Computer simulation of the Heisenberg spin glass with Ruderman-Kittel-Kasuya-Yosida–like coupling

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We report results of computer simulations on a three-dimensional Heisenberg spin-glass model, where the strength of the interactions falls off with the inverse third power of the distance, which should be a good model for systems with the Ruderman-Kittel-Kasuya-Yosida interaction. Our results show that this system is in a different universality class from the short-range model, in agreement with a suggestion of Bray, Moore, and Young. The data is also compatible with their proposal that the system is at its lower critical dimension, though we cannot rule out the possibility of a low but nonzero transition temperature.

I. INTRODUCTION

One surprising feature to emerge from recent studies on spin glasses is that the best studied systems, such as Cu-Mn and Ag-Mn, which have relatively little anisotropy and so are Heisenberg like, are better described by a short-range Ising model rather than a Heisenberg model. More precisely, while the experimental evidence[1] for a finite transition temperature, T_c, is very strong, theoretical studies indicate a finite T_c only for Ising systems,[2] whereas Heisenberg models[3–7] have $T_c=0$. In particular, Olive *et al.*[6] show that the nonlinear susceptibility of Ag-Mn (Omari *et al.*, Ref. 1) is quite similar to that obtained from a nearest-neighbor three-dimensional (3D) Ising model, but qualitatively different from a nearest-neighbor Heisenberg model. To fully explain this apparent paradox, it will probably be necessary to understand better the role of anisotropy.[5,8] However, there *is* a potentially important difference between many of the real systems and the theoretical models, namely that the metallic spin glasses have Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions which fall off as R_{ij}^{-3} where R_{ij} is the distance between sites i and j, whereas the models are usually confined to nearest-neighbor interactions. In fact, Bray *et al.*[9] recently proposed, on the basis of scaling arguments, that RKKY Heisenberg systems would be *at* their lower critical dimension, d_l, in contrast to the result[3–5] that $d_l \simeq 4$ for isotropic Heisenberg models. It is therefore clearly necessary to understand the role of RKKY interactions in order to explain experimental data. We have consequently undertaken numerical studies of a Heisenberg model with (essentially) RKKY interactions in order to test out the suggestion of Bray *et al.*[9]

We find that the nonlinear susceptibility increases much faster at low temperatures than for a short-range Heisenberg spin glass[6] (and faster than found by Chakrabarti and Dasgupta[7] for a similar model), in agreement with Bray *et al.*'s suggestion that the short range and RKKY Heisenberg models are in a different universality class. Our results are *consistent* with $d=3$ being the lower critical dimension but we are unable to simulate at low enough temperatures or large enough sizes to rule out the possibility that T_c is nonzero.

The plan of this paper is as follows. Section II describes the model, the quantities we calculate, and our method of analysis. In Sec. III we give the results and analysis, while Sec. IV summarizes our conclusions.

II. THE MODEL

Canonical spin-glass systems,[10] such as Cu-Mn and Ag-Mn have a small concentration of magnetic atoms interacting with the RKKY coupling

$$H_{\mathrm{RKKY}} = J_{\mathrm{RKKY}} \sum_{\langle ij \rangle} \epsilon_i \epsilon_j \frac{\cos(2k_f R_{ij})}{R_{ij}^3} \mathbf{S}_i \cdot \mathbf{S}_j \ , \tag{1}$$

where $\epsilon_i = 1$ or 0 depending on whether site i is occupied by a magnetic atom (e.g., Mn) or not, k_F is the Fermi wave vector, R_{ij} is the distance between sites i and j, and $\mathbf{S}_i$ is a Heisenberg spin. This Hamiltonian is rather awkward to simulate because, even for a rather low concentration of spins c, there will be some nearest neighbors on the lattice. These pairs do not play an important role in the physics but they have a much bigger coupling than do pairs of spins separated by the *typical* distance of a spin from its closest neighbor. This varies as $c^{-1/3}$ and so is much larger than one lattice spacing when c is small. Having such large couplings means that single spin-flip dynamics is rather inefficient in bringing the system to equilibrium because the two nearest-neighbor spins prefer to change their orientation together. Furthermore, the scaling behavior comes from the *long distance*, R_{ij}^{-3}, variation of the interactions,[9] though such strong short-range couplings may give important *corrections* to scaling. In contrast to Chakrabarti and Dasgupta[7] we have therefore not studied the model defined precisely by Eq. (1) but rather an Edwards-Anderson[11] model, with a spin on each site of a simple-cubic lattice, with Hamiltonian

