Finite temperature phase transition in the three-dimensional Heisenberg ±*J* spin glass model

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The three-dimensional Heisenberg spin glass model with ±*J* interactions is studied using an over-relaxed Monte Carlo algorithm. We have measured the correlation length ξ, and using the crossing of ξ/L for different L find a finite temperature spin glass transition, with $T_{SG}=0.220(5)$. In addition, we have varied the number of Monte Carlo steps used prior to, and during, thermal averaging to control the effects of finite time averaging. We find that the over-relaxation algorithm allows for an accurate measurements using as few as 300 Monte Carlo steps. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2670270]

Spin glasses have attracted a great deal of theoretical attention over the last 30 years, yet even the most fundamental issues remain unresolved. For example, the nearest neighbor three-dimensional (3D) Ising spin glass model was only recently shown to undergo a conventional, finite temperature second order phase transition.[1] The status of the spin glass transition in nearest neighbor 3D Heisenberg spin glass models has not been as controversial, as it has long been accepted that the model only orders at zero temperature.[2,3] It has been suggested that while the *spins* do not order at finite T, chiral degrees of freedom do.[4] However, recent Monte Carlo calculations of finite lattice correlation lengths showed that both spin and chiral degrees of freedom order at the *same* finite T_{SG} for a Gaussian distribution of bonds.[5] One reason given[5] for the erroneous conclusion that $T_{SG}=0$ was that the ordering occurs at temperatures too low to be accessible in prior Monte Carlo simulations. In the case of bimodal interactions it has also been suggested[6,7] that $T_{SG}\neq 0$, but the correlation length was not measured.

Evidence for the existence of a finite T_{SG} for Heisenberg spin glasses with bimodal ±*J* interactions has so far been based on rather exotic measurements, at least compared to the more studied Ising counterparts. These include measurements of the twist free energy[6] and an analysis of time correlation functions.[7] Both methods rely upon assumptions which make the conclusions somewhat suspect. Here we present measurements of the correlation length, ξ, for the ±*J* Heisenberg spin glass model. We demonstrate that a unique temperature exists where $\xi\propto L$, where L is the linear dimension of the finite sized lattice. The temperature for which $\xi \propto L$ is identified as T_{SG}. Having identified T_{SG}, we also make estimates of the critical exponents.

The Hamiltonian for the 3D ±*J* Heisenberg spin glass is $\mathcal{H}=-\sum_{\langle ij\rangle}J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j$, where $\mathbf{S}_i$ are three-dimensional unit vectors and the bonds J_{ij} take values ±1 at random, and with equal proportions. We study the model on a simple cubic lattice with periodic boundary conditions and $N=L^3$ spins, with sizes $L=4$, 6, 8, 10, and 12 (the same range of sizes used in Ref. 5). To simulate the model we use a Metropolis Monte Carlo algorithm incorporating over-relaxation updates.[8] Following every Metropolis update (one attempted update/site) we use five over-relaxation updates/site, which rotate the spins about the local internal field due to the coupling with nearest neighbor spins. Each Monte Carlo sweep then comprises N Metropolis updates and $5\,N$ over-relaxation updates. Details of our over-relaxation scheme are given elsewhere,[9] but we remark that for the noncollinear and frustrated ground state expected for the present model, the correlation times should be much reduced by the inclusion of an over-relaxation update except at the lowest temperatures. Indeed, as shown in the inset to Fig. 1, increasing the number of Monte Carlo steps by orders of magnitude has a little effect on our measurements, indicating that the correlation times have been greatly exceeded, except for the lowest T and largest L.

