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Dynamics of antiferromagnetic Ising model with fixed magnetization

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Abstract. The dynamical critical exponent z of the Ising antiferromagnet under the constraint of a fixed zero magnetization is verified by Monte Carlo simulations to be compatible with that of the usual Glauber dynamics of model A, while for positive magnetization the exponent seems different. We also determine the diffusivity of the magnetization and finite size effects.

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The kinetics of the normal Ising model without conservation laws (model A according to the standard classification [1]) is well studied in two and more dimensions [2]; and this also holds for the Kawasaki dynamics of an Ising ferromagnet with conserved magnetization m (model B). Less known is the case of an antiferromagnet when we keep the magnetization m (*i.e. not* the order parameter) fixed [3]. This case, perhaps together with an Ising ferromagnet at conserved energy, is model C. Renormalized field theories are in preparation [4] for finite-size dynamics in model C, analogous to those for model A [5]. Qualitatively, Fisher renormalisation is expected to explain changes in the critical exponents [6]. Reference [7] reviews older work for bulk systems, while reference [8] is a more recent dynamical study of this bulk model (but different from ours). Thus we simulate here the antiferromagnet with a fixed magnetization for future comparison with field theories. At zero magnetization, the Neel temperature T_{N} of the antiferromagnet agrees with the Curie temperature T_{c} of the corresponding ferromagnet, while for a fixed $m = 0.1$ we found $T_{\mathrm{N}} \simeq 0.93T_{\mathrm{c}}$ on the square lattice and $T_{\mathrm{N}}(m = 0.08) = 0.987 \pm 0.001T_{\mathrm{c}}$ on the simple cubic lattice. Here and later, T_{c} refers to the $m = 0$ Curie and Neel temperature.

As in Kawasaki spin exchange dynamics of ferromagnets, two neighbouring spins $S = \pm 1$ exchange their orientation according to Boltzmann's normalized probability provided they are antiparallel. Initially, exactly half of the spins (or another predetermined fraction) are up, and the others are down. Right at $T = T_{\mathrm{N}}$ the staggered magnetization (order parameter) m_{s} should decay with time t as $1/t^{\beta/\nu z}$ where z is the dynamic critical exponent (defined through: time proportional to length z), and β, ν are the usual static exponents of the Ising model. Above T_{N} we expect asymptotically a simple exponential decay $\propto \exp(-t/\tau)$. One Cray-T3E processor dealt with more than one spin pair per microsecond in geometric parallelization of our $L \times L \times (L+1)$ or $L \times (L+1)$ lattices. Three lattice lines or planes had to be shifted to neighbouring processors in both directions of our ring topology, during each sweep through the lattice, making parallelization with a large number of processors difficult.

Figure 1 shows bulk behaviour of large systems at and above T_{N} at $m = 0$ in two and three dimensions. Right at T_{N} we find $z \simeq 2.1 \pm 0.1$ in two and three dimensions, compatible with model A [2], while above T_{N} we find $\tau \simeq 2000$ on the square lattice with $T/T_{\mathrm{c}} = 1.02$ and $\tau = 250 \pm 15$ on the simple cubic lattice at $T/T_{\mathrm{c}} = 1.01$. For $m = 0.08$ in three dimensions at the T_{c} of the $m = 0$ system, and thus about 1.3 percent above the shifted $T_{\mathrm{N}}(m)$, we found a relaxation time of 190 ± 10 for $L = 1023$. These times may serve to normalize field-theoretical times [4]. Figure 2 shows the phase diagram, T_{N} *versus* m.

For finite sizes one expects a decay of the staggered magnetization $\propto \exp(-t/\tau(L))$ where $\tau(L) \propto L^z$ at $T = T_{\mathrm{N}}(m)$. In three dimensions we find in Figure 3 $z \simeq 2$ for $T = T_{\mathrm{c}}$ and $m = 0$, consistent with model A. (The discrepancy between the expected $z = 2.05$ and our slope 1.96 shows the errors in our simulation, partly due to the complicated algorithm which is much slower than that for model A.) For $m = 0.08$ we get instead $z \simeq 2.28$, presumably different from the 2.05 of model A [2] and roughly compatible with the theoretical [1,3] prediction $z = 2 + \alpha/\nu \simeq 2.158$. In two dimensions at $m = 0$ and $T = T_{\mathrm{c}}$ (Fig. 3) gives $z = 2.15$ consistent with model A [2,9].