$$H = -\sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \ , \tag{2}$$

where the interactions J_{ij} are given by

$$J_{ij}=\frac{c_L \epsilon_{ij}}{R_{ij}^3} , \quad (3)$$

where ϵ_{ij} is a random variable drawn from a Gaussian distribution with zero mean and unit variance, and c_L is defined for the lattice with $N=L\times L\times L$ sites by the requirement that

$$\sum_{j=1}^{N} J_{ij}^2=3 , \quad (4)$$

so that the mean-field[11] transition temperature is

$$T_c^{\rm MF}=1 . \quad (5)$$

Note that c_L depends weakly on L and tends to a constant for L large. To avoid surface effects, we compute R_{ij} from

$$R_{ij}=[(x_i-x_j)^2+(y_i-y_j)^2+(z_i-z_j)^2]^{1/2} ,$$

where the x_i, etc. are coordinates on the lattice, provided all the relative distances are less than $L/2$. If $x_i-x_j>L/2$ we replace x_i-x_j by $L-(x_i-x_j)$ to mimic the effect of periodic boundary conditions, and similarly for the other components. In other words, we periodically repeat the lattice and take R_{ij} to be the *shortest* possible distance between sites i and j, either in the same lattice or on adjacent repeats of it. We do not consider periodic boundary conditions in which the interaction between spin is summed over all periodic images. This geometry is expected to give similar results to the present ones.[12]

The main quantity that we calculate is the spin-glass susceptibility, $\chi_{\rm SG}$, defined by

$$\chi_{\rm SG}=\frac{1}{N}\sum_{ij}[\langle S_i\cdot S_j\rangle_T^2]_{\rm av} , \quad (6)$$

where $\langle\cdots\rangle_T$ denotes the statistical mechanical average for a given configuration of interactions, and $[\cdots]_{\rm av}$ indicates an average over all possible such configurations. In the paramagnetic phase $\chi_{\rm SG}$ is related[13] to the nonlinear susceptibility, the coefficient of h^3 in the expansion of the magnetization in powers of the magnetic field h.

In general $\chi_{\rm SG}$ is expected to diverge as

$$\chi_{\rm SG}\sim(T-T_c)^{-\gamma} \quad (7)$$

for a dimension d above the lower critical dimension, d_l, in which case T_c is nonzero. If the system is below the lower critical dimension ($d<d_l$) then Eq. (7) still holds, but now $T_c=0$, i.e.,

$$\chi_{\rm SG}\sim T^{-\gamma} . \quad (8)$$

Precisely at the lower critical dimension ($d=d_l$) one expects[9,14] an exponential divergence as $T\to 0$, i.e.,

$$\chi_{\rm SG}\sim \exp\left[\frac{C}{T^\sigma}\right] , \quad (9)$$

where σ is an unknown exponent, though McMillan[14] has argued that $\sigma=2$.

The exponent γ is given by

$$\gamma=(2-\eta)\nu , \quad (10)$$

where ν is the exponent of the spin-glass correlation length ξ for $T\gtrsim T_c$, and η describes the power-law decay of the correlation at T_c. Thus

$$G_2(R_{ij})\equiv[\langle \mathbf{S}_i\cdot\mathbf{S}_j\rangle_T^2]_{\rm av}\sim\frac{f(R_{ij}/\xi)}{R_{ij}^{d-2+\eta}} \quad (T\gtrsim T_c) , \quad (11)$$

where ξ diverges as

$$\xi\sim(T-T_c)^{-\nu} . \quad (12)$$

For $R\gg\xi$ one expects that $f(R/\xi)\sim\exp(-R/\xi)$. At $d=d_l$ the power-law divergence as $T\to 0$ is presumably replaced by the exponential variation in Eq. (9) but one can still define η by

$$\chi_{\rm SG}\sim\xi^{2-\eta} . \quad (13)$$

Thus, for a nonzero T_c, there are two independent static exponents in spin glasses, just as in uniform systems. Below the lower critical dimension d_l, the low-temperature behavior is governed by a zero-temperature critical point, as if the system had a transition at zero temperature ($T_c=0$). In this case, there is an additional relation[15] between the exponents *provided the ground state is nondegenerate* (aside from symmetry related states):

$$2-\eta=d \quad (T_c=0) , \quad (14)$$

so that

$$\gamma=d\nu \quad (T_c=0) . \quad (15)$$

Consequently, there is only one independent static exponent if $T_c=0$, provided that the ground state is not extensively degenerate.

