MONTE CARLO CALCULATIONS ON THE FINITE RANDOM ANISOTROPY MODEL

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Monte Carlo calculations on the random anisotropy model of Harris, Plischke, and Zuckermann[1,2] have been performed using free and periodic boundary conditions. The impact of these two different boundary conditions has been considered for calculations dealing with low temperatures and temperatures near the finite spin analog of the magnetic transition temperature (T_c). Although this paper has the somewhat limited object of studying the effect of boundary conditions on finite magnetic systems with random anisotropy, it is necessary to mention that two major questions are of interest. Does the random anisotropy model in equilibrium assume a spin glass state[3] below T_c? For an infinite system would the magnetic susceptibility and specific heat diverge, or at least have a maximum, as T_c is approached from above? For some examples of spin glasses,[4] the specific heat maximum occurs at a temperature above the temperature at which the magnetic susceptibility shows a maximum.

The Hamiltonian describing the random anistotropy model is[1,2]

$$H = -\frac{1}{2}\sum_{i,j=1}^{N} J_{ij}\vec{S}_i\cdot\vec{S}_j - D\sum_{i=1}^{N}(\hat{k}_i\cdot\vec{S}_i)^2 - \vec{B}\cdot\sum_{i=1}^{N}\vec{S}_i. \quad (1)$$

The first term is the exchange term, the second term is the anisotropy term and the third term is the Zeeman term. We will assume a simple cubic lattice with nearest neighbor coupling, where J_{ij} equals J for i and j referring to nearest neighbors and is zero otherwise. The spin located on site i is $\vec{S}_i$. All spins will be treated "classically" i.e. any orientation of the spins is allowed. Each spin will be assumed to have magnitude one, $|\vec{S}_i| = 1$. The $\hat{k}_i$ are unit vectors, randomly oriented, while D measures the strength of the random anisotropy term. In all of our calculations the magnetic field $\vec{B}$ will be set equal to zero, and J will be set equal to 1, which in effect determines the temperature scale.

We will evaluate four quantities. These are the rms magnetization m_r, the Edwards Anderson order parameter q, the specific

heat c, and the average magnetic susceptibility $\overline{\chi}$.

We define

$$m_x = \frac{1}{N}\sum_{i=1}^{N} S_{ix} \quad (2)$$

where N is the number of spins and there are similar equations for y and z. We only deal with classical spins and so the thermodynamic average for a canonical ensemble of any quantity A is given by

$$\langle A \rangle = \frac{\int e^{-\beta H} A\, d\Omega}{\int e^{-\beta H} d\Omega} \quad (3)$$

where

$$d\Omega = \prod_{i=1}^{N} \sin\theta_i \, d\theta_i \, d\phi_i \quad (4)$$

The angles θ_i and ϕ_i are the customary angles giving the orientation of $\vec{S}_i$ and $\beta = 1/(kT)$ where k is Boltzmann's constant and T is the temperature. We define the rms magnetization m_r as,

$$m_r = (\langle m_x^2 \rangle + \langle m_y^2 \rangle + \langle m_z^2 \rangle)^{1/2}. \quad (5)$$

The Edwards-Anderson order parameter q is defined as[5]

$$q = \frac{1}{N}\sum_{i=1}^{N} \langle \vec{S}_i \rangle \cdot \langle \vec{S}_i \rangle. \quad (6)$$

The specific heat per spin at constant field is given by[6]

$$c = (k\beta^2/N)\,[\langle H^2 \rangle - \langle H \rangle^2]. \quad (7)$$

The average susceptibility per spin at constant temperature is given by[6]

$$\overline{\chi} = \frac{1}{3}(\chi_{xx} + \chi_{yy} + \chi_{zz}), \quad (8)$$

where

$$\chi_{xx} = N\beta\,(\langle m_x^2 \rangle - \langle m_x \rangle^2), \quad (9)$$

with similar definitions for χ_{yy} and χ_{zz}.

All of the thermodynamic averages were evaluated using the algorithm of Metropolis et al.[7] in which we generate M systems $\{\alpha\}$ of an ensemble and thermodynamic averages are evaluated by

$$\langle A \rangle = \frac{1}{M} \sum_{\alpha=1}^{M} A_\alpha, \qquad (10)$$

where A_α is the value of the quantity A in the αth system. The techniques for generating the systems of the ensemble have been described elsewhere.[8,9] The averages defined by (3) are approximately calculated by (10).

