Phase Transition in the Ruderman-Kittel-Kasuya-Yosida Model of Spin-Glass

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The equilibrium behavior of a system of randomly distributed classical Heisenberg spins coupled via the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction is studied by Monte Carlo simulations. Finite-size scaling analysis of the results strongly indicates a zero-temperature critical point with the correlation length exponent $\nu = 0.87 \pm 0.08$. This conclusion is supported by the observed temperature and sample-size dependence of various relaxation times.

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Though spin-glasses have been the subject of extensive studies in recent years, whether a thermodynamic phase transition separating paramagnetic and spin-glass phases exists in three dimensions has not yet been established conclusively. From experimental studies[1] of the magnetic properties around the susceptibility cusp, it is not clear whether the system goes through a sharp phase transition or a progressive freezing of the spins. Although theoretical studies[2] of infinite-range Sherrington-Kirkpatrick[3] models of spin-glasses show true thermodynamic phase transitions for both Ising and Heisenberg systems, there exist several theoretical arguments[4] suggesting that short-range models of spin-glasses should not exhibit any phase transition in three dimensions. However, recent numerical studies[5] of Ising spin-glass models with nearest-neighbor interactions indicate a finite transition temperature in three dimensions, whereas a zero-temperature phase transition is indicated[6] for short-range Heisenberg models in three dimensions. None of these models provide a realistic description of metallic spin-glass alloys, in which randomly distributed Heisenberg spins are coupled via the long-range oscillatory Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. Theoretical investigations of realistic RKKY spin-glass models have mostly been confined to numerical studies. No definite conclusion about the existence of a phase transition can be drawn from the work of Ching and Huber.[7] Fernandez and Streit[8] do prescribe a transition at a finite temperature. However, their conclusion is not reliable because it is based on a method of analysis that also predicts[9] a transition for the two-dimensional Ising case where actually no such transition exists.[10] The numerical work of Walstedt and Walker[11,12] suggests that the model with only RKKY interactions does not show any transition and a small amount of anisotropy is needed to activate a clear-cut transition. These results, again, cannot be considered conclusive because of the following two reasons. The conclusion about the absence of a phase transition in the pure RKKY model was based on the observed behavior of quantities (such as the spin autocorrelation function and the components of the magnetization) which are not invariant under a uniform rotation of all the spins. Since the Hamiltonian for RKKY spin-glass is rotationally invariant, a Monte Carlo updating process will, in general, generate uniform rotations of the spins for finite samples. Unless care is taken to correct for the effects of uniform rotations, the long-time Monte Carlo averages of the quantities mentioned above will, therefore, vanish[13] irrespective of whether a phase transition takes place or not. This effect was not taken into account in the work of Walstedt and Walker [see discussion following Eq. (2) below]. Second, the fact that their simulations were carried out with a fixed time scale raises doubts about whether the measurements correspond to true equilibrium values, particularly at very low temperatures.

In this paper, we present the results of a detailed numerical study of the thermodynamics of the RKKY model. We have calculated equilibrium averages of various rotationally invariant quantities for a wide range of sample sizes, averaged over several realizations. Also, we have studied the temperature and sample-size dependence of the different relevant time scales of this system. Finite-size-scaling fits to the data for different sample sizes indicate $T=0$ as the only critical point. At this critical point, the correlation length diverges with an exponent $\nu = 0.87 \pm 0.08$. These results are firmly supported by our independent calculation of the moments of the distribution function of the Edwards-Anderson[14] (EA) order parameter and our calculation of the different time scales of the system.

The Hamiltonian of the system in this work is

$$H = -J_0 \sum_{j<i} [\cos(2k_F r_{ij})/r_{ij}^3] \mathbf{S}_i \cdot \mathbf{S}_j, \qquad (1)$$

where $\mathbf{S}_i$'s are classical Heisenberg spins of unit length randomly chosen on the sites of a $L \times L \times L$ fcc lattice with a concentration of 0.5 at.%, J_0 is an energy constant, k_F is the Fermi wave vector of the host metal, and r_{ij} is the distance between ith and jth spins. Periodic boundary conditions are imposed and the interaction is cut off at $L/2$. Parameters of the interaction are chosen representing Cu-Mn and the tempera-

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ture T is measured in units of $T_0=2\sqrt{2}J_0/10a_0^3k_B$ where a_0 is the fcc lattice constant.[15] In the Monte Carlo simulations for samples with number of spins $N=20$, 44, 81, 161, and 312, we used the standard Metropolis algorithm. For every value of N and T, the simulation was carried out for approximately 4 times the equilibration time which was estimated by monitoring various autocorrelation functions. The length of the Monte Carlo runs varied between 1000 and 60 000 Monte Carlo steps per spin, where each step corresponds to five consecutive attempts to move a spin. Configurational averages were taken over 30, 20, 15, 10, and 3 realizations for $N=20$, 44, 81, 161, and 312, respectively.

