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LETTER TO THE EDITOR

A Monte Carlo study of the kinetic Ising model with triplet interactions

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Abstract. Results of a Monte Carlo study of a kinetic Ising model with triplet interactions are presented. Effective exponents are determined for the static susceptibility and relaxation rate for the magnetisation time correlation function above the critical point. The results are consistent with Suzuki's concept of weak universality.

We present here results of a Monte Carlo study of a kinetic Ising model whose Hamiltonian contains pure triplet interactions on a triangular lattice, i.e.

$$H = -J \sum_{\langle ijk \rangle} \mu_i \mu_j \mu_k, \tag{1}$$

where $\mu_i = \pm 1$ and $\langle ijk \rangle$ form a triangle of nearest-neighbour interactions. The dynamical properties of this model are defined by a master equation (Glauber 1963) for the probability function $P(\mu_1 \ldots \mu_N, t)$, namely

$$\frac{\mathrm{d}}{\mathrm{d}t} P(\mu_1 \ldots \mu_N, t) = \sum_{j=1}^{N} (w_j(-\mu_j) P(\mu_1 \ldots -\mu_j \ldots \mu_N, t) - w_j(\mu_j) P(\mu_1 \ldots \mu_j \ldots \mu_N, t)), \tag{2}$$

where $P(\mu_1 \ldots \mu_N, t)$ is the probability that the systems will be in spin configuration $\{\mu_1 \ldots \mu_N\}$ at time t. The transition probability $w_j(\mu_j)$ for a spin μ_j to flip satisfies detailed balance and is chosen here to be

$$w_j(\mu_j) = \exp(2\beta \mu_j E_j), \qquad 2\beta \mu_j E_j < 0 \tag{3}$$

(in units of a free spin relaxation rate) and is otherwise zero. In (3) E_j is the local field at site j, such that

$$H = -\sum_j \mu_j E_j.$$

The dynamical properties of this model are of interest since it is known from the exact solution (Baxter and Wu 1973) for the free energy corresponding to (1) that this system belongs to a universality class other than that of the nearest-neighbour Ising model. In addition to the exact results for the specific heat and correlation length exponents ($\alpha = \nu = \frac{2}{3}$), it has also been conjectured (Baxter *et al* 1975) that the spontaneous order parameter exponent $\beta = \frac{1}{12}$, or equivalently that the static susceptibility exponent $\gamma = \frac{7}{6}$.

The latter is of relevance for the dynamical behaviour of the triplet model, since one knows that the exponent Δ_M, which characterises the divergence in the order parameter relaxation rate τ_M (with $\tau_M \sim \epsilon^{-\Delta_M}$, where $\epsilon = (K_c - K)/K_c$ with $K = (J/k_B T)$, satisfies the rigorous inequality (Kawasaki 1972) $\Delta_M \geq \gamma$. (The equality corresponds to the conventional theory of critical slowing-down, which in general is incorrect for two- and three-dimensional systems.) Thus unless there is an unusual anomaly in the kinetic coefficient, one would expect Δ_M to have a value only slightly greater than γ and consequently be considerably different from the nearest-neighbour model, for which (Yahata and Suzuki 1969) $\Delta_M \simeq 2$.

We have investigated this question using standard Monte Carlo techniques (Stoll *et al* 1973) and have studied the static and dynamical properties for a lattice of $N = 52 \times 52$ spins, using periodic boundary conditions. In particular, we have computed the time-dependent magnetisation correlation function

$$\phi_M(t) = \frac{N}{k_B T \chi} \frac{1}{t_m - t - t_n} \int_{t_n}^{t_m - t} (M(t') - \langle M \rangle)(M(t + t') - \langle M \rangle) \, dt,$$

where $M(t) = N^{-1} \Sigma_{i=1}^{N} \mu_i(t)$, and χ stands for the isothermal susceptibility.