In Fig. 1, we plot m_r^2/q vs. D/J for a fixed temperature $T = .3/k$. This temperature is well below the transition temperature T_c which for $D = 0$ and an infinite system is $T_c = 1.445/k$. Notice that $m_r^2/q = 1$ for a perfectly aligned ferromagnetic state and $m_r^2/q = 0$ for a spin glass state. The calculational results of Fig. 1 seem to indicate that the low temperature state is either

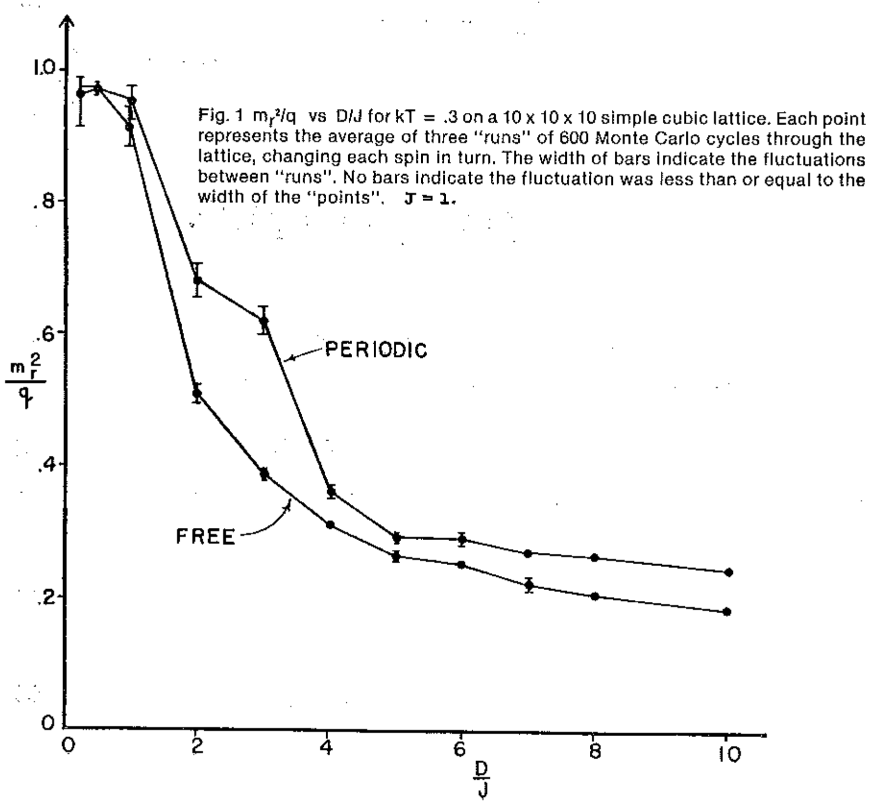


Fig. 1 m_r^2/q vs D/J for kT = .3 on a 10 x 10 x 10 simple cubic lattice. Each point represents the average of three "runs" of 600 Monte Carlo cycles through the lattice, changing each spin in turn. The width of bars indicate the fluctuations between "runs". No bars indicate the fluctuation was less than or equal to the width of the "points". J = 1.

ferromagnetic or asperomagnetic-like, depending on the value of D/J. It is possible that larger lattices than 10 x 10 x 10 would lead to different conclusions as has been pointed out by Jayaprakash and Kirkpatrick.[4] We believe, however, for *small* D/J even if the exact ground state is spin glass for an infinite system that for any calculationally reasonable finite system the ground state will appear to be ferromagnetic. There also may be metastable states for which m_r is sizeable. It is also worth noticing that the results differ, depending on whether periodic or free boundary conditions are used. This difference would indicate that the lattice is really not large enough. At least part of this difference can be interpreted as being due to a shift in the effective transition temperature due to a change in boundary conditions.[8]

Other calculations have been performed with different random numbers to define the anisotropy. At $kT = .3$ these led to fluctuations of order 10% in the calculated values of m_r^2/q, again an indication that a larger lattice would be desirable.