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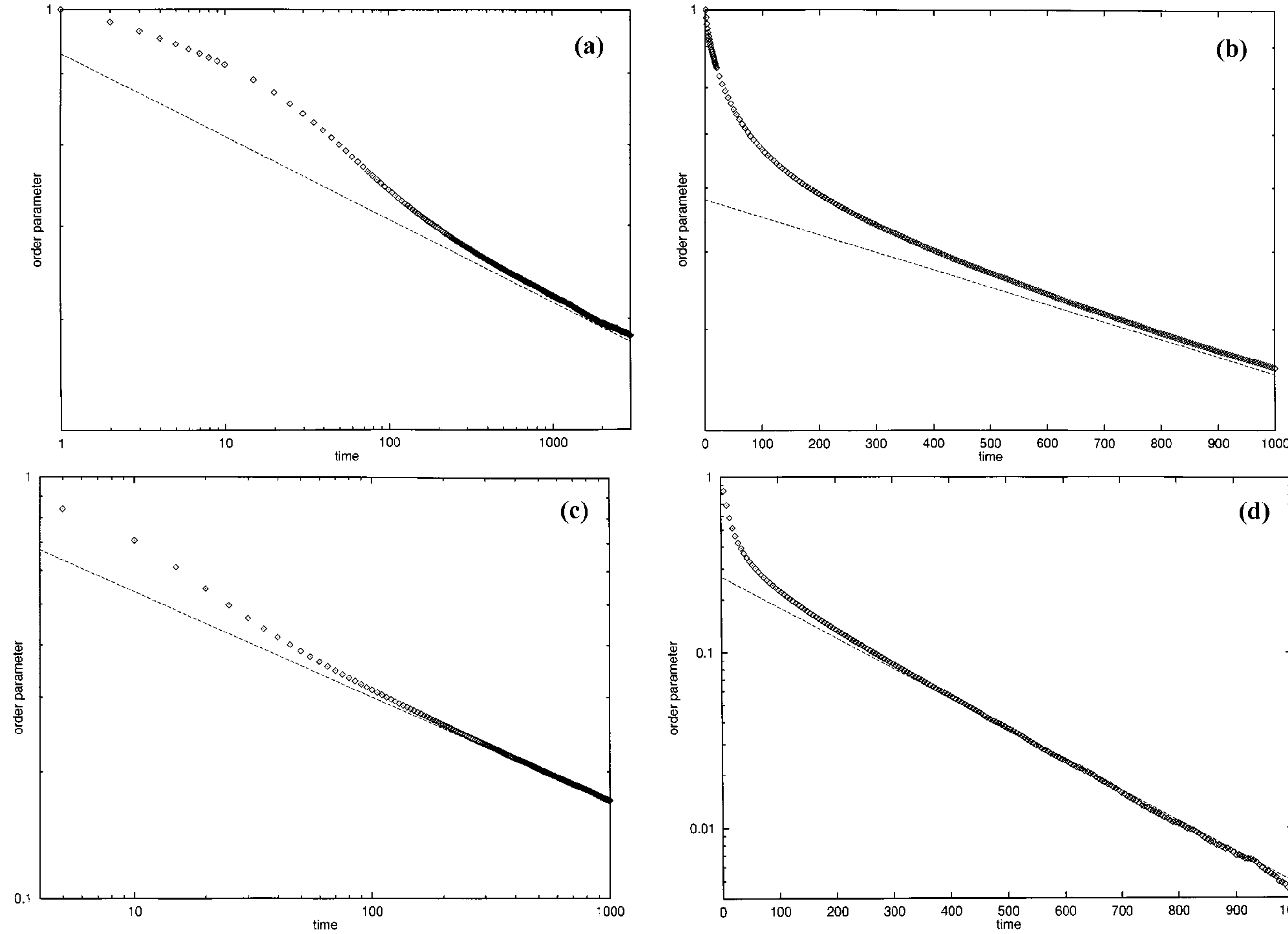

