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COMMENT

Critical dynamics of the spin-exchange model in quasilinear fractal geometries

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Abstract. We comment on the dynamic critical exponents recently reported by Leyvraz and Jan, in particular that for the spin-exchange kinetic Ising model in one dimension, $z=3$. This result is at variance with rigorous inequalities that z cannot be less than five for this model, i.e. $z \geq 5$. The source of the discrepancy appears to lie in the authors' Monte Carlo algorithm which subsumes a critically slow dynamical process, leading to an apparently faster dynamics in the critical region. In addition, the authors extend their finding for one dimension to the quasilinear (non-branching) fractal Koch curve, concluding $z=3d_f$, where d_f is the fractal dimension. We discuss the physical factors comprising the lower bound to the dynamic exponent in one dimension, $z=5$. We then obtain the generalised lower bound for spin-exchange dynamics on the non-branching Koch curve, $z=3d_f+d_w=5d_f$, where d_w is the random walk dimension.

In a recent comment, Leyvraz and Jan (LJ) (1986) discuss the critical dynamics of several discrete spin models in one dimension. For the four-state clock model and the three- and four-state Potts models with single spin-flip kinetics (model A, no conservation laws) LJ find the dynamic critical exponent $z=2$ and for the spin-exchange kinetic Ising model (SEKI) (model B, conserved order parameter), $z=3$. In addition, LJ extend these results to quasilinear, i.e. non-branching, fractal geometries, obtaining $z=2d_f$ and $z=3d_f$, respectively, where d_f is the fractal dimension. The purpose of this comment is twofold. We discuss these findings, arguing that the authors' results for model A are inconclusive, and more importantly, that the authors' conclusions for the SEKI model are at variance with rigorously known results. Secondly, after discussing the physics of the SEKI model in one dimension, we then obtain the generalised lower bound to the dynamic critical exponent for this model on the non-branching Koch curve, $z=3d_f+d_w=5d_f$ where d_w is the random walk dimension.

The conclusion that $z=3$ for the SEKI model in one dimension is incompatible with rigorous inequalities that z cannot be less than five for this model, i.e. $z \geq 5$. Within numerical accuracy, LJ obtain $z=3$ in a Monte Carlo (MC) simulation of the spin-exchange dynamics, which they note is consistent with the conventional result for model B (Hohenberg and Halperin 1977), $z=4-\eta$. We discuss below that 'standard' conventional theory does not hold at a zero temperature critical point, in that there is an 'anomaly' in the kinetic coefficient due to the freezing of the system. It is this 'extra' slowing down which leads to the larger value, $z=5$. The authors take as their unit of time the number of MC steps for spins at a domain wall to exchange. This interchange requires two bonds to be broken, proceeding at an energy cost of $4K$, which at low temperatures ($K \to \infty$) occurs at a critically slow rate. Thus, the authors' definition of the basic unit of time subsumes one of the mechanisms of critical slowing down for this problem, thereby yielding an apparently faster dynamics in the critical region. Below, we develop these arguments at greater length for the one-dimensional model, which we then extend to the fractal case. First, however, we discuss the authors' findings for model A.