In Fig. 2, we plot q, m_r, $(c)^{-1/2}$ and $(\bar{\chi})^{-1}$ versus temperature for $D/J = 3.0$. Since both q and c involve local or nearest neighbor properties we should expect the results for them to be approximately valid even for our relatively small lattice. These plots show that the apparent T_c for systems with free boundary conditions is below the T_c for systems with periodic boundary conditions, and in fact the shift in T_c is the major change. Also for both cases the maximum for $\bar{\chi}$ would appear to occur at a higher temperature than for c although convergence for $kT \cong 1.5$ is such as to make this point unclear, see Table 1. The fluctuations in the results increase as T_c is approached from above. Some similar calculations were done at $kT = 1.9$ with larger lattices (12^3 vs 10^3) and with different random numbers to define the anisotropy. Changes in size produced relatively appreciable fluctuations in results (10% or more) as did changes in the "random" anisotropy directions.

In Figs. 3 and 4 the values of q is plotted for each of the 10 x 10 layers in a cubic lattice with 10^3 spins. Notice that except at very low temperature there is an appreciable surface effect as well as effects attributable to a shift in apparent T_c. These results suggest that measurements of surface magnetization should be of interest. For D's which are not too large, such measurements could serve to indicate the appropriateness of the random anistoropy model.

For the results of Figs. 1, 2, 3, and 4 and Table I the first 1800 Monte Carlo cycles through the lattice were not recorded so as to eliminate any bias caused by selection of the initial state. Figs. 1, 2, 3, 4 then use averages of the next 1800 M.C. steps.

Fig. 2 m_r, q, $(\bar{X})^{-1}$, and $(c)^{-1/2}$ vs kT for D/J = 3.0 on a 10 x 10 x 10 simple cubic lattice. Results for both free and periodic boundary conditions are shown. J = 1.