Fig. 1. Order parameter relaxation in two (a, b) and three (c, d) dimensions at (a, c; log-log plots) and slightly above (b, d; semilogarithmic plots) the critical temperature, for lattices containing more than 10^9 spins. (In parts a and b, medium size for long times and large size for short times. The vertical axes vary from 1 down to 0.5 in a and 0.3 in b.) The dashed lines give the slopes expected for model A (parts a and c), $\tau = 2000$ (part b), and $\tau = 250$ (part d). Staggered magnetization at: (a) $T = T_c$ for 10031*10032 and 38399*38400, $m = 0$; (b) $T/T_c = 1.02$ for 14975*14976 and 38399*38400, $m = 0$; (c) $T = T_c$ for 1023*1023*1024, $m = 0$ and $0.95/x^{0.25}$; (d) $T/T_c = 1.01$ for 1151*1151*1152, $m = 0$ and $0.27/\exp(t/250)$.

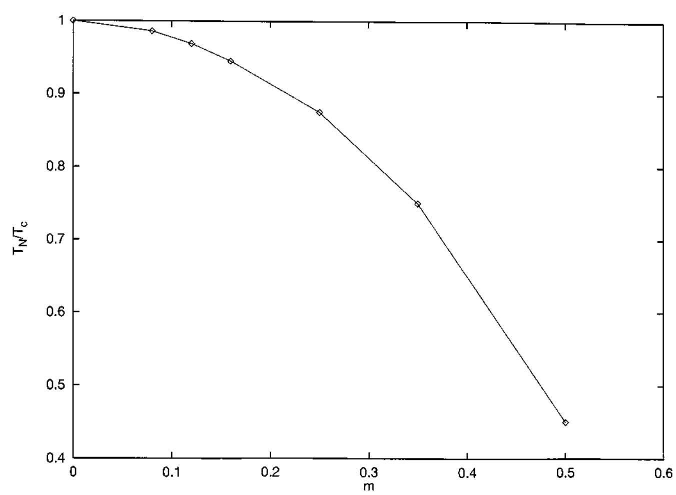

Fig. 2. Neel temperature $T_N(m)/T_c$ against m in three dimensions.

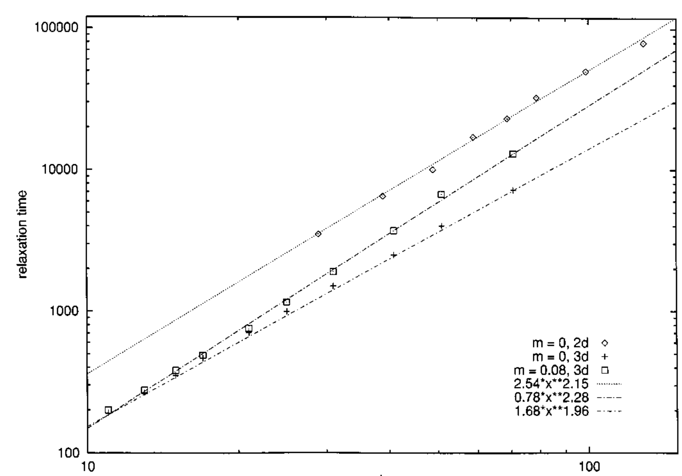

Fig. 3. The order parameter relaxation time τ at T_N *versus* the system size L is shown for two dimensions ($\diamond$, $m = 0$) and three dimensions (+ for $m = 0$, squares for $m = 0.08$). The best fit lines (from least square fitting) are also shown.

