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Non-universal critical behaviour in the 1D BEG model with Kawasaki dynamics

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Abstract. We investigate the one-dimensional BEG (Blume–Emery–Griffiths) model with Kawasaki dynamics, using domain-wall arguments (DWA) and Monte Carlo simulations (MCS) (conventional and Gillespie algorithm), after a quench from a disordered state to low temperatures. We observe that this model exhibits domain scaling behaviour, controlled by a universal exponent ($x = \frac{1}{3}$) as in other dimensions for model B. However, we find also that the critical exponent z is not universal and depends on the coupling constants of the Hamiltonian. The results of DWA are *consistent with those of* MCS.

1. Introduction

The problem of the critical dynamics in Ising-like systems has been the subject of many studies in recent years. The dynamic scaling hypothesis states that the relaxation time τ of a system near criticality is related to the correlation length ξ by [1]

$$\tau \sim \xi^z. \tag{1}$$

This exponent is typically less universal than the thermodynamic exponents, but nevertheless in dimensions greater than one z appears to depend on a small number of further attributes of the dynamics, in particular conservation laws. However, in one dimension it is now well known that the value of z may be less universal, depending upon ratios of coupling constants within the Hamiltonian and specific choices of rates (with the same conservation laws) [2]. The origin of this non-universality is that the critical temperature for these models is zero ($T_c = 0$) and the rates present Arrhenius-like singularities in this limit, arising from non-universal energy barriers.

By virtue of the fact that $T_c = 0$, the critical dynamics in one-dimensional models is directly related to the problem of domain growth after sudden cooling (quenching)

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from a high to low temperature, where a characteristic domain L size scales with time t according to the relation

$$L \sim t^x. \tag{2}$$

It has been found that the exponent x controlling this growth in one dimension is the same as in higher dimensions [3], being $\frac{1}{2}$ for non-conserved order parameter [4] and $\frac{1}{3}$ for conserved dynamics [5, 6].

The problem of reconciling the non-universal dynamic critical exponent with the universal growth exponent has recently been studied by two of the authors [7]. They find a relation between the two exponents and the energy barriers present in the system. However, in the case of spin-exchange dynamics, the widely accepted value of z for a system with spatially modulated coupling constants is inconsistent with this theory, implying either a much more complex scaling theory, with perhaps two relevant relaxation times, or a non-universal value for x.

The BEG model presents an interesting extension to the Ising model, in that there are two relevant order parameters and several distinct relaxation times, corresponding to different ordering processes. The critical dynamics of the one-dimensional BEG model with Glauber dynamics has been the subject of a recent publication by two of the authors [8]. The results of Monte Carlo simulations were found to be in good agreement with physical 'domain-wall' arguments, with a non-universal critical exponent z being a function of the coupling constants of the Hamiltonian.

In this paper, we study the spin-exchange ('Kawasaki' [9]) dynamics of the one-dimensional BEG model. We anticipate that some of the controversies relating to the z and x exponents in the Ising case will be resolved by studies of this system. Monte Carlo measurements of the z exponent in systems with such pathological critical slowing-down ($z \geqslant 5$) have been made feasible by the use of an unconventional Monte Carlo algorithm.

The paper is organized in the following way. After defining the Hamiltonian and the rates for the Kawasaki model, we present the analytic results by domain-wall arguments [10, 11] for both domain growth and critical dynamics. A scaling theory interpretation is presented. The results of domain-wall arguments are compared and agree with those from the Monte Carlo simulations.

2. The model

The BEG model, initially proposed by Blume *et al* [12] for the study of the He^3–He^4 λ transition, has been investigated extensively as an example exhibiting both first- and second-order phase transitions, as has been the effect of the single-ion anisotropy energy which affects the phase transition of this model. Here, we consider the one-dimensional case defined by the Hamiltonian

$$\mathcal{H} = -\sum_{i=1}^{N} [J\sigma_i\sigma_{i+1} + K\sigma_i^2\sigma_{i+1}^2 - D\sigma_i^2] \tag{3}$$

where N is the number of spins and $\sigma_i = \pm 1, 0$.

This model is characterized by two order parameters, the magnetization, $m = \langle\sigma_i\rangle$, and the quadrupolar average, $q = \langle\sigma_i^2\rangle$. This model obviously does not have a finite

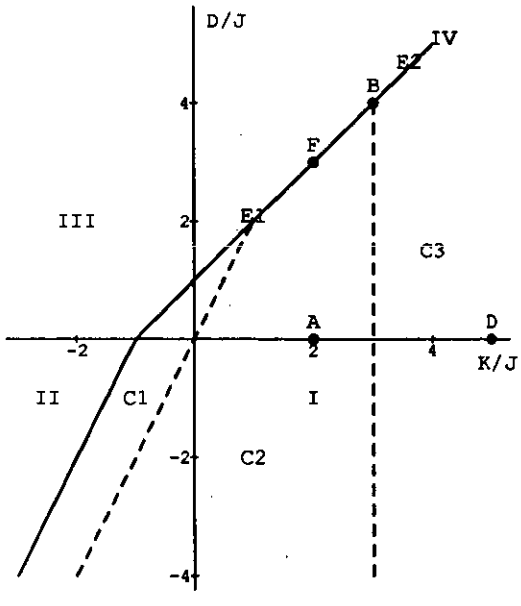

Figure 1. The phase diagram for the one-dimensional BEG model.

