Order of phase transition for systems with multispin interactions: Monte Carlo simulations

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A family of two-dimensional spin models with n-spin interactions in one direction and two-spin interactions in the other is studied by Monte Carlo simulations. Our results show that for the case where the variables are of the Ising (q-state Potts, $q>2$) type the transition is of first order for $n>n_c=3$ ($n>n_c=2$) in agreement with previous conjecture.

Lattice models with multispin interactions, although less studied than those involving two-spin interactions, are relevant in many physical situations.[1] The phase diagram of these systems may show a rich variety of critical behavior, the classical example being the exactly soluble eight-vertex model.[2]

Recently, an interesting class of one-dimensional quantum models involving multispin interactions has been introduced.[3,4] The models are described by the reduced Hamiltonian

$$\mathcal{H}=-\lambda\sum_i \sigma_i^z\sigma_{i+1}^z\sigma_{i+2}^z,\ldots,\sigma_{i+n}^z-\sum_i\sigma_i^x\ , \tag{1}$$

where λ is a coupling constant and σ_i^x,σ_i^z are Pauli matrices located at lattice site i. The case $n=2$ reduces to the exactly soluble transverse Ising model. This model is self-dual. Hence, the phase transition should occur at $\lambda=\lambda_c=1$, for all n, provided that the transition is unique. The invariance of the above Hamiltonian under the nonlocal symmetry corresponding to reversing the spins in any two of the n sublattices renders its ground state 2^{n-1} degenerate. The ground-state degeneracy and the structure of the low-lying levels suggested that these models should belong to the same universality class as the 2^{n-1}-state Potts model.[3,4] This conjecture implies that the triplet ($n=3$) model should have the same critical behavior as the 4-state Potts model and the Baxter-Wu model,[5] and the transition should be first order[6] for $n>3$. Attempts to test the conjecture for the triplet model have been made essentially only by finite-size scaling. Although the first calculations were inconclusive,[7,8] more recent results strongly support the conjectures.[9]

The question of the order as a function of n of the phase transitions was studied initially by mean-field theory (MFT)[3,7] and by finite-size scaling (FSS).[4] The MFT results state that for $n>n_c=2$ the transition is first order, which is not a surprise if we remember that for the q-state Potts model this type of calculation[10] also gives a first-order phase transition for $q>q_c=2$, which is clearly wrong. The FSS results suggest that $n_c=4$; however, as stated by these authors,[4] their FSS results should not be taken too seriously in the estimation of the order of the phase transition. More recently, the authors of Ref. 11, by improving the MFT and using a proposed criterion[12] to distinguish between continuous and discontinuous phase transitions, concluded that $n_c=3$, in agreement with the conjecture.

Motivated by the fact that Monte Carlo simulations have been proved to be a powerful tool in the determination of the nature of phase transitions for gauge[13] and spin systems[14,15] we decided to use this technique to analyze the order of the phase transition for the models (1).

The quantum Hamiltonian (1) may be considered as the time continuum limit[16] [$J_s\to 0$, $J_t\to\infty$, $\lambda=J_s\exp(J_t)$] of the classical model whose reduced Hamiltonian (action) is given by

$$\mathcal{H}=-\sum_{i,j}\left[J_s\prod_{k=0}^{n}\sigma(i+k,j)+J_t\sigma(i,j)\sigma(i,j+1)\right]\ , \tag{2}$$

where $\sigma(i,j)=\pm 1$ are classical Ising variables defined on a square lattice and J_s,J_t are the coupling constants in the horizontal (space) and vertical (time) direction, respectively. Because the long-distance properties are preserved in the above limit we expect the classical model (2) and quantum model (1) to belong to the same universality class. The Hamiltonian (2) is also self-dual,[3] which can be seen as a consequence of the fact that we have two interactions per lattice point.[17] The critical temperature, for the isotropic case, under the assumption that it is unique, is given by $J_s=J_t=\frac{1}{2}\ln(\sqrt{2}+1)$ for all n.