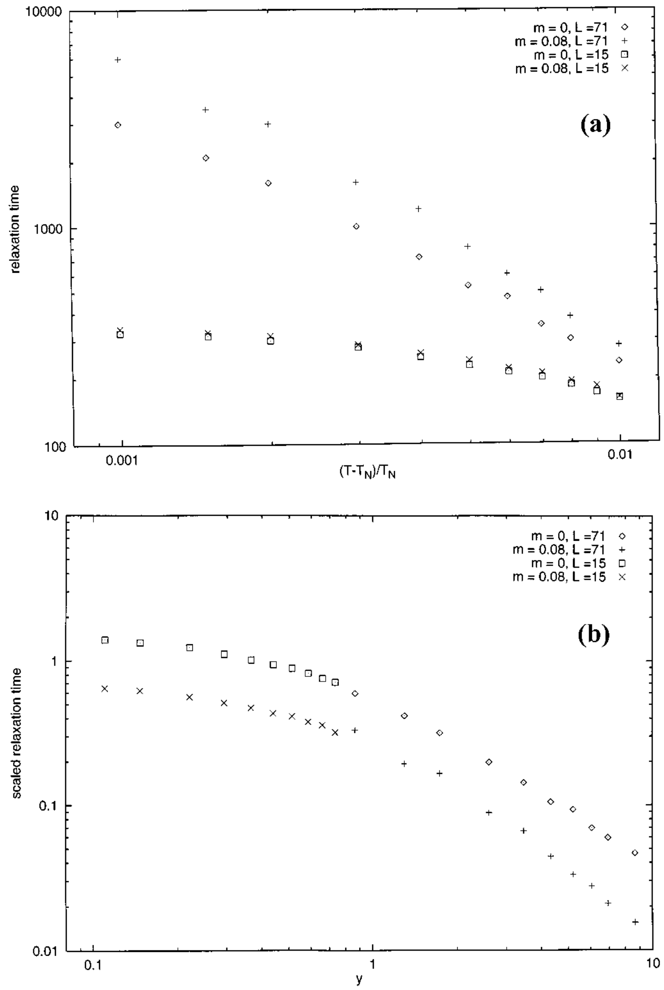

Fig. 4. (a) The order parameter relaxation time τ against $(T/T_{\mathrm{N}} - 1)$ is shown for two sizes $L = 15$ and $L = 71$ in three dimensions for zero and nonzero magnetization. (b) τ/L^z with $z(m = 0) = 2.0$, $z(m = 0.08) = 2.3$ against $y = (T/T_{\mathrm{N}} - 1)L^{1/\nu}$ for the same sizes are shown to be compatible with finite-size scaling hypothesis.

For $m = 0$ and 0.08 we have also studied the behaviour of τ with $(T - T_{\mathrm{N}})/T_{\mathrm{N}}$. Figure 4a shows the variation of τ for two system sizes $L = 15$ and $L = 71$. The curvature in the log-log plot clearly decreases with increasing system size. We have also plotted τ/L^z against $L^{1/\nu}(T - T_{\mathrm{N}})/T_{\mathrm{N}}$ for the same sizes in Figure 4b showing that the data is compatible with the scaling form $\tau = L^z f(L^{1/\nu}(T - T_{\mathrm{N}})/T_{\mathrm{N}})$. These data are specially relevant for comparison with the field theory studies.

Even for a constant magnetization as in this model, one can check for the diffusion of m, similar to heat conduction in a ferromagnet with conserved energy. As an alternative to Fourier transformation for the structure factor, we approximated the field theoretical approach [4] and assumed an initial magnetization density $m(x, t = 0) = m_0 + m_1 \sin(2\pi(x - 1)/(L - 1))$, which means we started with the smallest wavevector $k = 2\pi/(L - 1)$ in the x-direction that fits into our lattice. Then the overlap