For each realization of bonds J_{ij} we simulate two replicas of the system, 1 and 2. The elements of the overlap tensor are defined as

$$q^{kl}=N^{-1}\sum_i S^k_{i,1}S^l_{i,2}, \qquad (1)$$

where $k,l=x,y,z$ are the Cartesian components of $\mathbf{S}_{i,1}$ and $\mathbf{S}_{i,2}$. The order parameter q for the model is given as a time average $\langle\,\rangle$, itself averaged over configurations of disorder [ ],

$$q=\sum_{k,l}[\langle|q^{kl}|\rangle]. \qquad (2)$$

At T_{SG} finite size scaling theory predicts that $q\sim L^{-\beta/\nu}$, where β and ν are critical exponents. The spin glass susceptibility is

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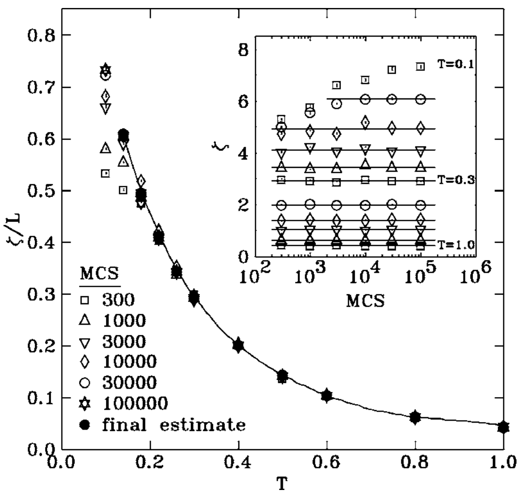

FIG. 1. Correlation length divided by system size, ξ/L, vs temperature as the number of Monte Carlo steps (MCSs) is increased during a simulated anneal ($L=10$). Also shown (●) are our final estimates of ξ/L. The inset shows ξ vs MCS for all temperatures studied. The range of MCSs used in the average for each T is shown by straight lines. At the lowest temperature, $T=0.1$, we do not observe a clear convergence.

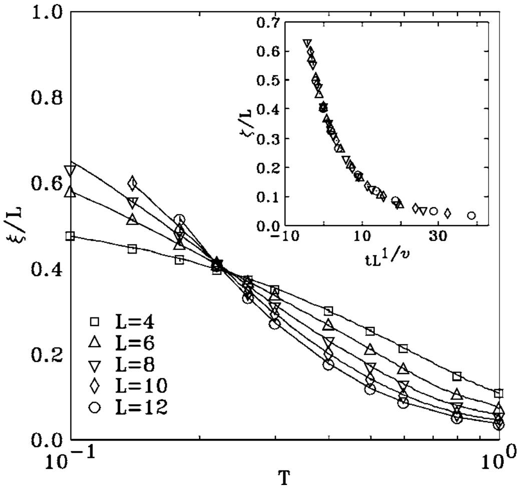

FIG. 2. Correlation length divided by system size, ξ/L, vs T for different L. A clear crossing is observed at $T_{SG}=0.22$. The inset shows the scaling of ξ/L according to Eq. (7) with $\nu=1.04$.

$$\chi = N^{-1}\sum_{k,l}\left[\left\langle\left|\sum_{i,j} q_i^{kl}q_j^{kl}\right|\right\rangle\right], \tag{3}$$

which diverges at T_{SG} as $\chi \sim L^{\gamma/\nu}$, with γ related to β and ν via hyperscaling ($\gamma = d\nu - 2\beta$), and d being the dimensionality.

The overlap between replicas can be generalized to wave vector **k**, allowing for the measurement of the correlation length. To do so, we define

$$q^{kl}(\mathbf{k}) = N^{-1}\sum_i S_{i,1}^k S_{i,2}^l e^{i\mathbf{k}\cdot R_i}, \tag{4}$$

where R_i is a vector connecting site i to an arbitrary origin. The spin glass susceptibility generalized to wave vector **k** is then

$$\chi(\mathbf{k}) = N^{-1}\sum_{k,l}\sum_{i,j}[\langle|q_i^{kl}q_j^{kl}e^{i\mathbf{k}\cdot\mathbf{r}_{ij}}|\rangle], \tag{5}$$

