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LETTER TO THE EDITOR

Breakdown of dynamic scaling at the percolation threshold

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Abstract. The critical dynamics of the two-dimensional Ising model at the bond percolation threshold is investigated by Monte Carlo simulations on a 64×64 lattice. Conventional dynamic scaling breaks down at low temperatures: the logarithm of the relaxation time depends quadratically upon the logarithm of the thermal correlation length. The coefficients of the quadratic and linear terms are 0.51 and 3.25, respectively. The results are compared with recent experimental and analytic work.

Although there is considerable knowledge about the static behaviour of the two-dimensional Ising model at the percolation threshold [1], for example, the exponents are believed to be known exactly, it is only recently that attention has turned to the critical dynamics of this system [2-4]. Assuming conventional dynamic scaling [5], Aeppli, Guggenheim and Uemara [2] were able to fit their data on the site dilute, two-dimensional Ising antiferromagnet $Rb_2(Mg_{0.41}Co_{0.59})F_4$ near the percolation threshold with an exceptionally large value for the dynamic exponent Z. Subsequently, standard dynamic scaling arguments [3] gave estimates for Z which agreed reasonably well with the experimental value. However, very recently, analytic work [4] on both non-random fractals and a randomly dilute two-dimensional lattice has led to suggestions that usual dynamic scaling breaks down at low temperatures; one has an effective dynamic critical exponent which diverges as the temperature is lowered. As the experimentalists [2] were restricted to relatively high temperatures ($T/T_c \geqslant 0.5$, where T_c is the transition temperature in the pure system), they were unable to see the predicted violation of dynamic scaling.

This letter adds numerical work to the discussion by presenting the results of Monte Carlo simulations of the two-dimensional Ising model on a square lattice at the bond percolation threshold. The Hamiltonian is given by [1]

$$H = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j \tag{1}$$

where $S_i = \pm 1$ are Ising spins situated on every site of an $L \times L (L = 64)$ lattice, $\langle \ldots \rangle$ indicates a summation over nearest neighbours only and the J_{ij} are quenched exchange interactions with probability distribution

$$P(J_{ij}) = (1-p)\delta(J_{ij}) + p\delta(J_{ij} - 1) \tag{2}$$

p being the bond concentration. Boltzmann's constant is set to unity. Throughout, the simulations are performed at the bond percolation threshold [6] $p_c = 0.5$ and periodic boundary conditions are imposed in all directions. The distributed array processor

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(DAP) at Queen Mary College, London, was used to perform the calculations. Approximately 7 million spins are updated per second. For any given temperature, T, the nearest-neighbour interactions are chosen according to equation (2) and the Hoshen-Kopelman [7] algorithm (with periodic boundary conditions) is used to check that the bonds percolate throughout the lattice. The spins, which are all pointing up at the start of the simulation, are allowed to evolve according to the Glauber [8] probability $(1+\exp(\Delta E/T))^{-1}$, where ΔE is the change of energy resulting from an update.

The magnetisation at time t is given by $M(t) = N^{-1}\Sigma_i S_i(t)$, where N is the number ($N = 4096$) of spins and $S_i(t)$ denotes the value of the ith spin at time t. Since the system described by equations (1) and (2) with $p = p_c = 0.5$ has a zero temperature phase transition [1], $T_c(p_c) = 0$, the magnetisation vanishes in equilibrium for $T \neq 0$. For each temperature investigated, $M(t)$ is seen to decrease with t and, eventually, $M(t = t_0 \geqslant \tau_0) = 0$, where τ_0 is a temperature-dependent decay time. The configuration at $t = t_0$ is taken as an initial state of the system and the spin-spin autocorrelation function $C(t) = N^{-1}\Sigma_i S_i(t_0)S_i(t+t_0)$ is measured for subsequent times. From $C(t)$, one defines a relaxation time τ by

$$\tau = \int_0^\infty C(t)\,\mathrm{d}t \tag{3}$$

where, in practice, $C(t) = 0$ for $t > t_0$. Data for τ were collected for $0.7 \leqslant T \leqslant 2.0$. For $T < 0.7$ the system does not achieve equilibrium within the available computer time. At the lowest temperature simulated, $T = 0.7$, a run of 10^6 Monte Carlo steps per spin was performed, of which the first 500 000 were required for equilibration. Note that during the simulations the value of t_0 was chosen liberally ($t_0 \simeq 2\tau_0$), so that one could be reasonably certain that equilibrium had been achieved. Averages over many (typically 36–200) samples were taken and statistical error bars ($\leqslant 7\frac{1}{2}\%$) evaluated from the sample-to-sample fluctuations. Once the system has attained equilibrium, evaluation of the spatial correlation function

$$\Gamma(n) = N^{-1}\sum_i \langle S_i S_{i+n}\rangle_T \tag{4}$$

where $\langle\ldots\rangle_T$ indicates a thermal average and $n (n = 0, 1, \ldots, 10)$ is the displacement in the x direction, yields information concerning the statics. For technical reasons, $\Gamma(n)$ was studied over a restricted temperature range, namely $1.05 \leqslant T \leqslant 2.0$.

