold to changes in the boundary conditions will be reported elsewhere. We note that with the Gaussian distribution used in the numerical simulation, the probability that one of the bonds is exactly zero is infinitesimally small. Nevertheless, the weak bonds may account for the diminished effective exchange couplings. In other aspects the numerical results for the disordered ferromagnet show that the one-dimensional approximation works well.

V. FERROMAGNET WITH RANDOM BOUNDARY CONDITIONS

As discussed in the Introduction, it may be argued that the imposition of periodic and antiperiodic boundary conditions on a spin-glass is similar to the imposition of random boundary conditions on a uniform ferromagnet. It may further be argued that such boundary conditions do not couple to the order parameter, and might under all circumstances yield an exponential decay of the characteristic free-energy scale of the sensitivity to boundary conditions. While it is not possible to prove that this is not the case for spin-glasses, the numerical data in Ref. 1 were consistent with an algebraic decay at $T=0$.

In this section we address the much simpler question of the effects of random boundary conditions on a uniform ferromagnet. We present a discussion of an Ising ferromagnet and numerical data on a two-dimensional Heisenberg ferromagnet which suggest that the sensitivity to appropriately chosen random boundary conditions may be used to obtain the correct LCD. We conclude this section with a brief discussion of the effects of introducing frustration at the boundary.

The two-dimensional uniform Heisenberg system with random boundary conditions is described by the Hamiltonian

$$H=-J\left[\sum_{i=1}^{L-1}\sum_{k=1}^{A}\vec{S}_{i,k}\cdot\vec{S}_{i+1,k}+\sum_{i=1}^{L}\sum_{k=1}^{A-1}\vec{S}_{i,k}\cdot\vec{S}_{i,k+1}\right]+H_B \tag{47}$$

with

$$H_B=-J\sum_{k=1}^{A}\vec{S}_{L,k}\cdot\vec{S}_{1,k}\eta(k)-J\sum_{i=1}^{L}\vec{S}_{i,A}\cdot\vec{S}_{i,1}\ , \tag{48}$$

where $\eta(k)=\pm 1$ randomly. Periodic and antiperiodic boundary conditions could be obtained by setting all of the η's equal to $+1$ and -1, respectively. There is no frustration in the bulk Hamiltonian given by Eq. (47). However, frustration is introduced at the boundary whenever $\eta(i)\eta(j)=-1$, where i and j represent nearest-neighbor sites. Such frustration effects yield a beyond the bulk contribution to the free energy.

To study the influence of changes in the boundary conditions on the free energy of the system, it is clearly desirable to choose a conjugate pair of boundary conditions, such that the amount of boundary frustration with both boundary conditions is identical. Starting with a given random boundary condition $\eta(k)$, one can readily obtain its partner $\eta'(k)$ by the operation

$$\eta'(k)=-\eta(k)\ . \tag{49}$$

Clearly, periodic and antiperiodic boundary conditions form a conjugate pair.

We now discuss a d-dimensional Ising ferromagnet with a conjugate pair of random boundary conditions. As a first step let us consider the system as being a set of independent Ising chains. A given chain with an η of $+1$ has all of its spins aligned parallel to each other. A chain with an η of -1, on the other hand, has as its ground state one domain wall. In the independent chain approximation the domain wall can be positioned at any site along the chain. Taking into account the ferromagnetic coupling between the chains results in the optimal ground state having all of the domain walls pushed to the end of the sample. In other words, the ground state of the system is one in which all of the spins are parallel and the ground-state energy is higher than the ground-state energy with periodic boundary conditions by an amount proportional to the number of -1's in the $\eta(k)$. The key point, therefore, is that the energy with any given boundary condition is independent of the length of the system. One can now consider the energy difference obtained from the imposition of a pair of conjugate boundary conditions. The characteristic *total* free-energy difference at $T=0$ is proportional to A and is independent of the length of the system. To obtain the area dependence, systems with the same length L and different areas have to be considered. Let $\tilde{A}$ represent the area of the smallest such system. The area dependence is then found by studying systems of area $A=\tilde{A}m^{d-1}$ with $m=1, 2, 3,\ldots$. Such a treatment enables one to periodically repeat the random boundary conditions of the smallest unit. For example, in $d=2$ we require that

$$\eta(k+\tilde{A})=\eta(k)\ . \tag{50}$$

Note that periodic and antiperiodic boundary conditions satisfy (50) with any $\tilde{A}$. We arrive then at the expected result that the LCD of the Ising ferromagnet is 1.