We use finite-size scaling[16] to extract the maximum amount of information from our simulations. This predicts that $\chi_{\rm SG}$ should vary with L and ξ as

$$\chi_{\rm SG}=L^{2-\eta}\bar{\chi}[(L/\xi)^{1/\nu}] , \quad (16a)$$

$$=L^{2-\eta}\bar{\chi}[(T-T_c)L^{1/\nu}] . \quad (16b)$$

For a $T=0$ transition $\chi_{\rm SG}$ is given by

$$\chi_{\rm SG}=L^d\bar{\chi}[TL^{1/\nu}] \quad (17)$$

if $d<d_l$, so ν is finite, whereas for $d=d_l$ Eqs. (9), (13), (15), and (16a) give

$$\chi_{\rm SG}=L^d\tilde{\chi}\left[L\exp\left[\frac{C/d}{T^\sigma}\right]\right] . \quad (18)$$

Precisely at $T=0$ we have

$$\chi_{\rm SG}=\frac{L^d}{3} , \quad (19)$$

where the factor $\frac{1}{3}$ comes from the fact that we have a Heisenberg model and the spins point randomly in all directions. As discussed by Chakrabarti and Dasgupta,[7] there are corrections to Eq. (9) for small sizes because neighboring spins have some preference for parallel or antiparallel alignment. However, we find that these corrections appear to be small even for the smallest lattices that we study.

The Monte Carlo simulations used a heat bath algorithm, which is described in Ref. 6. This has the advantage that a move is made every step, as opposed to the Metropolis algorithm where no change is made for a certain fraction of attempts. We used an $L \times L \times L$ simple-cubic lattice with sizes $4 \le L \le 16$ at a range of different temperatures, and tested that the system was equilibrated using the techniques of Bhatt and Young.[2,17] This involves computing χ_{SG} both from a four-spin correlation function at different times (which should give too large an answer if the simulation is too short) and from the correlation at equal times of spins in two independent copies of the system with the same interactions (which should give too small an answer if the simulation is too short). If the two estimates agree, this should therefore be the equilibrium value. We checked that the results did agree for all the data points which we present. Because every spin couples to every other one, the number of interactions is N^2, which requires more memory for $L=16$ than available on the Cray Research X-MP computer where the computations were performed on the largest sizes. We therefore packed 16 different ϵ_{ij}'s, defined in Eq. (3), into one word of computer memory, so there were four bits per bond. Hence for $L=16$, and only for this size, the distribution was actually a discretized Gaussian with $2^4=16$ possible values. We checked that the effect of this discretization was less than the statistical errors by doing some runs for $L=11$ with both the full and discretized distributions.

III. RESULTS

Figure 1(a) depicts the spin-glass susceptibility χ_{SG} as a function of temperature for different systems sizes in a log-log form. The points represent an average of between 11 and 300 bond configurations. Note that the studied temperature range is somewhat limited, particularly for the largest sizes ($T \ge 0.5$ for $L=16$), because relaxation times increase very rapidly as the temperature is lowered or the size increased. Comparing Fig. 1(a) with 1(b), which shows analogous results for the nearest-neighbor model,[6] we see that χ_{SG} increases much more rapidly as T is reduced for the system with RKKY interactions. In fact, whereas the data for the short-range model show rather convincingly that $T_c=0$, we shall see that we are unable to rule out a nonzero value of T_c for the RKKY system. As a result, the RKKY data are much more affected by finite-size corrections than the short-range data, which will make the analysis more difficult.

