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LETTER TO THE EDITOR

Dynamics of interface width in the three-dimensional Q2R Ising model

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Abstract. The Q2R cellular automaton is used to simulate the growth of the liquid-vapour interface in the 3D Ising model. At the critical point we find that its width increases with time in a power law manner with an exponent of $0.34_5 \pm 0.01_5$; below the critical temperature we study the size dependence of the equilibrium width.

The Q2R algorithm [1-3] of cellular automata seems to approximate reasonably the Ising model, though some deviations were also observed [1]. Its simplicity and speed make it particularly attractive for computer simulations. Basically, a spin is flipped if and only if such a spin flip does not change the interaction energy of the spins. Thus the Q2R algorithm approximates a microcanonical simulation of the Ising model, with fixed energy but fluctuating magnetisation.

We apply this technique here to the liquid-gas interface in the lattice gas model, i.e. to a domain wall in the Ising magnet. In the upper half of our $L \times L \times H$ simple cubic lattice the spins are initialised randomly as mostly up, and in the lower half as mostly down; an initial concentration p of up spins corresponds to a thermal energy density of $12p(1-p)$ in units of the nearest-neighbour exchange energy. Two additional buffer planes, at the top with all spins up and at the bottom with all spins down, were maintained in order to ensure the presence of an interface. In the horizontal plane periodic (helical) boundary conditions were used.

We then let the system evolve according to the Q2R rule mentioned above and see how the initially quite sharp interface between vapour and liquid broadens in the course of time. (The time t is the number of computer sweeps through the whole lattice.) In particular, we want to know whether the width $W(t)$ depends on time t in a power law manner or as $\log t$ [4-8], in the region where W is much smaller than the equilibrium width for infinite times, and much larger than unity. Also, we check if, for the equilibrium width, the Q2R algorithm gives the logarithmic size dependence well known [9, 10] for the usual Ising model.

Storing one spin per word we needed 5 μs per simulation step on a SUN3/260 work station; simulating ten systems simultaneously, with ten spins per word, we reached 0.6 μs per step. Usually we took H as 96 and worked with lengths L up to 99 in our $L \times L \times H$ lattices. For a given configuration, with isolated holes and droplets, one cannot uniquely define a reasonable interface position z; thus our width was

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determined via averages over all heights z, involving the shape of the magnetisation profile. The squared width W^2 was determined as $[\langle z^2\rangle - \langle z\rangle^2]$, with the height z, and z^2 weighted proportionally to the magnetisation gradient as explicitly defined in [9, equation (4)] and [10, equation (1)]. (Results for $W(t)$, qualitatively similar to the ones described below, are also obtained using local interface energy density as a weight, but the accuracy using the magnetisation gradient is better.)

For values of $p < p_c = 0.2125$, the width seems to increase with t before saturating to its equilibrium value.

As an example of the size dependence of the equilibrium width, figure 1 shows W^2_{sat} against log L at $p = 0.03$ and 0.1, corresponding to $T/T_c = 0.7$ and 0.89, respectively. As expected from the earlier studies [9, 10], W^2_{sat} seems to increase linearly with log L.

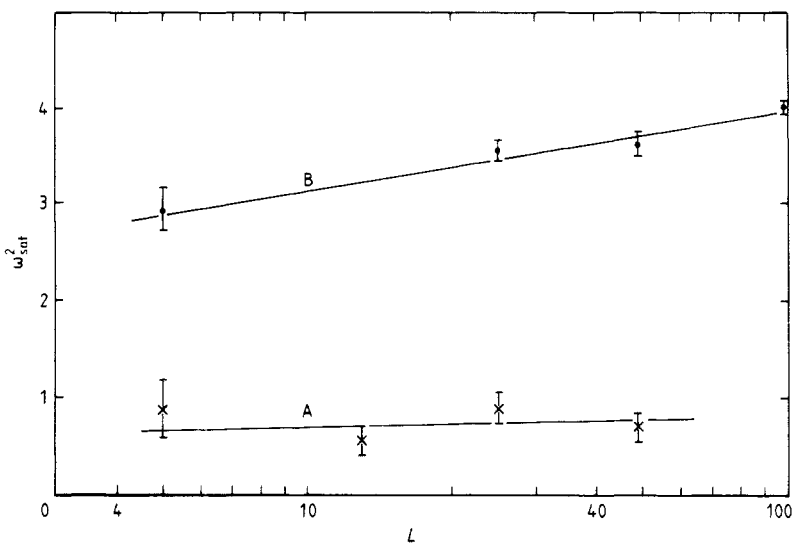

Figure 1. Variation of the squared saturation width W^2_{sat} with L (note the semilogarithmic plot) for (A) $p = 0.03$ ($T/T_c = 0.7$) and (B) $p = 0.1$ ($T/T_c = 0.89$). The results are averages over 100 runs for $L \times L \times H$ systems with $H = 96$ and 24.

At $T = T_c$, corresponding to $p = 0.2125$, the interface width should diverge in equilibrium. This makes it easier to study its time dependence at intermediate times than for p below p_c. In figure 2 we show $\ln(W^3(t))$ against $\ln(t)$ at the Curie point $p = p_c$. The data appear to fit a straight line with a slope of about 0.7. Thus we infer that $W(t)$ behaves like $t^{0.35}$. A linear fit to the data for $99 \times 99 \times 96$ and $99 \times 99 \times 48$ systems with an average over 1300 runs for the former and over 110 runs for the latter leads to a slope of 0.37 ± 0.02. A subset of these data, shown in figure 2, for the $99 \times 99 \times 96$ system with an average over 1000 runs leads to a slope of $0.34_5 \pm 0.01_5$. The error bars in these values of slope are purely statistical; due to other possible systematic errors, a slope of $\frac{1}{3}$ is not ruled out.

For temperatures less than T_c, a log t behaviour of the squared width for a three-dimensional system has been expected theoretically [4, 6]. Here we find a power law behaviour for the width at $T = T_c$.

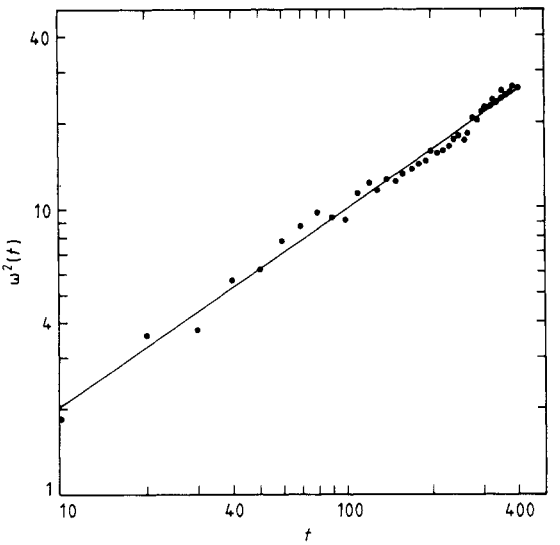

Figure 2. Variation of $W^2(t)$ against t (note the logarithmic plot) at the Curie point, $p = 0.2125$, for $L = 99$ and $H = 96$. The results are averages over 1000 runs. Results for smaller systems gave roughly the same result.

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