First-order phase transitions of Ising models with multispin interactions

O. G. Mouritsen and S. J. Knak Jensen
Department of Physical Chemistry, Chemical Institute, Aarhus University, DK-8000 Aarhus C, Denmark

B. Frank
Department of Physics, Sir George Williams Campus, Concordia University, 1455 de Maisonneuve Boulevard West, Montreal, Quebec, H3G 1M8, Canada

(Received 28 April 1980)

Ising models on fcc lattices with pure three-spin or pure four-spin interactions are shown by Monte Carlo calculations to exhibit only one phase transition which is of first order. The transition temperature of the model with pure four-spin interactions differs from the Onsager result. This implies that the model is likely not to possess a self-dual property as claimed by Wood.

Much attention is currently devoted to phase transitions and critical phenomena of lattice models with many-body interactions, e.g., three-body and four-body interactions. In particular, the question is raised whether the critical properties of such models differ from the critical properties of models with pure pair interactions. In two dimensions, the exact solution of the Baxter model[1] reveals nonuniversal critical behavior, and the exact solution of the Ising model on a triangular lattice with pure three-spin interactions[2] leads to a critical behavior different from that of the Ising model with pure pair interactions. Three-dimensional Ising models on cubic lattices with three-spin (triplet) and four-spin (quartet) interactions have been investigated by Griffiths and Wood (GW)[3–8] using dual transformations and series analysis. For models with pure triplet and pure quartet interactions on fcc lattices GW[6,7] find the critical exponents to differ appreciably from the exponents of the three-dimensional Ising model with pure pair interactions. Furthermore, the series result for the critical temperature of the quartet model on the fcc lattice, which is believed to be self-dual with respect to the chosen quartet interactions,[4] is at variance[5] with the Onsager result. Provided that the self-dual property holds, this has the important implication that the uniqueness postulate should be invalid for this model.

The series result of GW are based on the assumption that the phase transition of the models is *continuous.* In this paper we shall demonstrate that the phase transition of Ising models on fcc lattices with pure triplet and pure quartet interactions is of *first order.* The transition temperature of the quartet model differs from the Onsager result. This, in conjunction with the fact that we observe only one phase transition, implies that the model is likely not to be self-dual, in contrast to Wood's conjecture.[4]

Our results are derived from Monte Carlo calculations of the ferromagnetic order parameter (the magnetization per spin),

$$m = N^{-1}\left\langle \left| \sum_{i=1}^{N} \sigma_i \right| \right\rangle , \tag{1}$$

and the internal energy per spin, $E = \langle H \rangle / N$, of the two Ising models defined by the Hamiltonians

$$H_3 = -J_3 \sum_{\{i,j,k\}} \sigma_i \sigma_j \sigma_k \tag{2}$$

and

$$H_4 = -J_4 \sum_{\{i,j,k,l\}} \sigma_i \sigma_j \sigma_k \sigma_l \ . \tag{3}$$

The models are arrayed on fcc lattices consisting of N sites subjected to toroidal periodic boundary conditions. $J_3 > 0$ and $J_4 > 0$ are coupling parameters, and $\sigma_i = \pm 1$ is the spin variable at the ith lattice site. The sums in Eqs. (2) and (3) comprise all elementary triangles $\{i,j,k\}$ and tetrahedra $\{i,j,k,l\}$, respectively, formed by nearest-neighbor bonds of the fcc lattice. The ground state of the triplet model is uniquely the ferromagnetic state. The ground-state manifold of the quartet model contains in the limit $N \rightarrow \infty$ infinitely many states, one of which is the ferromagnetic state.

We have applied a conventional Monte Carlo importance-sampling technique to calculate for a prescribed temperature a canonical ensemble corresponding to the Hamiltonians in Eqs. (2) and (3). The ensemble averages are calculated from coarse-grained averages[9] which are averages over a small number of systems of the ensemble. In addition, we have calculated the distribution functions of the internal energy and the order parameter. The distribution functions, which give the relative occurrence of a given energy and order of the systems comprising the ensemble, as well as the coarse-grained averages, are useful in detecting metastable states close to first-order transitions.[10–12] The calculations are carried out on lattices consisting of $N = 2L^3$ spins with $L = 4$, 8, and 10. In order to estimate the numerical uncertainties and to detect possible metastable states we have performed the Monte Carlo calculations several times for each temperature using different chains of random numbers and starting from different initial spin configurations. Furthermore, we have calculated increasing as well as decreasing temperature series. The data in the transition region are obtained using 5000 MCS/S (≡ Monte Carlo steps per site), while 500 MCS/S are used outside the transition region.