We wish to ascertain whether the short-range and RKKY models are in different universality classes or not. Clearly they are not in the same universality class if $T_c \neq 0$ for RKKY interactions. We will therefore first assume that $T_c=0$ and ascertain whether the more rapid increase in χ_{SG} seen in Fig. 1(a) is due to a different exponent γ (which implies a different universality class) or whether γ is the same in the two cases but the amplitude is larger for the RKKY system (which would mean the same universality class). Later we will see what bounds we can put on T_c. Even without a finite-size scaling analysis we can deduce a lower bound on γ if we assume that, for the infinite system, the slope of the log-log plot in Fig. 1(a) monotonically increases as T is lowered, and that the slope is never greater than this for a finite system. With these reasonable assumptions the lower bound on γ is the largest slope of the curves of Fig. 1(a). From a cubic spline fit we find that this occurs at $L=16$ and $T=0.62$ and gives

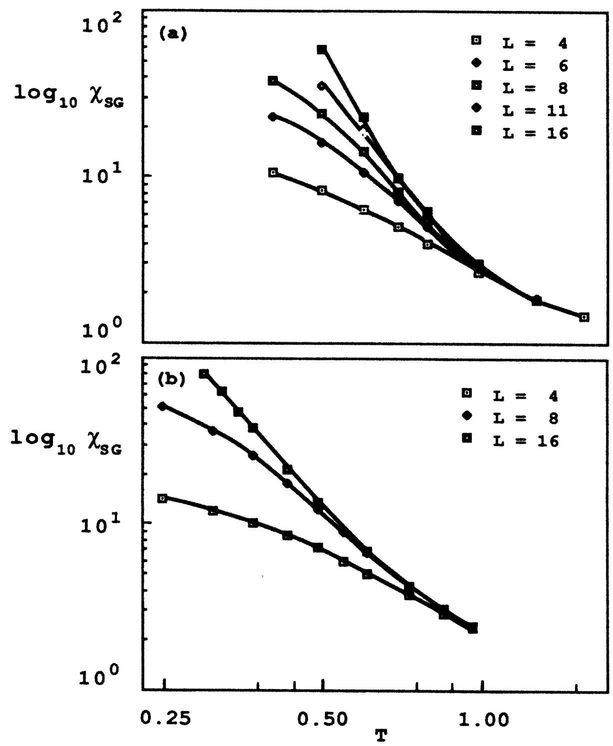

FIG. 1. (a) log-log plot of the spin-glass susceptibility as a function of temperature for different system sizes as indicated. (b) Same as Fig. 1(a) but for the short-range model [Olive *et al.* (Ref. 6)]. Note the slower increase of χ_{SG} with decreasing T. As in 1(a), T is given in units of the mean-field transition temperature.

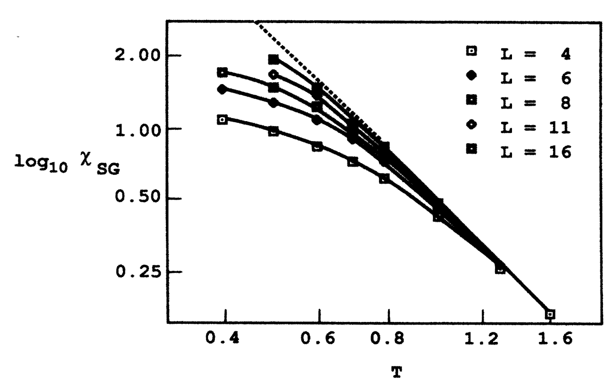

FIG. 2. Lower critical dimension scaling plot: $\log_{10}\chi_{SG}$ against T on a log-log scale. The dashed line corresponds to $\chi_{SG}=\exp(1.1/T^{2.2})$, i.e., an essential singularity in χ_{SG} at $T_c=0$.

$$\gamma > \gamma_{min} \approx 5.8 \ . \quad (20)$$

Note that finite-size effects are significant at this temperature so we expect that the slope for the infinite system would be larger than our bound of 5.8, and would probably continue to increase at lower temperatures. However this value is already larger than the result of Olive *et al.* for the short-range Heisenberg spin glass,[6]

$$\gamma_{\text{short range}} = 3.42 \pm 0.06 \ , \quad (21)$$

and larger still than the estimate $\gamma \approx 2.6$ of Chakrabarti and Dasgupta[7] for the RKKY model. [We obtained this last figure by taking the values of ν in Ref. 7 and using Eq. (15).] Hence we agree with the suggestion of Bray, Moore, and Young[9] that RKKY and short-range Heisenberg spin glasses are in a different universality class.