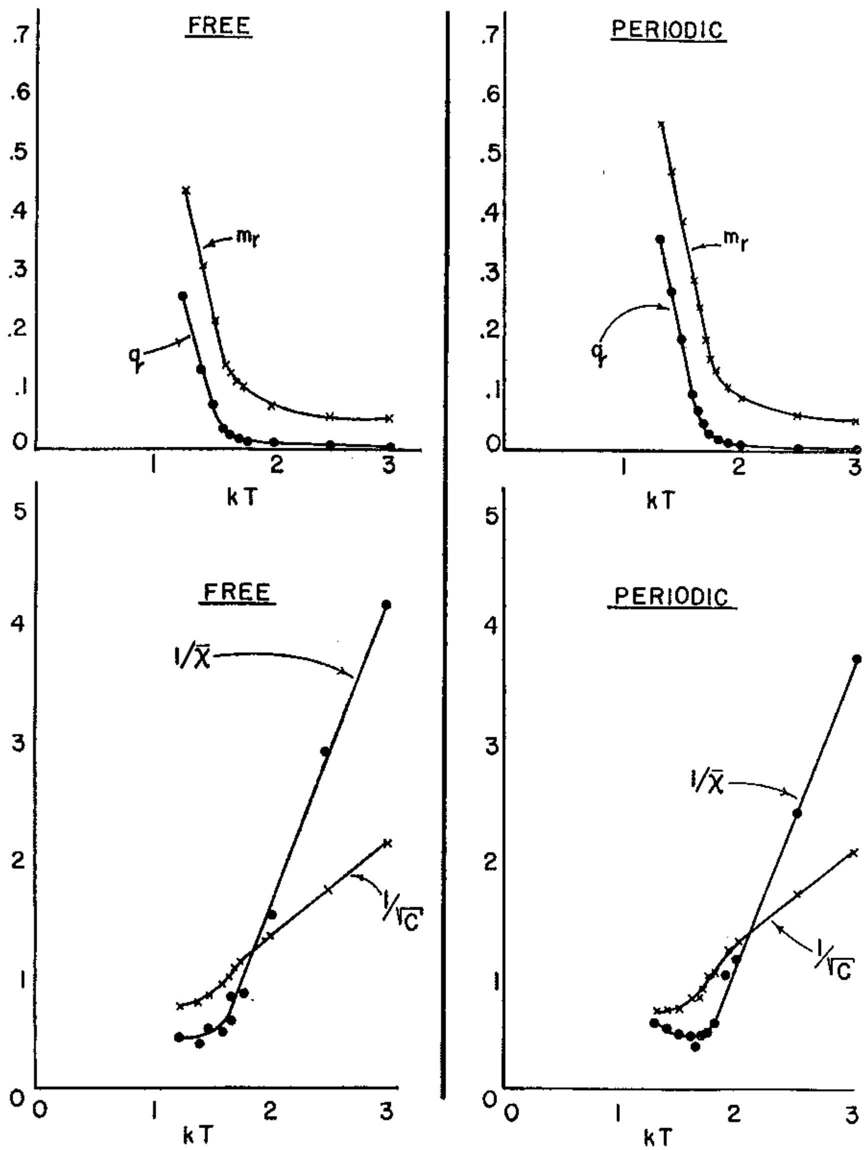
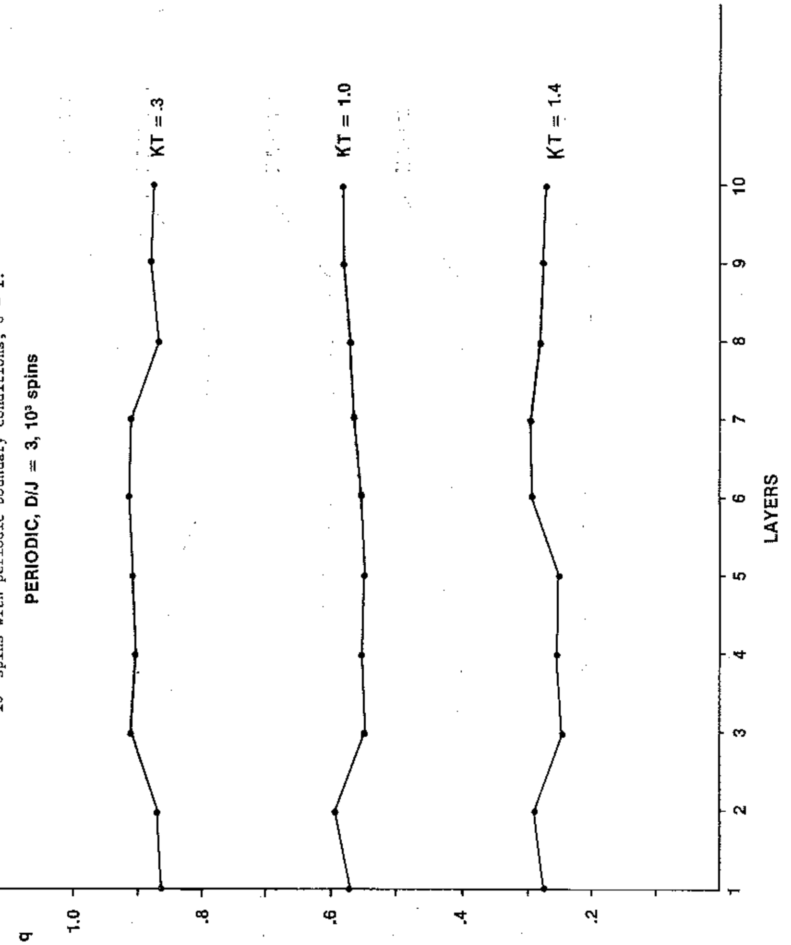


Fig. 3 Edwards-Anderson order parameter q for 10 layers on lattice of 10^3 spins with periodic boundary conditions, J = 1.