We have calculated $E(T)$ and $m(T)$ over an extended range of temperatures. The temperature dependence of these properties, as well as of the corresponding fluctuation quantities, clearly indicates that each model exhibits only one phase transition.

In Fig. 1 we present the Monte Carlo data for $E(T)$ and $m(T)$ in the transition region for the triplet model. Both properties exhibit metastabilities demonstrating that the phase transition of the triplet model is of *first order*. The metastabilities are observed in the Monte Carlo experiments as (i) shifts between the ordered and the disordered phase during the evolution of the Monte Carlo experiment for temperatures in the transition region, and as (ii) hysteresis in $E(T)$ and $m(T)$ when calculated for increasing and decreasing series of temperatures. The effect of increasing the lattice size is to enhance the gap in E and m in the transition region and to reduce the frequency of shifts between the two coexisting phases. In the transition region the shift frequency for the $N = 128$ system is as high as 1 per 20 MCS/S, which makes necessary the use of the distribution functions when estimating the equilibrium values of E and m. In the disordered phase $m(T)$ possesses an unphysical tail due to finite-size effects. From Fig. 1 we estimate the discontinuities of the internal energy and the order parameter to be approximately $\Delta E/E_0 \approx 65\%$ and $\Delta m \approx 88\%$.

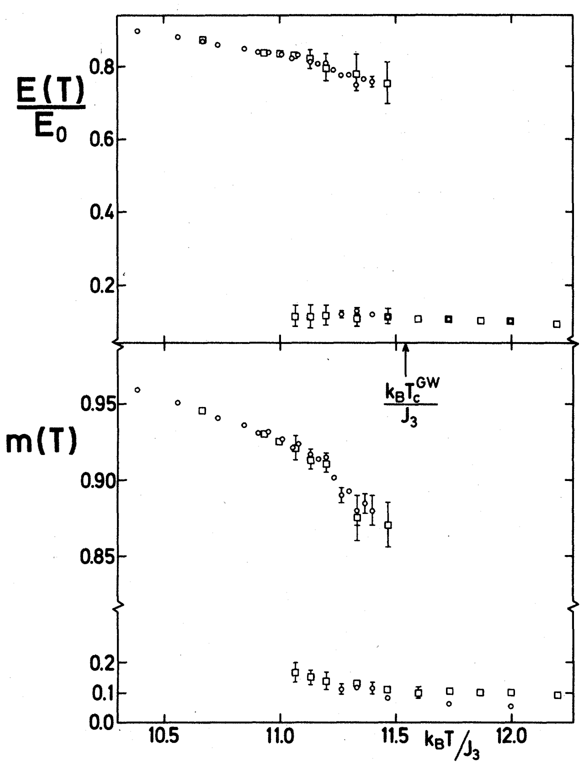

FIG. 1. Temperature dependence of the normalized internal energy, $E(T)/E_0$, and the ferromagnetic order parameter, $m(T)$ Eq. (1), for the pure *triplet* model, Eq. (2). E_0 is the energy of the ground state. The results are obtained from Monte Carlo calculations on fcc lattices with N spins. □: $N = 128$, ○: $N = 2000$. T_c^{GW} is the transition temperature from the series analysis by Griffiths and Wood.

Figure 2 shows the Monte Carlo data for $E(T)$ and $m(T)$ in the transition region for the quartet model. Also for this model there is clear evidence of metastabilities. Thus the transition of the quartet model is of *first order*. The upper branch of the $m(T)$ curve is calculated for increasing temperatures starting from a ferromagnetic ordered state. Due to the high degeneracy of the ground state for this model it is impossible to determine the actual long-range order for decreasing temperatures starting from a disordered state. Neither is it possible to determine the actual long-range order in the transition region if the system during the course of the Monte Carlo experiment shifts from the ferromagnetic state to the disordered state or to any other ordered state. The lower branch of the $m(T)$ curve in Fig. 2 derived from the ferromagnetic order parameter in Eq. (1) is therefore an underestimate of the actual finite-size rounding. However, a clear discontinuity in $m(T)$ is observed for increasing temperatures, simultaneously with the jump in the internal energy. The energy curve remains the same as in Fig. 2 when one starts at low temperatures from a ground state different from the ferromagnetic state. Only for the smallest system, $N = 128$, is it possible in decreasing temperature series starting from a disordered state to make the system enter the ordered phase within reasonable computer time. For the larger systems the metastable disordered states have lifetimes larger than 10^4 MCS/S for all temperatures investigated. We interpret this as evidence of the lack of large fluctuations, indicating that the model does not go critical for any temperature. This accords with the first-order nature of the transition. We estimate the discontinuities for the quartet model to be $\Delta E/E_0 \approx 58\%$ and $\Delta m \approx 98\%$.