They also propose that the RKKY interactions are sufficiently long ranged so that the present model is *at* its lower critical dimension, for which Eq. (9) should apply. To test this possibility, we plotted $\log_{10}\chi_{SG}$ versus T in a log-log plot in Fig. 2. If the susceptibility has an essential singularity at $T_c = 0$ as in Eq. (9), we should get a linear behavior in Fig. 2. Although this is not quite the case for the sizes and temperature ranges plotted, presumably because of finite-size effects discussed below, the behavior of the curves suggests that for large enough sizes all the curves could lie on a straight line, close to the dashed one, which has a slope $\sigma \approx 2.2$ and from the intercept we obtain $C \approx 1.1$. Whereas our present data are not sufficient to rule out all other possibilities, they are certainly compatible with the system being at its lower critical dimension and the spin-glass susceptibility having an essential singularity as in Eq. (9).

Next we consider finite-size effects. In Fig. 3 we show a scaling plot of the data in a form where curves for different sizes would lie on top of each other if the finite-size scaling formula for the lower critical dimension, Eq. (18), is correct. We used the values $\sigma = 2.2$ and $C = 1.1$ obtained from Fig. 2. On this plot the straight-line region on the right is for large enough sizes that finite-size corrections do not occur and the temperature dependence is given by Eq. (9). However, the curves for different sizes break away from this line at different points, indicating that finite-size scaling is not working. We should point out, however, that the data is not for very low temperatures, so that if $T_c = 0$ we may well not be in the asymptotic scaling region. Furthermore, corrections to finite-size scaling are particularly large at $d = d_l$. These reasons could account for the lack of scaling in Fig. 3.

In Fig. 3 we assumed that η is given by Eq. (14). If, however, we relax that restriction, which is equivalent to assuming a degenerate ground state, and allow η to be an adjustable parameter we can obtain a much better fit. A plot with $\eta = 0$ is shown in Fig. 4, which clearly scales much better than Fig. 3. Nonetheless we see no reason why the ground state should be degenerate and feel that a more likely explanation for the relatively poor fit in Eq. (3) is that the temperature is rather high so the asymptotic scaling region has not been reached.

We would nevertheless like to ascertain whether or not the finite-size corrections confirm that the RKKY system

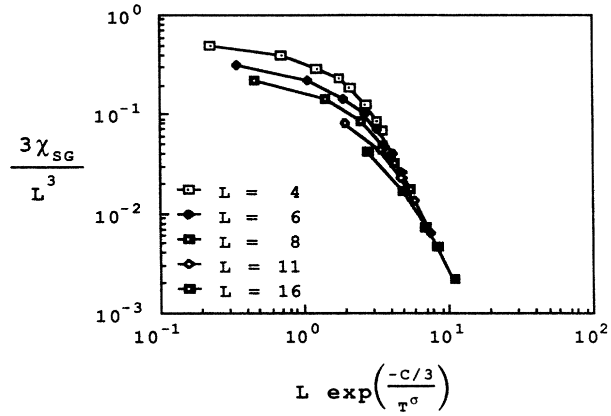

FIG. 3. Finite-size scaling plot with the assumption that the system is at its lower critical dimension, ($d = d_l = 3$). The values $\sigma = 2.2$ and $C = 1.1$ were taken from the dashed line in Fig. 2.

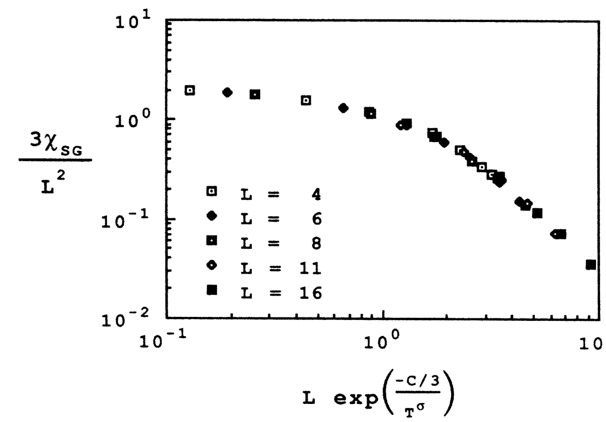

FIG. 4. Same as Fig. 3 but with the additional assumption that the ground state is degenerate and $\eta = 0$.