where $\mathbf{r}_{ij}=\mathbf{R}_i-\mathbf{R}_j$. Using this definition of $\chi(\mathbf{k})$ the correlation length is calculated[1,5] using

$$\xi = \frac{1}{2\sin(|\mathbf{k}_{min}|/2)}\left[\frac{\chi(0)}{\chi(\mathbf{k}_{min})}-1\right]^{1/2}, \tag{6}$$

where $\mathbf{k}_{min}=(2\pi/L,0,0)$ is the minimum wave vector allowed by our choice of boundary conditions. For $T \gg T_{SG}$, ξ should be independent of size while for low temperatures, $\xi \sim \sqrt{N}$. At T_{SG} one expects $\xi \sim L$ *if* the transition is second order. Thus a plot[1] of ξ/L for various L will cross at T_{SG}, fanning out both above and below T_{SG}. This method was used to determine T_{SG} in Ising[1] and Heisenberg[5] spin glasses with Gaussian bond distributions, and has also been shown to work well in $\pm J$ frustrated Heisenberg ferromagnets[9] where a comparison can be made between various independent measures of T_C.

A difficulty experienced in Monte Carlo simulations of spin glass models is the slow convergence at low temperatures. To investigate convergence we simulate the model with increasing numbers of Monte Carlo sweeps, m, used both prior to and during thermal averaging. For each L and m we simulate $n=100$ disorder configurations beginning in the paramagnetic state and cooling to low temperatures (simulated annealing). Different disorder configurations are used for each L and m in order to check that our choice, $n=100$, produces consistent results. The number of Monte Carlo steps range from $300 \le m \le 10^5$.

As there are two principal and independent sources of error, a thermal error and a disorder error, we expect that with increasing m and n the total error σ should behave as $\sigma = (\sigma_m^2/m + \sigma_n^2/n)^{1/2}$. With n fixed, a lack of sufficient thermal averaging should show up as a decrease in the error with increasing m. On the other hand, if the correlation time has been greatly exceeded and $\sigma_m^2/m \ll \sigma_n^2/n$, then σ should be approximately constant and the data for different m will agree within the stated error, provided n is large enough.

Our expectations are borne out in Fig. 1 where we show the simulation data for $L=10$, the smallest L for which a lack of convergence could be observed. For $T \ge 0.18$, the calculated ξ are independent of m, as are the errors. The results at $T=0.14$ with $m=300$ and $m=1000$ are clearly underestimated; the data at $T=0.14$ remain correlated with the previous measurement at $T=0.18$, evidence that the appropriate correlation time has not been exceeded. At $T=0.1$, ξ continues to increase with increasing m, and for this reason we cannot make an estimate of ξ at this temperature. For $L=12$ we did not observe a convergence for $T=0.1$ and $T=0.14$, which, based on the behavior at $L=10$, is entirely expected. We make final estimates of $\xi(T,L)$ using a weighted average of those results deemed to have converged, as shown in the inset of Fig. 1 by straight lines spanning those measurements used in the average.

In Fig. 2 we have plotted ξ/L vs T. For a conventional, finite temperature, second order phase transition, the data should cross at T_{SG}, the temperature for which $\xi \propto L$. A clear crossing is observed at $T=0.22$. The data show little to no shift in the crossing point as L increases. To demonstrate the clear crossing we show in Fig. 3(a) plot of $\log(\xi)$ vs $\log L$ at