The terminals of the upper and lower branches of the $E(T)$ and $m(T)$ curves in Figs. 1 and 2 constitute an upper and a lower limit, respectively, of the

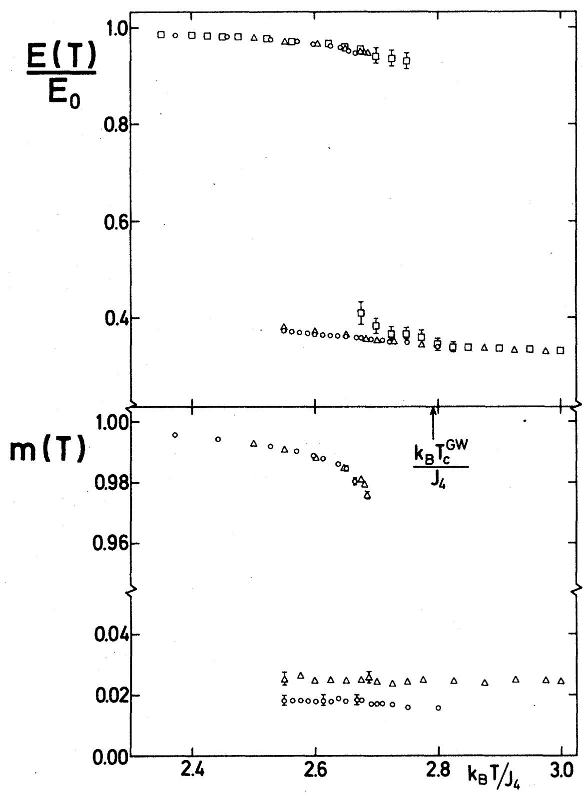

FIG. 2. Temperature dependence of the normalized internal energy, $E(T)/E_0$, and the ferromagnetic order parameter, $m(T)$ Eq. (1), for the pure *quartet* model, Eq. (3). E_0 is the energy of the ground state. The results are obtained from Monte Carlo calculations on fcc lattices with N spins. □: $N=128$, Δ: $N=1024$, ○: $N=2000$. $T_c^{\rm GW}$ is the transition temperature from the series analysis by Griffiths and Wood. The lower branches of the curves for the larger systems are somewhat arbitrarily broken off around $k_BT/J_4 \sim 2.55$.

transition temperature. The upper limit decreases with increasing lattice size. This leads us to estimate from the figures the transition temperatures for the triplet model and the quartet model to be $k_BT_c/J_3=11.33\pm0.05$ and $k_BT_c/J_4=2.66\pm0.01$, respectively. The corresponding values from the series analysis by GW[5,6] are $k_BT_c^{\rm GW}/J_3=11.54$ and $k_BT_c^{\rm GW}/J_4=2.79\pm0.01$, respectively. For both models the series estimate of "the critical temperature" lies above the true transition region. The transition temperature of the quartet model is markedly different from the Onsager result, $k_BT_c/J_2 = -2/\ln(\sqrt{2}-1)\simeq 2.27$. Recently Mitran[13] has calculated "the critical temperature" for the quartet model to be $k_BT_c/J_4=2.795$ by using a product average decomposition approximation in conjunction with a generalized nonuniform magnetic field method. This approach appears to be based on the assumption that the transition is continuous. It should be noted that due to the long lifetimes of the metastable disordered states for the quartet model the estimate of the lower limit of $T_c^{\rm MC}$ is based solely on the Monte Carlo data for the small system. If the finite-size dependence of this limit is qualitatively different from that of the triplet model (and various well-known pair-interactions models where the lower limit increases with N) it cannot be excluded that the transition temperature may be lower than the value quoted above.

