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COMMENT

Test of three-dimensional Q2R Ising algorithm

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Abstract. Simulation results of Q2R cellular automata on the simple cubic lattice are compared with usual Monte Carlo simulations of the Ising model. Curie temperature, spontaneous magnetisation and specific heat agree, but at low temperatures the susceptibility and the distribution of local energies differ.

In Q2R cellular automata one flips a spin if and only if this flip does not change the energy [1, 2]. Simulations showed [3] that this method reproduces the spontaneous magnetisation of the two-dimensional Ising model well, but at low temperatures problems appear [4]. The simplicity of this method allows high-speed simulations with up to 4300 million spin flip attempts per second [5]. The present work tries to check if the Q2R algorithm also gives Ising model results in three dimensions.

Initially we set the spins randomly up with probability p and down with probability $1-p$; the average energy (in units of the nearest-neighbour exchange energy J) is then larger than the ground-state energy -3 by $12p(1-p)$ on the simple cubic lattice. We then go through the lattice in a regular fashion, except that we divide the lattice into two sublattices treated consecutively [1-5]. Twenty spins were stored in one 60 bit computer word. The Curie point [6] corresponds to a concentration $p_c = 0.2125$ and infinite temperatures to $p = 0.5$. The magnetic field is always zero in this microcanonical algorithm.

The equilibrium magnetisation M measured in this way agrees well with that of the standard Metropolis type calculations [7], as shown in figure 1. Here we use the empirical energy-temperature relationship of [7] to compare our data at fixed energy with those of Landau for fixed temperature. Figure 2 also shows good agreement for the specific heat, where the temperature scale is now determined via $M(T)$. On the other hand, the fluctuations in the magnetisation measured through

$$\chi = (\langle M^2 \rangle - \langle M \rangle^2)/k_B T$$

differ strongly below the Curie point from the Ising model results, figure 3. Apparently the complete lack of energy fluctuations also reduces the magnetisation fluctuations in the Q2R method. The energy, figure 4, seems to work adequately. (Since we cannot determine the correct temperature directly in this microcanonical algorithm, we used the known relation between energy and temperature when we checked our results for the magnetisation, and the known relation between magnetisation and temperature when we checked our results for the energy. The specific heat is found by numerical differentiation of the energy curve, since the usual determination via energy fluctuations cannot work here.)

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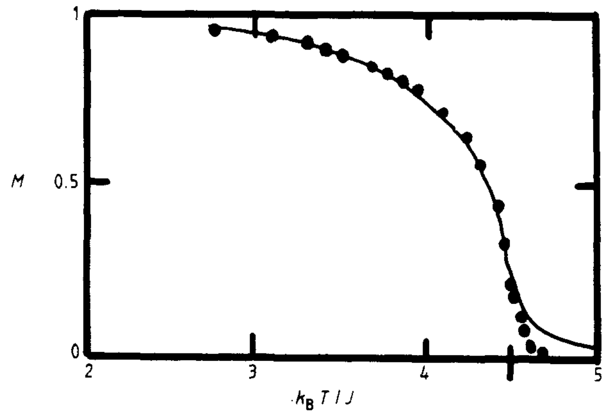

Figure 1. Spontaneous magnetisation plotted against $k_B T/J$. The full curve gives Landau's results for the Ising model.

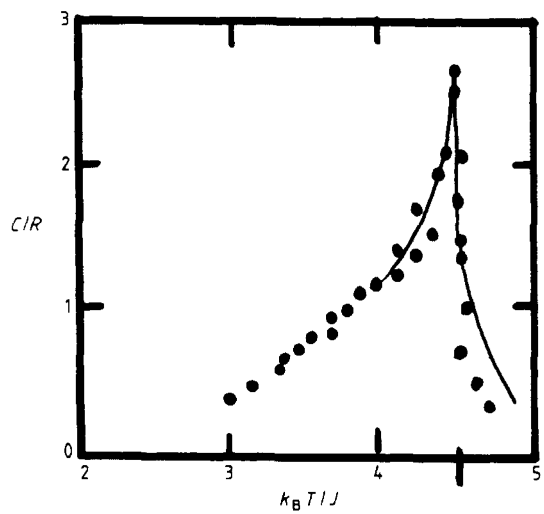

Figure 2. As figure 1, for the specific heat.

A direct way of determining the temperature T in the Q2R algorithm is to look at the local energy distribution. In the usual canonical ensemble, the probability that a site surrounded by six up neighbours is up itself must be larger by a factor $\exp(12J/k_B T)$ than the probability that this centre spin is down. Ratios of $\exp(8J/k_B T)$ and $\exp(4J/k_B T)$ must be valid for the case of five up and one down neighbour, or four up and two down neighbours, respectively. We found that above and at T_c these relations are well confirmed, but below T_c they are strongly violated. Similar effects were also found on a square lattice.

In summary, some aspects of the Ising model are described correctly by the Q2R algorithm, and others below the Curie temperature are not: 'handle with care'.

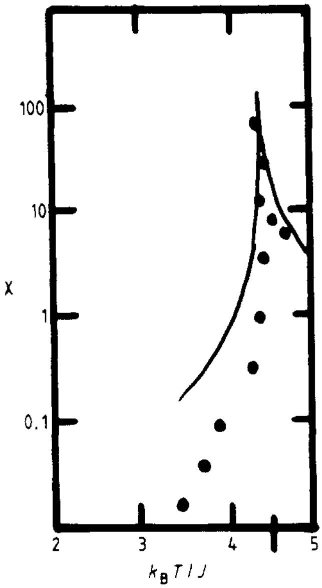

Figure 3. As figure 1, for the 'susceptibility'.

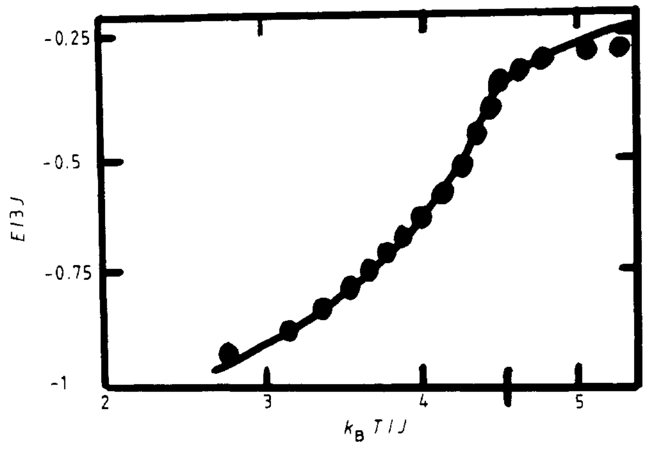

Figure 4. As figure 1, for the energy.

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