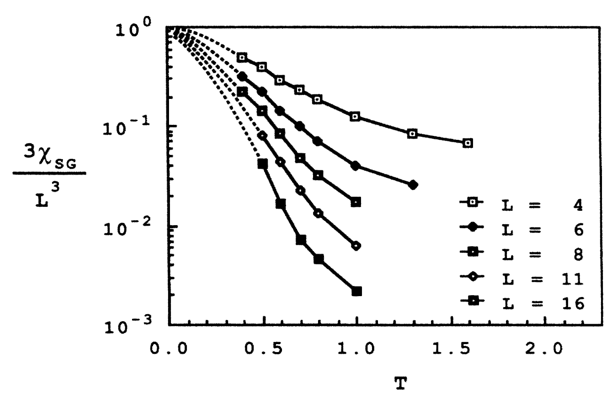

FIG. 5. Logarithmic plot of the normalized spin-glass susceptibility $\hat{\chi}_{SG} = (3\chi_{SG}/L^d)$ as a function of T for different system sizes. The dashed lines indicate the expected low-temperature behavior.

is in a different universality class from short-range systems, as we already found from the maximum slope in Fig. 1. We therefore plot in Fig. 5 the normalized susceptibility $\hat{\chi}_{SG}=(3\chi_{SG}/L^d)$ as a function of T for different system sizes. From Eq. (19) $\hat{\chi}_{SG}$ should tend to unity as $T\rightarrow 0$. The actual data are represented by the symbols, and the low-temperature behavior is roughly suggested by the extrapolated dashed line. To see if we can obtain a bound on the exponents ν and γ we try to scale $\hat{\chi}_{SG}$ as a function of T and L in the following form:

$$\hat{\chi}_{SG}(T,L)=F(T/T(L)) \ . \tag{22}$$

For each linear size L we determine the characteristic temperature $T(L)$ from the condition that all data points lie on the same curve when $\hat{\chi}_{SG}$ is plotted against $T/T(L)$. To achieve this, we have chosen a number of specific values of $\hat{\chi}_{SG}$, found the corresponding temperature values, $T_i(L)$, for all sizes by using cubic-spline interpolation, and required that all data points lie as close to each other as possible, i.e., we found the minimum of

$$\sum_i \sum_{L,L'} \left[\frac{T_i(L)}{T(L)} - \frac{T_i(L')}{T(L')} \right]^2 \ . \tag{23}$$

This method works very well if all the data scales properly.[6] It is somewhat arbitrary, however, if not all data lie in the scaling region. For our data the latter is true, so we have a certain freedom in choosing the values of $\hat{\chi}_{SG}$, at which the curve collapsing is performed. From Eq. (17) we see that for $d<d_l$ the scaling prediction for $T(L)$ is

$$T(L)\sim L^{-1/\nu} \ . \tag{24}$$

Figure 6 shows a scaling plot which places emphasis on the low-temperature behavior. It suggests that our higher-temperature data points are not yet in the $T\rightarrow 0$, $L\rightarrow\infty$ scaling regime. If that is accepted, the curves can be interpreted in terms of scaling at low temperatures. The corresponding characteristic temperatures $T(L)$ are plotted in Fig. 7 in a log-log form. The curve is not a straight line, as would be the case for scaling at $d<d_l$ [see Eq. (24)], but it is curved in a way that the *effective* exponent $\nu_{\text{eff}}(T)$, defined as the inverse of the slope in Fig. 7, increases at lower temperatures. If we make the plausible assumption that $\nu_{\text{eff}}(T)$ monotonically increases as T decreases we can get a lower bound for ν from the inverse of the minimum slope in Fig. 7, i.e., where the temperature is lowest and the size the largest. This gives

$$\nu>2.3 \ , \tag{25}$$

which, from the scaling law Eq. (15), gives

$$\gamma>6.9 \ . \tag{26}$$

Both this result and the direct estimate in Eq. (20), which did not allow for finite-size corrections, show that the present long-range model is in a different universality class from the short-range one.[6]

We would like to comment on the above mentioned arbitrariness of this fitting procedure. By requiring that the curves of Fig. 5 collapse as well as possible when data at