Cordery *et al* (CST) (1981) have shown for both models A and B that one can understand the physics of the one-dimensional dynamic critical exponent in terms of the motions of the boundary separating low temperature domains. For example, in the case of Glauber dynamics domain boundaries perform independent random walks, which to cover a distance N require in one dimension N^2 steps. Hence, this physical argument yields $z=2$. The method can also be applied to fractal geometries of ramification order $R=2$. Luscombe and Desai (1985) have previously employed the argument of CST to obtain the generalisation $z=d_w=2d_f$ for Glauber–Ising dynamics on the non-branching Koch curve. Below, the argument is extended to model B for Ising spins on the Koch curve as well. It should be noted that the conclusion $z=d_w$ is exact on the Koch curve, since the Glauber model can be solved independently of the CST argument. Strictly, however, this type of argument provides only a lower bound to the actual exponent since it identifies the lowest energy barrier, and hence the fastest mode, for domain motion to occur (consistent with constraints imposed by the dynamic universality class). The Glauber model aside, the other models mentioned above have not been solved exactly in one dimension. LJ base their conclusion $z=2$ for model A dynamics on a consideration of domain wall random walks. We note then that such arguments do not in themselves determine, but can only make plausible, a given value of z in one dimension. For this reason, the authors should present their numerical evidence in support of their values for z. We note that $z=2$ is undoubtedly the correct lower bound for the relaxational models LJ have considered. A second more serious consideration, however, is the fact that LJ have not presented the master equation transition probabilities for the models they investigate. In one dimension there can be non-universal contributions to z induced by the particular form of the transition probability. Detailed balance is not a unique constraint in defining stochastic spin models and non-universal factors in the transition probability can produce critical effects at zero temperature. Dynamic universality classes in one dimension have been previously established for Ising spins by Haake and Thol (1980) and more recently for Potts spins by Weir *et al* (1986). For example, Haake and Thol show that, for certain models, the value of z is model dependent and can assume any value between two and four. Thus, in the present context, unless a well defined dynamical model is specified, the value of z obtained is inconclusive. By way of illustration, Weir and Kosterlitz (1986) also obtain $z=2$ for Potts spins, while Lage (1985), using another model, obtains $z=3$, also for model A Potts dynamics in one dimension. We now turn to the main consideration of this comment: the SEKI model.

As stated above, the one-dimensional spin-exchange model cannot be solved exactly. Even in the non-interacting (high temperature) limit, the dynamics is non-trivial due to the dynamic coupling needed to maintain spin diffusion (Mazenko and Oguz 1982). However, certain results are well known for this model. Rigorous inequalities can be established for dynamical quantities derived from a Hermitian master equation (Kawasaki 1972, Halperin 1973, Mazenko and Valls 1981). In particular, the Kawasaki inequality (KI) states that the initial response rate of the system forms an upper bound to the subsequent system response. The main application of the KI is to provide a rigorous lower bound to the dynamic critical exponent. Luscombe and Desai have used the KI to establish for Glauber–Ising dynamics that $z \geqslant d_f$ for finitely ramified fractal geometries, e.g. the Sierpinski gasket. In the present context, the KI applied to the one-dimensional spin-exchange model yields $z \geqslant 5$. Haake and Thol (1980), using a variational technique, also obtain $z \geqslant 5$ for the general spin-exchange model. Zwerger (1981) obtains $z = 5$ in a particular model for which certain non-linearities in the equations of motion vanish in the hydrodynamic limit (Mazenko and Oguz 1982). The domain boundary diffusion argument of CST for model B also yields $z = 5$ (see discussion below). Note that the CST result conforms with the lower bound. Thus, the authors' finding of $z = 3$ is at variance with previously established results for the one-dimensional spin-exchange kinetic Ising model.

The agreement of the authors' result with the conventional theory of dynamic critical phenomena for model B, $z = 4 - \eta$, is specious. In conventional theory, to which the lower bounds above correspond, the characteristic response frequency at wavevector k,

$$\omega_c(k) = \Gamma_k \chi_k^{-1} \tag{1}$$

is given by the ratio of a transport coefficient to the order parameter susceptibility. In the case of model B, for large wavelength

$$\Gamma_k = \Gamma_0 k^2 + O(k^4) \tag{2a}$$

where the k^2 dependence signifies that the order parameter is conserved. At criticality,

$$\chi_k^{-1} \sim k^{2-\eta} \tag{2b}$$

and the standard conventional exponent, $4 - \eta$ is obtained. The argument, however, presupposes that the coefficient Γ_0 remains finite at T_c which, in the absence of mode-mode coupling effects, would be true except if the phase transition happens to occur at zero temperature. In the present context, Γ_0 is the canonical average of the spin-exchange transition probability (see Mazenko and Oguz 1982)