The pure system [9] ($p = 1$) has $T_c \simeq 2.27$ in the units used in this letter (where the exchange interaction is set to unity). Consequently, the simulations described here are over the range $0.31 \leqslant T/T_c \leqslant 0.88$, whereas the experiment [2] was performed for $T/T_c \geqslant 0.5$.

As at $p = p_c$ the percolation correlation length is infinite, the correlation length, $\xi(p_c, T)$, is given by the thermal correlation length ξ_T[1]. For asymptotically large $n (n \gg \xi_T)$ the spin-spin correlation function, equation (4), can be fitted by $\Gamma(n) \sim \exp(-n/\xi_T)$, thereby enabling one to extract ξ_T. Figure 1 shows a plot of $\ln \xi_T$ against $1/T$ for $1.05 \leqslant T \leqslant 2.0$. The linear fit shown there implies that

$$\xi_T = \xi_0 \exp(2\nu_T/T) \tag{5}$$

where ν_T is the thermal exponent and ξ_0 is a constant. The result $\nu_T = 1.33 \pm 0.05$ obtained in the simulations confirms the prediction [10] of a crossover exponent of 1 and is in excellent agreement with the exact result [1, 11] $\nu_T = \nu_p = \frac{4}{3}$, where ν_p is the percolation exponent. If one fits the experimental [2] value of ξ_T at $T = 50$ K

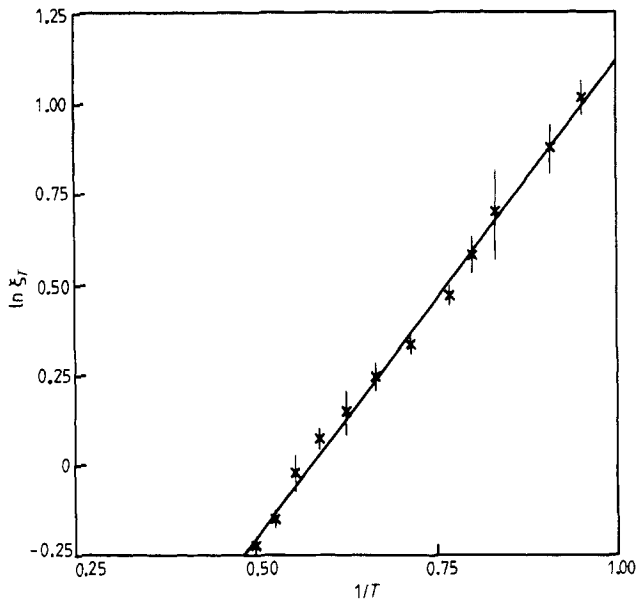

Figure 1. Plot of $\ln \xi_T$ against $1/T$ for $1.05 \leqslant T \leqslant 2.0$. The error bars are from statistical fluctuations. The weighted line of best fit is also shown. This has gradient $= 2.66 \pm 0.09$ and intercept $= -1.52 \pm 0.02$; from the gradient one gets $\nu_T = 1.33 \pm 0.05$ and from the intercept $\xi_0 = 0.22 \pm 0.01$ (see text). Assuming $\nu_T = 1.33$ and $\xi_0 = 0.22$, one gets $\xi_T(T = 0.7) = 9.83$ lattice spacings.

to equation (5) with $\nu_T = \frac{4}{3}$, one obtains [12] $\xi_0 = 0.39$ which is, of course, near the site percolation threshold. At $T/T_c = 0.46$, the lowest temperature at which $\Gamma(n)$ is evaluated, $\xi_T = 2.76$ and by extrapolation one expects that at $T/T_c = 0.31$, $\xi_T = 9.83$. So, at low temperatures, although $\xi_T \gg$ lattice spacing (assumed to be 1), one always has $L \gg \xi_T$. Consequently, one does not expect the results of the simulations to be influenced by finite size effect.

Ordinary dynamic scaling [5] would imply that along $p = p_c$ in the neighbourhood of the bicritical point, $(T, p) = (0, p_c)$, the relaxation time $\tau \sim \xi_T^Z$, where Z is a dynamic critical exponent. On fitting the experimental data [2] to this hypothesis one gets $Z = 2.4 \pm 0.1$. However, within conventional theory one has $Z = 2 - \eta_T$ for a system without conserved order parameter [13] and, further, as $\eta_T \simeq 0.33$ for the diluted antiferromagnet studied by Aeppli, Guggenheim and Uemura [2, 14], one sees that $Z \simeq 1.67$. It has been argued [2, 3] that the percolating network is the underlying cause for the discrepancy between the experimental and theoretical values. Subsequently, arguments [4] have been proposed which suggest that the self-similarity of the lattice at p_c has a far more drastic consequence for the dynamics of the system: at low temperatures conventional dynamic scaling [5] fails and one instead has that [4]

$$\tau = \tau_0 \xi_T^{A \ln \xi_T + B} \tag{6}$$

where τ_0 is a constant, A and B are new exponents and ξ_T is the thermal correlation length discussed previously. Combining equations (5) and (6) gives

$$\ln \tau = C_1/T^2 + C_2/T + C_3 \tag{7}$$

where $C_1 = 4A\nu_T^2$, $C_2 = 2\nu_T(B + 2A \ln \xi_0)$ and $C_3 = \ln \tau_0 + B \ln \xi_0 + A(\ln \xi_0)^2$. Figure 2