It is straightforward to generalize the above arguments to define γ_m and γ_w in the case of a disordered Ising ferromagnet. As discussed in Sec. III, in the paramagnetic phase the characteristic free-energy difference would have an exponential dependence on the length. It is interesting to note that if one did not choose a conjugate pair of boundary conditions (such that the surface frustration is different in the two cases) one would still obtain an algebraic law at $T=0$ which would persist even in the paramagnetic phase.

A similar analysis can be carried out for a Heisenberg ferromagnet. Unlike the Ising case, the ground state, while unique, does not have all of the spins aligned parallel to each other. We have performed numerical calculations on a two-dimensional Heisenberg ferromagnet with several different sets of conjugate pairs of boundary conditions. In each case, a behavior similar to the one obtained with periodic and antiperiodic boundary conditions is observed. In fact, for any given pair of conjugate boundary conditions we find that

$$\Delta f\sim\frac{1}{L^2} \tag{51}$$

and is independent of A, in the sense defined by Eq. (50). Equation (51) again confirms that the LCD of the Heisenberg ferromagnet is 2.

It is interesting to consider what happens if one carries out an ensemble average over a set of random boundary conditions. Let f_ν represent the free energy per spin with a random boundary condition labeled by ν. We define

$$\gamma = \langle (f_\nu - \langle f_\nu \rangle_\nu)^2 \rangle_\nu^{1/2} , \qquad (52)$$

where $\langle\ \rangle_\nu$ denotes an average over the boundary conditions.

Such a procedure, as discussed earlier in this section, produces a boundary frustration so that one may expect an algebraic law for γ at all finite temperatures. It is interesting to note, however, that one obtains the correct LCD by using γ as the characteristic free-energy scale in the problem. This follows readily for the Ising model as $\gamma \sim L^{-1} A^{-1/2}$ [since an ensemble average over the boundary conditions is being taken we do not use the restrictive prescription (50) in this procedure]. The total characteristic free-energy scale is independent of the length and again results in the LCD being 1.

Figure 3 shows a plot of the size dependence of γ for the two-dimensional uniform Heisenberg ferromagnet at $T=0$. Since we are able to average over a limited set (50) of boundary conditions, we have adopted a weighting scheme. The number of adjacent pairs of η's having a product of -1 is enumerated and the number of different ways of obtaining such a configuration is determined. A weighting factor proportional to this number has been used in obtaining the averages. Substantially similar results are found when a simple arithmetic average is performed. The data in Fig. 3 show that

$$\gamma \sim \frac{1}{L^{3/2} A^{1/2}} . \qquad (53)$$

Following Ref. 1, the characteristic total free-energy sensitivity of the system to a change in boundary conditions is given by $\gamma L^d \sim L^{(d-2)/2}$, leading to an LCD of 2 for the Heisenberg system. We emphasize again that γ is not expected to be useful in distinguishing between the ferromagnetic and paramagnetic phases. It is further possible that the correct result for the LCD, as obtained from (53), is a mere coincidence.

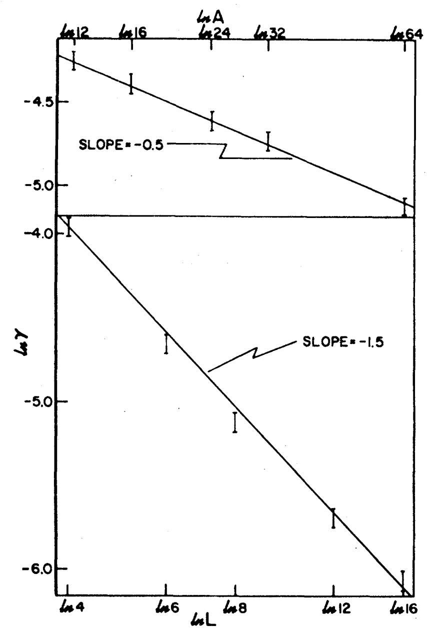

FIG. 3. Plot of $\ln\gamma$ vs $\ln L$ and vs $\ln A$ for a two-dimensional uniform Heisenberg ferromagnet with random boundary conditions. The length dependence is for $A=64$, whereas the area dependence is for $L=8$.

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