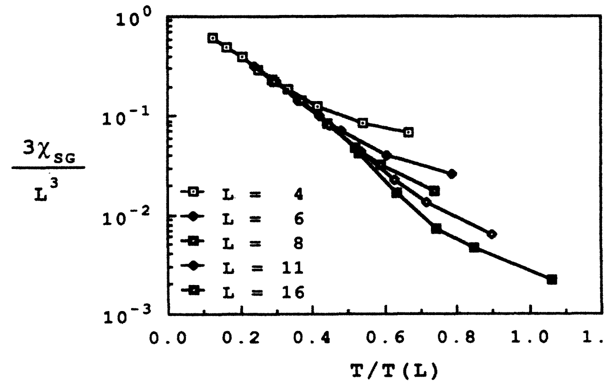

FIG. 6. Scaling plot of the normalized spin-glass susceptibility $3\chi_{SG}/L^d$ against $T/T(L)$. The characteristic temperatures $T(L)$ are fit parameters.

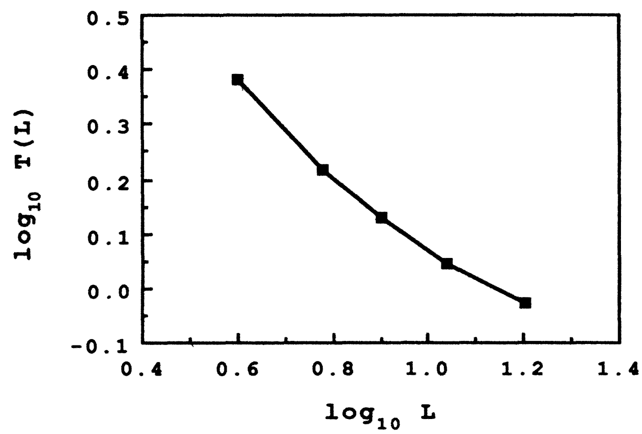

FIG. 7. log-log plot of the characteristic temperatures $T(L)$ from Fig. 6 against the linear system size L.

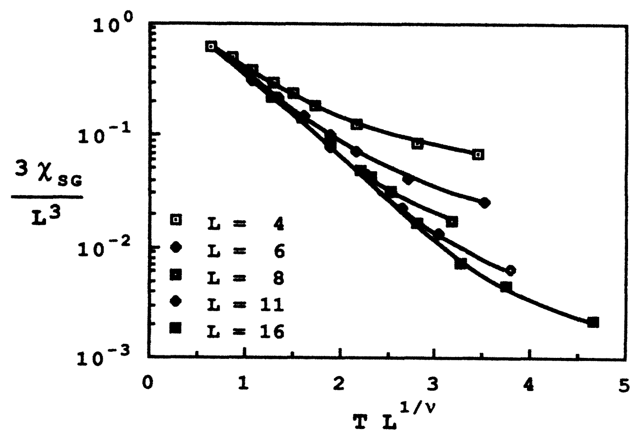

FIG. 8. Finite-size scaling plot with the assumption that the system is below its lower critical dimension, $(d_l>d=3)$. The fit parameters are $\eta=-1$ and $\nu=1.8$. The latter implies $\gamma=5.4$.

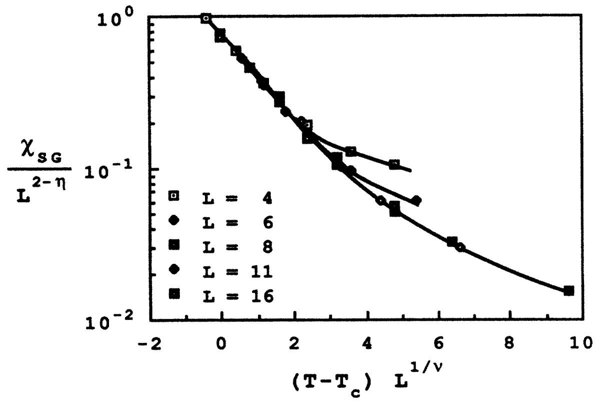

FIG. 9. Finite-size scaling plot with the assumption that T_c is finite. The fit parameters are $T_c=0.4$, $\eta=0.1$, and $\nu=1.0$.

higher temperatures than those in Fig. 6 are included, one changes the scaling plot and the numerical value of $T(L)$. However, the variation of $T(L)$ with L is qualitatively very similar, and the numerical estimate for ν is changed by only about 10%, which still implies that the RKKY system is in a different universality class from short-range models.