One quantity of interest is the single-spin autocorrelation function

$$q(t)=\left\langle\left\langle \max\left[\frac{1}{N}\sum_{i=1}^{N}\mathbf{S}_i(0)\cdot\mathbf{R}\cdot\mathbf{S}_i(t)\right]\right\rangle\right\rangle_c, \tag{2}$$

where $\langle\ \rangle$ is the Monte Carlo (thermodynamic) average, $\langle\ \rangle_c$ is the configurational average over different realizations of the interaction, and $\mathbf{R}$ is a general SO(3) matrix whose inclusion corrects for any uniform rotation of the spin system.[16] We find that the "unrotated"-spin autocorrelation function,

$$q'(t)=\left\langle\left\langle \frac{1}{N}\sum_{i=1}^{N}\mathbf{S}_i(0)\cdot\mathbf{S}_i(t)\right\rangle\right\rangle_c,$$

always goes to zero within the observation time, whereas $q(t)$ approaches a constant value ($\simeq 0.7$ for $N=312$ at $T^*=0.01$) at long times. The observed decay of $q(t)/q'(t)$ with time is consistent with the form expected[13] for uniform spin rotations. These results indicate that the vanishing of the EA order parameter observed by Walstedt and Walker[11,12] is a consequence of uniform spin rotations. We also computed the two-spin time-correlation function

$$q^{(2)}(t)=\left\langle\frac{2}{N(N-1)}\sum_{i>j}^{N}\langle[\mathbf{S}_i(0)\cdot\mathbf{S}_j(0)][\mathbf{S}_i(t)\cdot\mathbf{S}_j(t)]\rangle\right\rangle_c, \tag{3}$$

which is invariant under an overall rotation of the system. The EA order parameter,

$$q=\langle(1/N)\textstyle\sum_i|\langle\mathbf{S}_i\rangle|^2\rangle_c, \tag{4}$$

is obtained from $q(t)$ as

$$q=\lim_{t\to\infty}q(t), \tag{5}$$

and

$$q^{(2)}(t\to\infty)\equiv q^{(2)}=\left\langle\frac{2}{N(N-1)}\sum_{j<i}\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle^2\right\rangle_c \tag{6}$$

is related to the spin-glass susceptibility,

$$\chi_{sg}=(N-1)[q^{(2)}-\tfrac{1}{3}q^2]+1-q^2. \tag{7}$$

Note that $q(0)=1$ and if, at any given instant, the spins are distributed uniformly on the unit sphere, then $q^{(2)}(0)=\frac{1}{3}$. In the simulation we find appreciable deviations form this value of $q^{(2)}(0)$ at low temperatures. Since the magnitude of the RKKY interaction is large for small values of r_{ij}, the close neighbors of a particular spin tend to be either parallel or antiparallel to it, thus making $q^{(2)}(0)$ for finite samples larger than $\frac{1}{3}$ at low temperatures. This finite-size $[O(1/N)]$ effect, which also affects the value of $q^{(2)}(t)$, was approximately taken into account by defining a "normalized" value of $q^{(2)}(t)$, given by

$$q^{(2)}_{\text{norm}}(t)=q^{(2)}(t)/3q^{(2)}(0). \tag{8}$$

Also computed was the probability distribution function for q given by

$$P(q)=\frac{1}{t_0}\sum_{t=\tau}^{t_0+\tau}\langle\delta(q-q(t))\rangle_c, \tag{9}$$

where τ is the equilibration time and t_0 was taken between 3τ and 4τ for different sample sizes. It has been shown[5] that the sample-size dependence of the ratio of the moments of this distribution yields useful information about the existence of a phase transition. If we assume a second-order phase transition at $T=T_c$, then finite-size-scaling arguments[5,17] enable us to write $P(q)$ as

$$P(q)=L^{\beta/\nu}\tilde{P}(qL^{\beta/\nu},\ L^{1/\nu}(T-T_c)), \tag{10}$$

where β is the order parameter exponent and ν is the correlation-length exponent. The L-dependent prefactor can be eliminated by considering appropriate ratios of moments of $P(q)$. We calculated the quantity

$$\rho=[(\langle q^4\rangle_{\text{av}}/\langle q^2\rangle^2_{\text{av}})-1]^{1/2}, \tag{11}$$

where the $\langle\ \rangle_{\text{av}}$ represents an average over $P(q)$. This quantity is expected to have the scaling form

$$\rho=\tilde{\rho}(L^{1/\nu}(T-T_c)). \tag{12}$$

For transitions with a diverging correlation length, curves of ρ vs T for various L should intersect at T_c, since ρ will be independent of L at $T=T_c$. Our results for ρ vs T for various system sizes are shown in Fig. 1. The curves do not intersect each other at any point and hence indicate that no phase transition takes place for