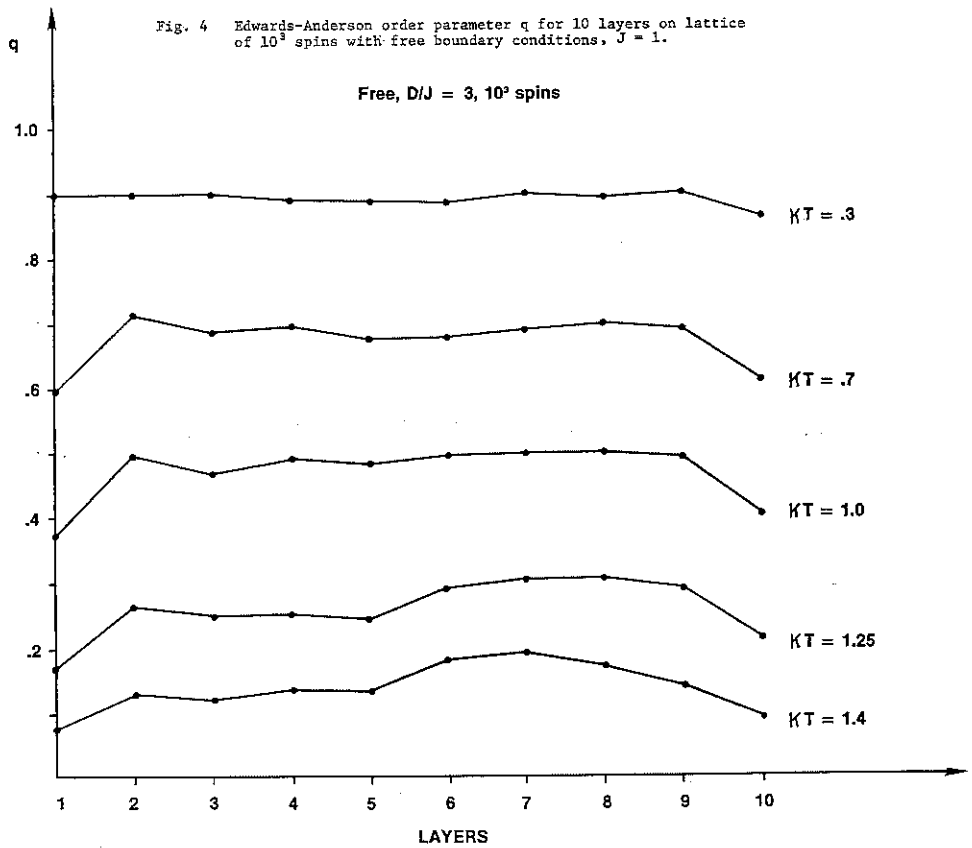


Fig. 4 Edwards-Anderson order parameter q for 10 layers on lattice of 10^3 spins with free boundary conditions, J = 1.

Table I

	kT	Δq	q	$\Delta q/q$	Δm_r	m_r	$\Delta m_r/m_r$	Δc	c	$\Delta c/c$	$\Delta\overline{\chi}$	$\overline{\chi}$	$\Delta\overline{\chi}/\overline{\chi}$
Periodic	3	.0003	.005	.06	.003	.054	.06	.040	.222	.18	.013	.266	.05
	2.5	.0007	.006	.12	.006	.062	.10	.061	.327	.19	.034	.412	.08
	2	.0031	.011	.28	.013	.093	.14	.052	.555	.09	.150	.830	.18
	1.5	.020	.187	.11	.017	.393	.04	.365	1.719	.21	.469	1.803	.26
Free	3	.0001	.005	.02	.002	.051	.04	.033	.217	.15	.017	.239	.07
	2.5	.0003	.006	.05	.004	.057	.07	.068	.322	.21	.023	.342	.07
	2.0	.0009	.009	.10	.006	.076	.08	.050	.522	.10	.065	.655	.10
	1.5	.013	.073	.18	.016	.222	.07	.577	1.294	.45	.070	1.690	.04

Fluctuations in thermodynamic quantities at various temperatures for free and periodic boundary conditions. The fluctuations Δq, Δm_r, Δc, and $\Delta\overline{\chi}$ are those found in 3 "runs" of 600 cycles through the lattice. The values q, m_r, c, and $\overline{\chi}$ are the averages of the 3 "runs." J = 1.

Several previous calculations have been done on the random anisotropy model[10-13] and new papers are continuing to appear.[4,14,15] After an initial sequence of confusion it appears to be accepted that the ground state is spin glass for any D/J. Because of the numerical difficulty, for finite systems, in obtaining low temperature spin glass states we believe that magnetized states must be very near in energy to spin glass states and so they may be as accessible experimentally as the true ground state. Thus from a practical point of view the fact that the ground state may be spin glass may be of less importance.

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