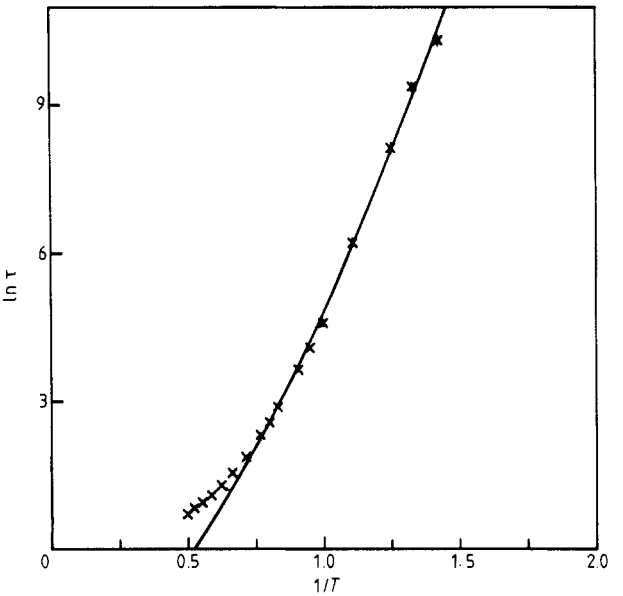

Figure 2. The results for the relaxation time shown as a plot of $\ln \tau$ against $1/T$ for $0.7 \leqslant T \leqslant 2.0$ ($0.31 \leqslant T/T_c \leqslant 0.88$). The full curve is the best quadratic fit to the data for $0.7 \leqslant T \leqslant 1.5$ ($0.31 \leqslant T/T_c \leqslant 0.66$). Letting $y = C_1x^2 + C_2x + C_3$, where $y = \ln \tau$, $x = 1/T$, one has $C_1 = 3.60$, $C_2 = 4.59$ and $C_3 = -3.36$ for the fit indicated above. These coefficients imply $A = 0.51$, $B = 3.25$.

shows the results for $\ln \tau$ against $1/T$ for $0.7 \leqslant T \leqslant 2.0$. Clearly, as $T \to 0$, $\ln \tau$ diverges much faster than $1/T$. As one expects equation (7) to be true for $T/T_c \ll 1$, the best quadratic fit to the data over $0.31 \leqslant T/T_c \leqslant 0.66$ ($0.7 \leqslant T \leqslant 1.5$) is also shown; for this one has $A = 0.51$, $B = 3.25$. Using a recursive argument, Harris and Stinchcombe [4] (see also Stinchcombe [4]) have suggested that $A = 0.54$. As was mentioned above, the experimental results [2] for $T/T_c \geqslant 0.5$ were fitted to $\tau \sim \xi_T^z$. If one fits the data from the computer simulations for $T \geqslant 1.1$ ($T/T_c \geqslant 0.48$) to standard dynamic scaling one gets $Z \simeq 2.71$.

The error bars shown in figure 2 were obtained from statistical fluctuations. The values of A and B depend on the temperature range chosen for the quadratic fit. For example, if one fits the data over the whole range ($0.31 \leqslant T/T_c \leqslant 0.88$), one gets $A = 0.68$, $B = 2.62$.

Universality would demand that the exponents A and B are the same for any diluted two-dimensional Ising system. It is interesting to note that the value of A obtained in the computer simulations—on a square two-dimensional lattice at the bond percolation threshold—is approximately the same as that obtained by the real space calculation of Harris and Stinchcombe [4] and Stinchcombe [4] on a two-dimensional honeycomb lattice with bond dilution; further, the experimental data [2], which was obtained on a square two-dimensional lattice near the site percolation threshold, when fitted to equation (7) also gives a similar value for A, namely $A = 0.5 \pm 0.2$ (see Harris and Stinchcombe [4]).

To conclude, by performing Monte Carlo simulations at low temperatures, it has been shown that conventional dynamic scaling breaks down for the two-dimensional Ising model at the percolation threshold. It is suggested that the new dynamic behaviour

should also be seen in the experimental system for $T/T_c \leqslant 0.4$. The computer simulations have confirmed recent analytic work and, further, have enabled estimates for both A and B to be given.

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