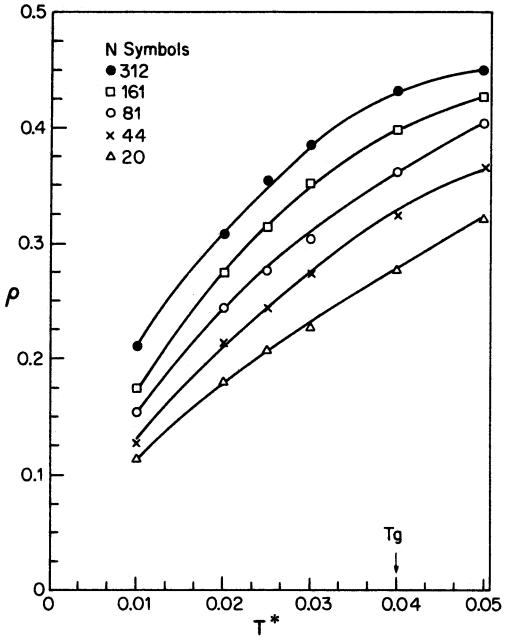

FIG. 1. Plot of ρ as defined in Eq. (11) vs reduced temperature $T^* = T/T_0$ (see text) for various sample sizes. Solid lines are guides to the eye. The position of the experimental value of T_g is indicated by the arrow.

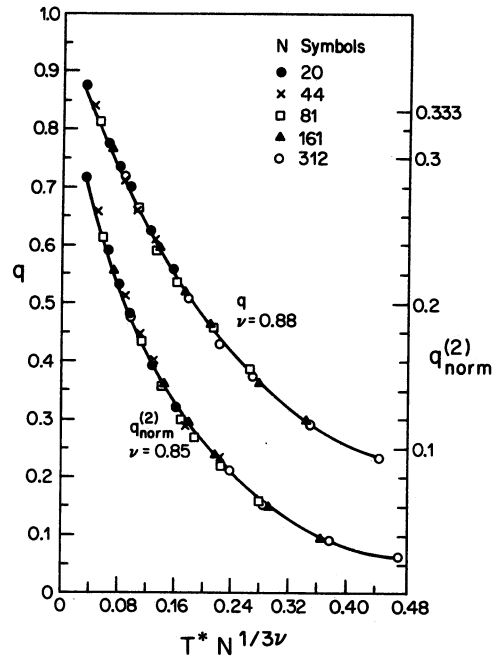

FIG. 2. Finite-size-scaling curves for q and $q^{(2)}_{\rm norm}$ and the value of ν found in each case. Solid lines are guides to the eye.

$T > 0.01\,T_0$, which is $\simeq \frac{1}{4}$ of the experimentally observed T_g. This leads us to consider the possibility that $T_c = 0$. For a zero-temperature critical point, $\beta = 0$ and this implies $d - 2 + \eta = 0$. Hence for $d = 3$ we get $\eta = -1$, and $\gamma = \nu(2-\eta) = 3\nu$. Then, finite-size scaling predicts that

$$q \simeq T^{\beta}\tilde{q}(L/\xi) \simeq \tilde{\tilde{q}}(TN^{1/3\nu}), \tag{13}$$

where $\xi \simeq T^{-\nu}$ is the correlation length. Also, $q^{(2)}$ is expected to exhibit the scaling behavior

$$q^{(2)} \simeq \tilde{q}^{(2)}(TN^{1/3\nu}). \tag{14}$$

Our results for q and $q^{(2)}_{\rm norm}$ can be fitted very well by the scaling forms, Eqs. (13) and (14). The scaling curves for q and $q^{(2)}_{\rm norm}$ and the values of ν found in each case are shown in Fig. 2.