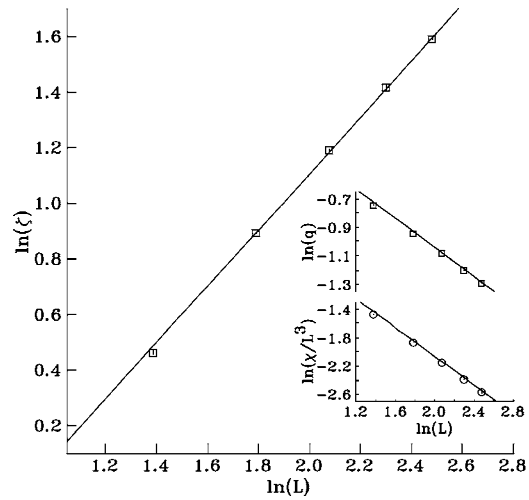

FIG. 3. Double logarithmic plot of ξ vs L at $T_{SG}=0.22$. A fit omitting the $L=4$ point yields a slope $s=1.012(15)$. The proximity to $s=1$ shows that $T_{SG}\sim 0.22$ and that finite size corrections are small. The inset shows double logarithmic plots of q and χ/N vs L. The slopes obtained from the two fits, omitting $L=4$, yields our estimates $\beta/\nu=0.509(8)$ and $\gamma/\nu=1.990(33)$.

$T=0.22$. If ξ is proportional to L at this temperature, then the data should fal on a straight line with slope $s=1$. Fitting for $L\geqslant 6$ gives $s=1.012(15)$, consistent with $s=1$. The proximity of our result to $s=1$ shows that we are very close to the critical temperature, and our estimate of the transition temperature is $T_{SG}=0.220(5)$.

According to standard finite size scaling theory

$$\xi/L=\mathcal{F}(tL^{1/\nu}), \tag{7}$$

where $t=(T-T_{SG})/T_{SG}$ is the reduced temperature and ν the exponent of the correlation length. An estimate of $1/\nu$ can be made from the slope of ξ/L by noting that, at T_{SG}, $\log[d(\xi/L)/dT]\propto(1/\nu)\log(L)$. A fit to this form, for $L\geqslant 6$, yields $1/\nu=0.96(6)$. In the inset of Fig. 2 we show the collapse according to Eq. (7) using $\nu=1.04$, and we point out that the collapse is excellent over the entire temperature range studied.

Further support for our assertion that $T_{SG}=0.220(5)$ is found in the scaling of the order parameter q and the spin glass susceptibility χ. According to standard theory, at T_{SG} we should have $q=aL^{-\beta/\nu}$ and $\chi=bL^{\gamma/\nu}$, while from hyperscaling $d=2(\beta/\nu)+\gamma/\nu$. Fits of the data in log-log form provide the exponent ratios, and using $L\geqslant 6$ we get $\beta/\nu=0.509(8)$ and $\gamma/\nu=1.990(33)$. The inset to Fig. 3 shows the fits of $\log(q)$ vs $\log(L)$ and $\log(\chi/N)$ vs $\log(L)$. The data at $L=4$ clearly suffer from finite size effects, and it would be desirable to have results for larger L to confirm the large L behavior. In addition, hyperscaling is well satisfied with $2(\beta/\nu)+\gamma/\nu=3.01(4)\sim 3$.

Our results are in good agreement with those of other authors who conclude that $T_{SG}\neq 0$. The twist free energy calculation[6] of Endoh *et al.* gives $T_{SG}=0.19(2)$, although it was necessary to assume a particular scaling form for the size dependent shift of their observed crossing point. Our results show no shift in the crossing point, except perhaps at $L=4$. Nakamura and Endoh estimated[7] $T_{SG}=0.22^{+0.01}_{-0.04}$, $\nu=1.1(2)$, $\gamma=1.9(4)$, and $\beta=0.72(6)$. These results compare reasonably well with ours, $T_{SG}=0.220(5)$, $\nu=1.04(6)$, and $\gamma=2.1(1)$, with the exception of our results $\beta=0.53(3)$.

In conclusion, we have shown that the nearest neighbor, $\pm J$ Heisenberg spin glass undergoes a conventional, second order phase transition in 3D, with $T_{SG}=0.220(5)$. Our data cannot accommodate a zero temperature transition since the correlation length diverges at $T\neq 0$. Lastly, we have shown that the use of over-relaxation updates along with standard Metropolis updates allows one to study the model at T_{SG} using as little as 300 Monte Carlo updates.

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