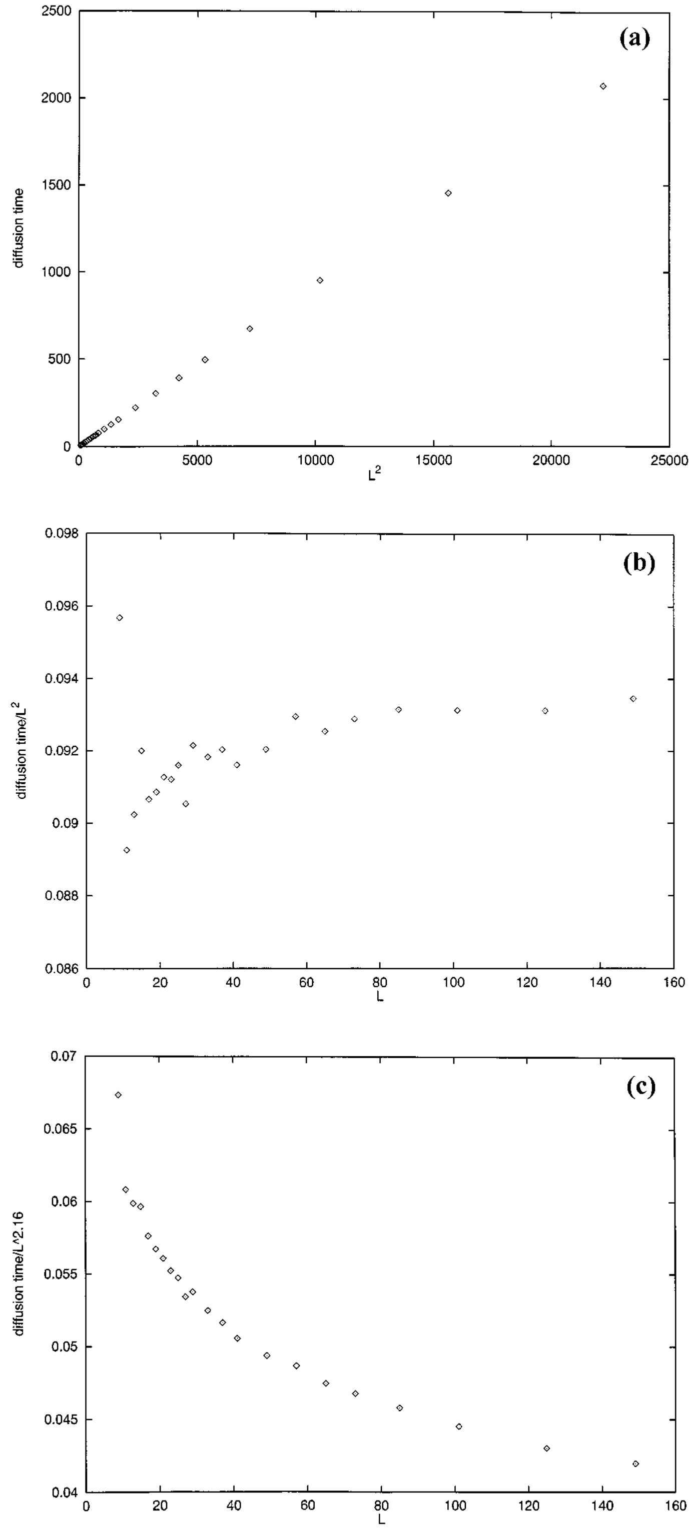

Fig. 5. (a) The relaxation time τ_{d} for the diffusion of the magnetization is shown to vary as L^2 ($m = 0.08$, $T = T_{\mathrm{N}}$). (b) τ_{d}/L^2 against L shows only small deviations from constant behaviour. (c) Same data plotted as $\tau/L^{2+\alpha/\nu}$ *versus* L. Now the variation is stronger but monotonic.

$\psi = \sum_x (m(x,t) - m_0)(m(x,0) - m_0))$ decays as $\exp(-Dk^2 t) = \exp(-t/\tau_d)$, where D is the spin diffusivity we are looking for. For $m = 0.08$, Figures 5 show our results for intermediate system sizes and the finite-size scaling behaviour, at $T_N(m)$. The corrections to the leading power law (as a function of size) are small if we look at Figure 5b but large if we look at Figure 5c; the latter one presumably corresponds to the asymptotically correct behaviour. The reason for the more constant behavior in Figure 5b is not clear at present.

In summary, we confirmed theoretical expectations for bulk behaviour in model C and found some finite-size effects for diffusion.

Note added in proofs

Different exponents were found for Ising ferromagnets with exactly conserved energy (non-ergodic q2r cellular automata simulation): D. Stauffer, Int. J. Mod. Phys. C **7** (in press).

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