We also studied the temperature and sample-size dependence of the various relevant time scales of the system. Through definition of a quantity

$$\Delta q(t) = q(t) - q, \tag{15}$$

the longest relaxation time, $\tau_{\rm max}(T)$, of the system at any particular temperature can be defined as

$$\Delta q(t \geq \tau_{\rm max}(T)) = 0. \tag{16}$$

Also, to characterize the average thermal relaxation time, $\tau_{\rm av}(T)$ we write $\delta q(t) = \Delta q(t)/\Delta q(0)$ in terms of a distribution of relaxing modes, $Q(\tau)$:

$$\delta q(t) = \int_0^{\infty} d\tau\, Q(\tau) e^{-t/\tau}, \tag{17}$$

which implies that

$$\tau_{\rm av}(T) \equiv \int_0^{\infty} Q(\tau)\tau\, d\tau = \int_0^{\infty} \delta q(t)\, dt. \tag{18}$$

Another time scale of interest is $\tau_{\rm hop}(T)$ which is the typical time between successive hops from one metastable equilibrium configuration (EC) to another. This time scale can be defined only for samples having more than one EC (e.g., $N = 312$, 161, and 81).[18] We computed this in the following way. At each point of the time evolution we computed the overlap of the evolved state $\{\mathbf{S}_i(t)\}$ with each nonequivalent EC $\{\mathbf{S}_i^{\alpha}\}$ as

$$\max[(1/N)\textstyle\sum_i \mathbf{S}_i(t)\cdot\mathbf{R}\cdot\mathbf{S}_i^{\alpha}], \tag{19}$$

where $\mathbf{R}$ is a general O(3) matrix, remembering that states connected by simple rotations and/or inversions would be equivalent. From the observed time dependence of the overlaps, it is easy to determine the time the system spends in the neighborhood of a particular EC before making a transition to the vicinity of a different one. The average value of $\tau_{\rm hop}(T)$ was calculated from the average of the logarithm of these time intervals over the whole run. Our results for the three different time scales for $N = 161$ are shown in Fig. 3. As can be seen, the time scales of the system do not increase as fast as $e^{\alpha/T}$, indicating that no barriers develop. Another important result is that even at very low temperatures, the time scales do not increase with N as $\exp(AN^x)$. Thus, the nonergodic behavior[19] expected in a spin-glass phase is not present in the

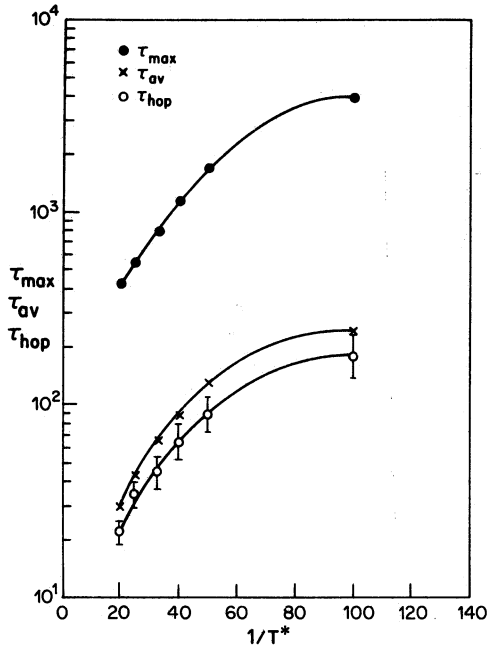

FIG. 3. Semilog plots of the various relevant time scales (see text) in units of Monte Carlo steps per spin vs the inverse of the reduced temperature of $N=161$. Solid lines are guides to the eye.

RKKY model. The observed N dependence of the time scales is even slower than a power law, indicating that the correlation length is finite at all nonzero values of the temperature.

In summary, we conclude that the RKKY model shows a critical point at $T=0$ and that only RKKY exchange cannot account for the experimental observations[20] of time scales increasing faster than an Arrhenius law at low temperatures. Actually real-life spin-glasses contain weak randomly anisotropic Dzyaloshinsky-Moriya interactions[21] and it has been suggested by various authors[22] that a small amount of anisotropy can induce a crossover to Ising-type behavior. These mean-field calculations predict a nonzero T_c for the isotropic case and therefore, are not directly applicable to the RKKY model. However, it is quite plausible that Ising-type behavior will result when the rotational symmetry of the RKKY interaction is broken by the presence of anisotropy. As simulations of three-dimensional short-range Ising spin-glass indicate a transition at a finite temperature, we expect that the introduction of anisotropy in the RKKY model will bring the transition temperature to a nonzero value. Some evidence indicating the existence of such a finite-temperature phase transition has been provided by the work of Walstedt and Walker.[11,12] A comprehensive study of this question is currently in progress.

The numerical computation was performed on the University of Minnesota Cray 1 computer. It required approximately 30 h of central processing unit time. The use of the Cray computer was made possible by a grant from the University of Minnesota Supercomputer Institute. This work was also supported by the Alfred P. Sloan Foundation.

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