$$\Gamma_0 = \alpha \langle W_{i,j} \rangle \tag{3}$$

where i and j are the exchanging spins and α is the exchange rate for non-interacting spins. Γ_0 *must vanish* for a system in equilibrium as the temperature approaches zero since the spins become predominantly aligned with their neighbours. If we say Γ_0 vanishes in the critical region like ξ^{-x}, then the conventional exponent for one dimension will be given by $z = 4 + x - \eta$. For a wide class of spin exchange models (Haake and Thol 1980, Zwerger 1981, CST)

$$\Gamma_0 \sim \alpha\, e^{-4K} \sim \alpha \xi_1^{-2} \tag{4}$$

and hence $x = 2$ (ξ_1 is the one-dimensional correlation length). Note however that for the model of Mazenko and Oguz (1982), $x = 3$. The point here though is that the smallest dynamic exponent for conserved order parameter dynamics in one dimension is $z = 5$. It should be noted that conventional theory results from projecting the order parameter out of the full non-linear equations of motion. The KI states that the 'orthogonal' non-linearities can in principle lead to a slower critical dynamics than the projected linear equations of motion, which is why the full dynamic exponent is always larger than the conventional exponent (see Mazenko and Valls 1981). For the Glauber model the order parameter equation of motion is already linear. In this sense conventional theory is exact for the Glauber model, and yet the exponent is not given by the analogous conventional expression for model A, $z = 2 - \eta$. Again, one must account for the vanishing of the kinetic coefficient at zero temperature, $z = 2 + x - \eta$, with $x = 1$ for the Glauber model.

We now outline the CST argument for spin exchange dynamics, modified to the fractal curve. A spin at a domain boundary exhanges into the 'wrong' domain at energy cost $4K$, occurring at the critically slow rate (equation (4)) $\alpha\, e^{-4K} = \alpha\xi^{-2d_f}$, where ξ is the fractal correlation length $\xi = \xi_1^{1/d_f}$ (Gefen *et al* 1983). Each succeeding exchange of this spin further into the domain occurs as a random walk, and the probability of the reversed spin exchanging through the domain and not returning to its starting point is, as shown by CST, N^{-1} where N is the number of domain sites as measured along the fractal. N is related to ξ via $N \sim \xi^{d_f}$. Thus the rate of one spin passing through the domain, and the entire domain shifting one unit, is $\alpha\xi^{-3d_f}$. For the domain itself to move a net distance ξ requires on the fractal geometry ξ^{d_w} steps. Hence, the domain will traverse the distance ξ in a time $\sim \xi^{d_w+3d_f}$, implying $z = d_w + 3d_f$. For reasons stated above this is a lower bound to the actual exponent. To the best of our knowledge, this is the first time this expression has been derived.

As stressed above, the authors should specify their dynamical model, i.e. transition probability, if meaningful conclusions are to be drawn. To obtain $z = 3$ would require a model in which Γ_0 remains finite at zero temperature. Such a model, however, cannot satisfy detailed balance since the dynamics must stop in this limit. The authors, through their MC algorithm, in effect absorb Γ_0 into an overall temperature-independent exchange rate. Thus, it is not surprising they obtain a reduced exponent. However, the 'waiting time' for domain wall spins to exchange is part of the physics of the problem since there is an energy barrier for this motion to occur, but which is neglected in the authors' MC procedure.

In summary, the finding by Leyvraz and Jan of the dynamic critical exponent $z = 3$ for the spin-exchange kinetic Ising model in one dimension is misleading, since the authors' unit of time itself undergoes critical slowing down. This discrepancy is related to the neglect of the activation barrier for domain boundary spins to exchange, leading to an apparently faster dynamics in the critical region. In addition, we have formulated the domain diffusion argument for spin-exchange dynamics on a quasilinear fractal obtaining the lower bound to the dynamic exponent $z = d_w + 3d_f = 5d_f$.

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