Our Monte Carlo simulation is performed by employing the heat-bath algorithm[13-15] for the isotropic case $J_s=J_t=J$ of the classical model (2). The nature of the phase transitions for these models can be investigated[13-15] by comparing, at critical temperature, long simulations of an initially ordered state and an initially totally disordered state. Figures 1(a)–1(c) show the evolution of the energy per spin for those simulations in the cases $n=2$ (Ising model), $n=3$, and $n=4$, where by iteration we mean one Monte Carlo step per spin. We clearly see in Fig. 1(c) that after a short relaxation time (of the order of 100 iterations) each one of the configurations reached the equilibrium at two clearly distinct values of the average energy. This implies the existence of a large latent heat, proportional to the difference between the energy of those final configurations, which render the transition first order for the case $n=4$. In sharp contrast we show in Fig. 1(a) the same simulation for the Ising model ($n=2$), and we clearly see that the two final energies are equal, consistent with a continuous phase transition. In Fig. 1(b) we show such simulations for the triplet ($n=3$) case. In this case the evolution of the two states is consistent with the absence of latent heat but with a large divergence in the

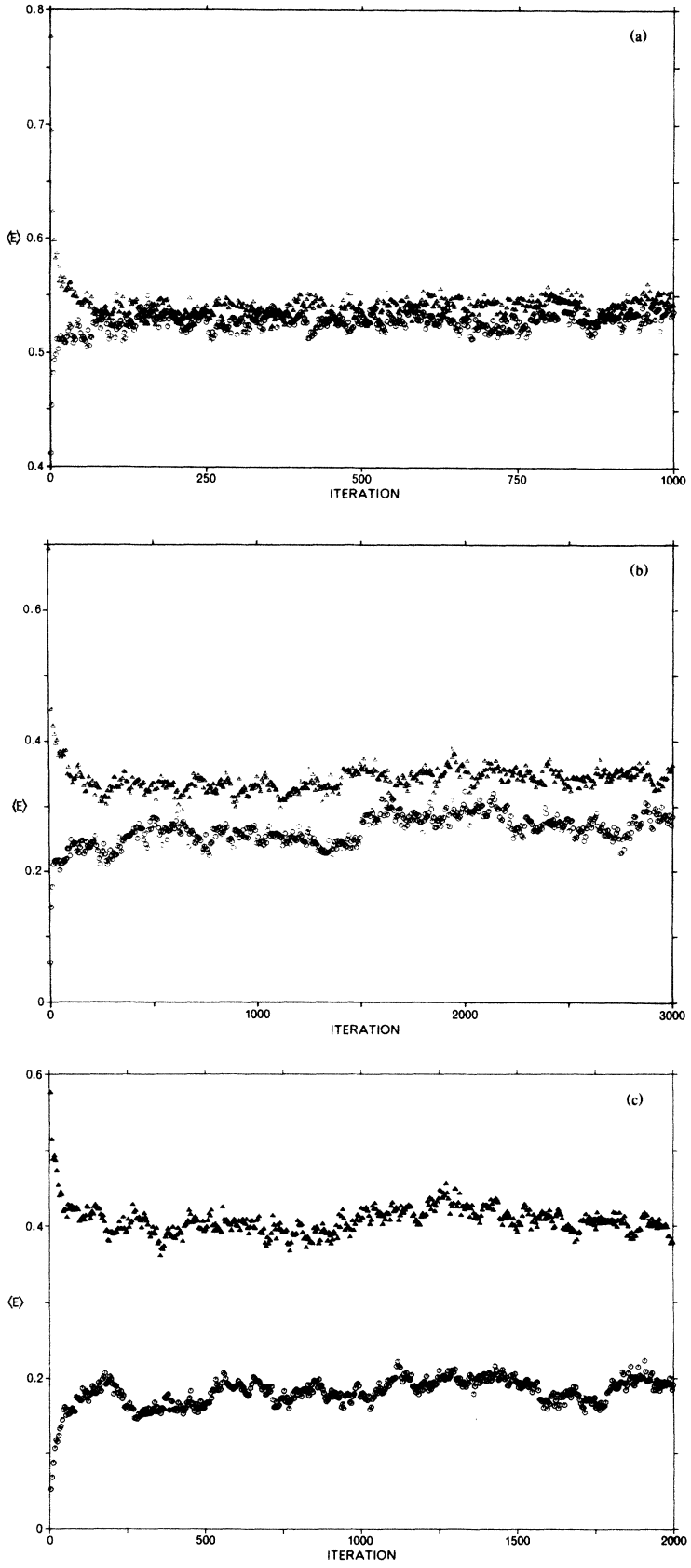

FIG. 1. Evolution, at the critical temperature $J=\frac{1}{2}\ln(\sqrt{2}+1)\cong 0.44$, of an initially disordered state (triangles) and an initially ordered state (circles). The lattice size is 132×132 and the energy is normalized to be 1 (zero) for infinite (zero) temperature. These simulations refer to the Ising multispin system described by the Hamiltonian (2) for the cases (a) $n=2$, (b) $n=3$, and (c) $n=4$.