In general we follow the procedure and notation of Stoll *et al*; in particular, the time interval $t_m - t_n$ is one during which all configurations assumed by the system are equilibrium configurations. The static quantities, C_H, the specific heat, and χ, the isothermal susceptibility, can be computed (Stoll *et al* 1973) from expressions analogous to (4). The relaxation time τ_M for the magnetisation correlation function is obtained as an integral of $\phi_M(t)$ over the interval from $t = 0$ to $t = t_m - t_n$. As a practical matter, defining the relaxation function as above leads to a value of $\phi_M(t)$ which is negative for some value of $t = t^*$ (Muller–Krumbhaar and Landau 1976). The integration of $\phi_M(t)$ was therefore carried out over the interval from $t = 0$ to $t = t^*$. The error introduced by this procedure is quite small.

A minimum of 400 Monte Carlo Steps (MCS) were eliminated before any equilibrium averages were calculated. Averages were calculated over a minimum of 1200 MCS. It was found necessary to eliminate 4000 MCS and average over the next 12 000 MCS in the 'critical' region studies, corresponding to $0{\cdot}02 \leq \epsilon \leq 0{\cdot}1$, in order to obtain accurate estimates of the time constant τ_M in this domain. For values of $\epsilon < 0{\cdot}01$, finite-size rounding effects can be detected (Fisher 1971, Suzuki 1977).

As a check on our method we have computed the average energy and specific heat and compared them with the exact Baxter–Wu (1973) solution. The calculated values for the energy are always in close agreement with the exact results, the error being about 2% in the critical region. The situation with respect to the specific heat is quite similar, except that in the critical region the difference between the computed and exact C_H increases, as one would expect, and the error becomes of the order of 10% for equilibrium averages computed from 1200 MCS. More important, however, is that in this domain the exact specific heat does not display its asymptotic behaviour corresponding to an $\alpha = \frac{2}{3}$, but rather, as can be seen from figure 1, has an 'effective' exponent of 0·72, due to the influence of non-negligible correction terms. Thus the region which we can in practice study using Monte Carlo methods is not the asymptotic region, and we can therefore expect corrections to the leading singularity to be present in the static susceptibility and relaxation time. At present, therefore, we can only determine 'effective' values for γ and Δ_M. However, since the difference between the 'effective' exponent α in the region of our study and the exact α is small, we might expect the corrections to the leading singularity in χ and τ_M also to be small.

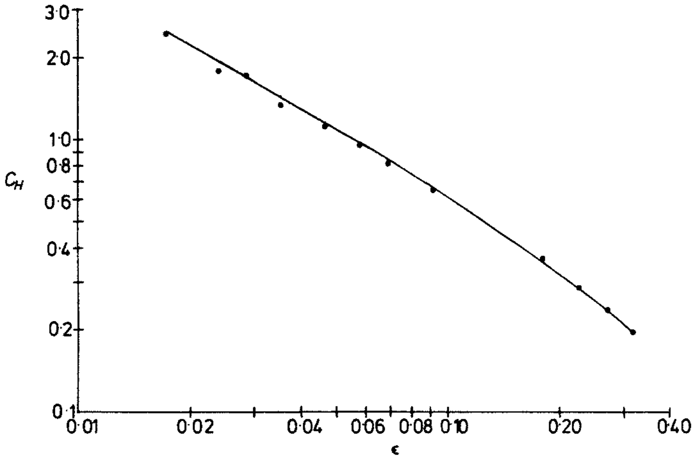

Figure 1. Specific heat C_H as a function of reduced temperature ϵ. The full line represents the exact solution (Baxter and Wu 1973). The full circles represent the Monte Carlo results.