For a further comparison of the Monte Carlo results with the "critical properties" derived from the series study of the two models, we have estimated the "effective exponent" $\beta_{\rm eff}$ by fitting the function $m(T)\sim(T_c^{\rm GW}-T)^{\beta_{\rm eff}}$ to the Monto Carlo data. The asymptotic slopes of $\log m(T)$ vs $\log(T_c^{\rm GW}-T)$ plots lead to $\beta_{\rm eff}=0.045\pm0.010$ and $\beta_{\rm eff}=0.013\pm0.002$ for the triplet and the quartet model, respectively. These values are consistent with the respective series estimates[5,6] 0.0538 and 0.0133. It thus appears that the series analysis in terms of power-law singularities may effectively describe properties in the vicinity of the first-order transitions.

In summary, we have presented conclusive evidence for the first-order nature of the phase transitions of Ising models on fcc lattices with pure triplet and pure quartet interactions. This makes irrelevant the classification[5,8] of the models in universality classes different from the universality class of the three-dimensional Ising model with pure pair interactions. Our finding of only one phase transition with a transition temperature different from the Onsager result implies that the quartet model is likely not to possess a self-dual property as claimed by Wood.[4] To resolve this apparent discrepancy between the Monte Carlo result and Wood's duality conjecture we note that Wood in establishing the self-dual property of the quartet model explicitly assumes the ground state to be ferromagnetic,[4] thereby making possible a correspondence between the high-temperature and low-temperature graphical expansions of the partition function. However, as the ground state is highly degenerate this assumption is not justified, and the status of the self-dual relation therefore remains unclear.

We finally wish to comment on the expected influence on the critical properties of admixtures of many-body potentials to ordinary pair potentials. The models considered in this paper, when including pair interactions, do not fulfill the Kadanoff-Wegner criterion[14] for nonuniversality, and their critical behavior is therefore expected to be determined solely by the pair-potentials. Renormalization-group studies[15,16] lend support to this expectation. In contrast, the series analysis by Griffiths and Wood leads to critical exponents varying continuously with the interaction parameters.[7,8] However, the results presented here, as well as mean-field[17] and renormalization-group calculations,[15,16] are consistent with the hypothesis that the models possess a tricritical point, and that the phase transition changes from a continuous transition to a first-order transition when a many-body interaction parameter becomes sufficiently large. It would be of importance to investigate the validity of this hypothesis in order to assess whether these three-dimensional models violate the universality postulate.

The authors wish to express their gratitude to the Danish Natural Science Research Council for supporting this project. B.F. would like to thank NSERC of Canada for continuing support.

[1]R. J. Baxter, Phys. Rev. Lett. 26, 832 (1971).

[2]R. J. Baxter and F. Y. Wu, Phys. Rev. Lett. 31, 1294 (1973).

[3]D. W. Wood and H. P. Griffiths, J. Math. Phys. 14, 1715 (1973).

[4]D. W. Wood, J. Phys. C 5, L181 (1972).

[5]H. P. Griffiths and D. W. Wood, J. Phys. C 6, 2533 (1973).

[6]D. W. Wood and H. P. Griffiths, J. Phys. C 7, 1417 (1974).

[7]D. W. Wood and H. P. Griffiths, J. Phys. C 7, L54 (1974).

[8]H. P. Griffiths and D. W. Wood, J. Phys. C 7, 4021 (1974).

[9]O. G. Mouritsen and S. J. Knak Jensen, Phys. Rev. B 18, 465 (1978).

[10]O. G. Mouritsen, S. J. Knak Jensen, and P. Bak, Phys. Rev. Lett. 39, 631 (1977).

[11]S. J. Knak Jensen, O. G. Mouritsen, E. Kjaersgaard Hansen, and P. Bak, Phys. Rev. B 19, 5886 (1979).

[12]S. J. Knak Jensen and O. G. Mouritsen, Phys. Rev. Lett. 43, 1736 (1979).

[13]O. Mitran, J. Phys. C 12, 557, 4871 (1979). Note that an inconsistency in the approach of Mitran has recently been pointed out by B. Frank, J. Phys. C 12, L595 (1979).

[14]L. P. Kadanoff and F. J. Wegner, Phys. Rev. B 4, 3989 (1971).

[15]A. Aharony, Phys. Rev. B 9, 2416 (1974).

[16]M. Gitterman and M. Mikulinsky, J. Phys. C 10, 4073 (1977).

[17]V. M. Matveev and E. L. Nagaev, Sov. Phys. Solid State 14, 408 (1972).