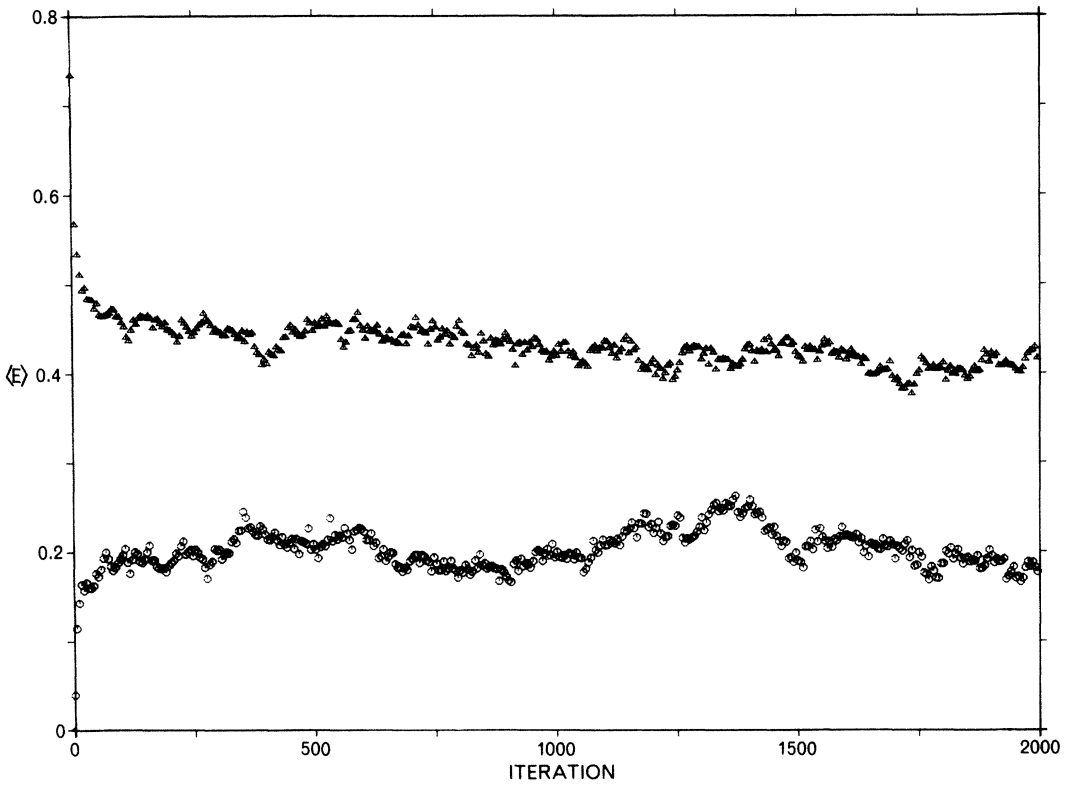

FIG. 2. Same as Fig. 1 for the triplet 3-state Potts model [$n=3$, $q=3$ in Eq. (3)] at the critical temperature $J_s=J_t=\ln(\sqrt{3}+1)\cong 1.005$.

specific heat. This is exactly what we should expect if the triplet model belongs to the same universality as the 4-state Potts and Baxter-Wu models, where the specific-heat divergence is peculiarly large ($\alpha=\frac{2}{3}$).[2,6] The same type of simulation in the Baxter-Wu models shows[14] similar results to those in Fig. 1(c).

We also investigate the order of the transition for the q-state Potts version[7] of the multispin Hamiltonian (2):

$$\mathcal{H}=-\sum_{i,j}\left[J_s\delta_q\left(\sum_{k=1}^{n}n(i+k,j)\right)+J_t\delta_q(n(i,j)+n(i,j+1))\right], \tag{3}$$

where $n(i,j)=0,1,\ldots,q-1$ and δ_q is a Kronecker δ function, modulo q. Like the two-body Potts model the above models are also self-dual[7,17] with the critical coupling expected to be $J_s=J_t=\ln(\sqrt{q}+1)$. In Fig. 2 we show the simulations for the triplet ($n=3$) model, which shows that the transition is already of first order (the ground state is sixfold degenerate in this case). Similar simulations reveal that the difference between the final states increases with n and q.

In summary, by performing Monte Carlo simulations, we have shown in this paper that the multispin models (1) exhibit a first-order phase transition for $n>n_c=3$ in agreement with the conjecture that those models belong to the same universality class as the 2^{n-1}-state Potts models. The generalization (3) of these models has $n_c=2$ for all q.

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