Our results for the static susceptibility and relaxation rate are displayed in figures 2 and 3 respectively. The effective exponents in this region are given approximately by $\gamma = 1{\cdot}0$ and $\Delta_M = 1{\cdot}3$. Although an accurate estimate of the error is difficult to obtain, fluctuations in the data lead to an error estimate for the exponents of approximately 10%. Within the precision of our studies, our results are consistent with the conjectures that $\gamma = \frac{7}{6}$ and $\Delta_M \geqslant \gamma$. The most important qualitative conclusions which we can draw from our work are that the dominant contribution to τ_M comes from the static susceptibility (i.e. that the anomaly in the kinetic coefficient is small) and that the relaxation rates for the triplet and nearest-neighbour-like models are strikingly different.

Our result $\Delta_M \sim \frac{4}{3}$ is in fact in good agreement with the concept of weak universality in dynamics, as proposed by Suzuki (1978). According to this, the ratio Δ/ν should be

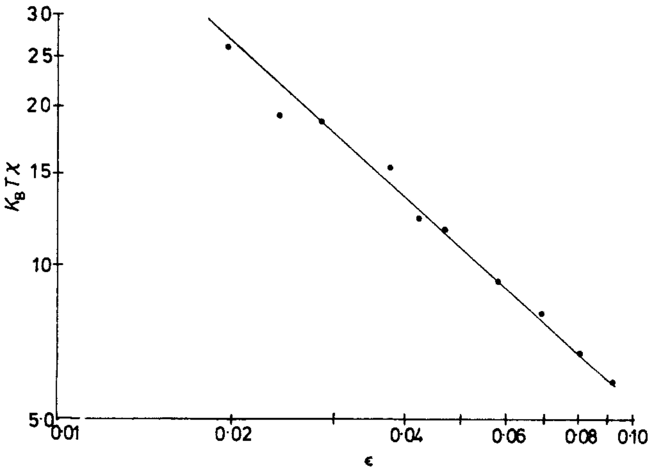

Figure 2. Monte Carlo results for magnetic susceptibility plotted against the reduced temperature ϵ.

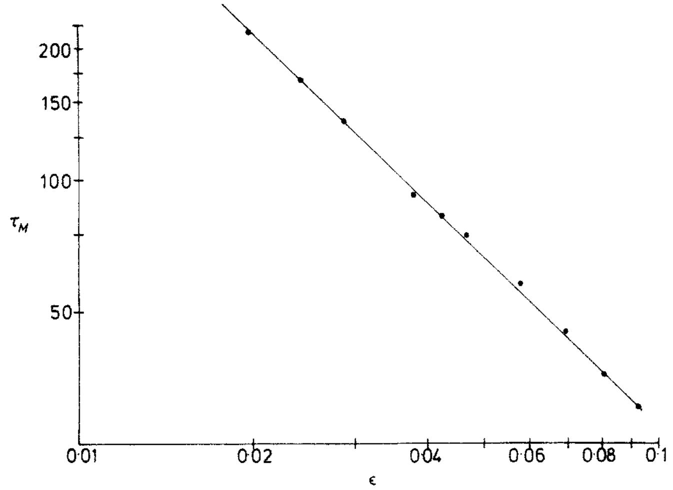

Figure 3. Monte Carlo results for the relaxation rate τ_M of the magnetisation time correlation function $\phi_M(t)$, plotted against the reduced temperature ϵ.

the same for the nearest-neighbour and triplet models. Therefore using the estimate $\Delta_M = 2$ for the nearest-neighbour model, and the known values $\nu = 1$ and $\nu = \frac{2}{3}$, leads to the prediction $\Delta_M = \frac{4}{3}$ for the triplet model.

Apart from improving the precision of our results by increasing the number of MCS used in computing equilibrium averages and obtaining data closer to the critical point, many interesting problems deserve future study. In particular, the low-temperature properties are of considerable interest, due to the existence of several competing ground states. In addition, the problem of the crossover to nearest-neighbour-like behaviour, which should occur in the correlation functions when nearest-neighbour interactions are included in (1), is also worthy of investigation. Our work is just the first step in understanding the dynamical properties of this model.

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