We have also tested to what extent our data can be fitted to the finite-size scaling ansatz, Eq. (17), appropriate for $d<d_l$. The best fit, shown in Fig. 8, is for $\nu=1.8$, which implies $\gamma=5.4$. The quality of the fit is not very good but we note that the value of γ is again larger than the short-range value given in Eq. (21).

We now discuss the possibility that T_c may be finite. A fit to Eq. (16b) with $T_c=0.4$, $\nu=1.0$, and $\eta=0.1$ is shown in Fig. 9. The quality of the fit is not excellent but given the difficulties encountered in scaling with $T_c=0$ we do not feel that this value of T_c can be ruled out. Higher values of T_c do not work as can be seen from the curvature of the data in Fig. 1(a) for $T\geq 0.5$. Lower T_c's fit somewhat less well than $T_c=0.4$ but also cannot be ruled out. Finally we have tested the possibility of an exponential divergence at a finite temperature. This occurs,

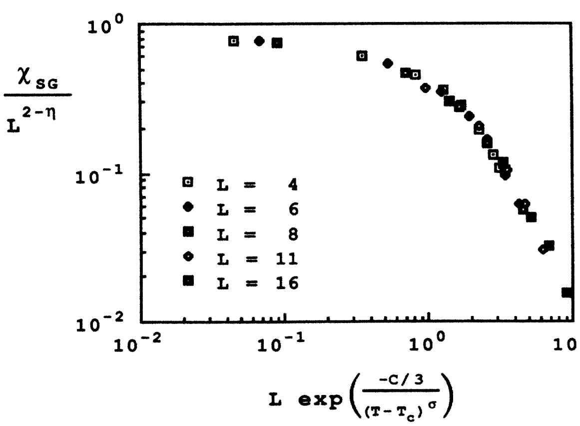

FIG. 10. Finite-size scaling plot with the assumption of an exponential divergence at finite temperature. The fit parameters are $T_c=0.2$, $\eta=0.1$, $C=1.2$, and $\sigma=1.5$.

for example, in the two-dimensional XY ferromagnet.[18] The finite-size scaling ansatz to this would be like Eq. (18) but with T replaced by $T-T_c$. A corresponding scaling fit is shown in Fig. 10 for $T_c=0.2$. While the fit is good, we note that there are four adjustable parameters compared with three in Fig. 9 and only two in Fig. 3. There are no theoretical arguments for this behavior but clearly our numerical results cannot rule it out.

IV. CONCLUSIONS

We have carried out extensive simulations of the 3D Heisenberg spin glass with RKKY-like couplings. These provide sound evidence that the RKKY system is in a different universality class from the short-range model. Our conclusions differ from those of Chakrabarti and Dasgupta,[7] who model a site dilute system. However, our sizes are substantially larger than theirs, $N\leq 4096$ compared with $N\leq 312$. Furthermore, we have already discussed that the very strong nearest-neighbor coupling in their model may give large corrections to scaling. We believe that our results are strong evidence that the spin-glass susceptibility of RKKY systems diverge more strongly than that of short-range Heisenberg spin glasses. Our results are quite consistent with $d=3$ being the lower critical dimension and with the resulting exponential divergence of χ_{SG}. We are unable, however, to rule out other possibilities such as $d=3$ being just above or just below d_l. In the latter case T_c would be finite and we can rule out any T_c greater than 0.4 in units of the mean-field transition temperature. Although our results are not as conclusive as we would have liked in deciding the question of the lower critical dimension, we should emphasize that the RKKY Heisenberg spin glass remains a very hard problem which is difficult to treat by other techniques, such as high-temperature series expansions or transfer matrices, because of the long-range interaction.

We believe that our results must be included, along with an accurate treatment of anisotropy, in any detailed comparison with experiments on the nonlinear susceptibility.[1] In fact Bray and Moore[8] have suggested, that RKKY Heisenberg systems are so sensitive to any small anisotropy (because of the exponential divergence of the nonlinear susceptibility in the isotropic system), that one will never see short-range Heisenberg behavior for any reasonable value of the anisotropy. This is indeed in accordance with observation. It would be clearly useful to perform more detailed studies on insulating spin glasses to isolate experimentally the role of RKKY couplings.

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