critical temperature; however, at $T = 0$ the ferromagnetic system ($J > 0$) is characterized by different types of ordering, with the ground-state properties being a function of the coupling constants of the Hamiltonian. Essentially one finds four different regions (figure 1); the first one (I) ($2K + 2J - D > 0$, $K + J - D > 0$) is characterized by a long-range ferromagnetic order at low temperatures, with spin domains in $\sigma_i = 1$ and $\sigma_i = -1$ states. In this region the only correlation length (typical measure of the length size) that diverges is the one associated with the correlations of the order parameter m ($\langle\sigma_i\sigma_j\rangle$), and behaves

$$\xi_m^{-1} \sim e^{-2J}(1 + e^{-(2K-D)}). \tag{4}$$

The second region (II) ($2K+2J-D < 0$, $D < 0$), is characterized at low temperatures by alternative domains of $\sigma_i = 0$ and $|\sigma_i| = 1$, with only the correlation length associated with the correlations of the q order parameter ($\langle(\sigma_i^2 - \langle\sigma_i\rangle^2)(\sigma_j^2 - \langle\sigma_j\rangle^2)\rangle$) diverges. In region (III) ($K - D < -J, D < 0$), the paramagnetic region, all spins are in the state $\sigma_i = 0$ and no divergence of the correlation length is observed. Region (IV) ($K - D = -J$, $K > -J$) is a tricritical line where the two correlation lengths ξ_m and ξ_q diverge. At low temperatures both lengths diverge in the same way:

$$\xi_{m,q}^{-1} \sim e^{-2J}(1 + e^{-(K-3J)/2}). \tag{5}$$

This spin system interacts with a heat bath allowing spin flips. We consider here the case of the spin-exchange dynamics [9], where processes can only occur if the two nearest-neighbour spins are in different states. This system is described by a master equation for the spin-exchange dynamics in the conventional way:

$$\frac{dP(\{\sigma\},t)}{dt} = -\sum_i (1 - \hat{p}_{i,i+1})\, W_i(\{\sigma\},t)\, P(\{\sigma\},t). \tag{6}$$

Here $\hat{p}_{i,i+1}$ is an operator that exchanges the spins σ_i and σ_{i+1}. The condition of detailed balance is insufficient to constrain the choice of the transition probabilities $W_i = W(\sigma_i, \sigma_{i+1} \to \sigma_{i+1}, \sigma_i)$ fully. We adopt the following choice:

$$W_i = \frac{1}{2}\left[1 - \tanh\left(\frac{\beta\Delta\mathcal{H}}{2}\right)\right]$$

$$= \frac{1}{2\tau} f(\sigma_i, \sigma_{i+1})\left[1 - \tanh\left(-\frac{J}{2}(\sigma_i - \sigma_{i+1})(\sigma_{i-1} - \sigma_{i+2})\right.\right.$$

$$\left.\left. - \frac{K}{2}(\sigma_i^2 - \sigma_{i+1}^2)(\sigma_{i-1}^2 - \sigma_{i+2}^2)\right)\right] \tag{7}$$

where $f(\sigma_i, \sigma_{i+1})$ is a factor that is zero when σ_i and σ_{i+1} are in the same state, and one in all other cases.

3. Domain-wall arguments

It is usually impossible to solve equation (6) analytically. However, the study of domain-wall motion [10, 11] provides a simple *analytical* approach which has been very successful in predicting both the x [6] and the z exponent in some one-dimensional models. First, the DWA were thought to give a lower bound to the critical exponent, but in fact in some cases it gives the correct value, principally in the case of homogeneous chains [13]. This argument is based on a physical description of the long-time behaviour of the one-dimensional kinetic models. We know that the correlation length diverges when the temperature goes to zero. Near $T = 0$ the system splits into large domains of type '+', '−' and '0'.

3.1. Domain growth x exponent

After a rapid quench from high to low temperature, the domains are initially much smaller than the characteristic equilibrium size ($\sim \xi$). These domains will grow by the nucleation of mobile domains of size one, which then perform random walks until they meet a neighbouring domain wall; the domains themselves therefore perform random walks, until they coalesce with a neighbouring domain of the same type. In the BEG model, we have three types of domain (0, +1 and −1), though by symmetry the domains of '+' will have the same characteristic size as domains of '−'.

We shall first discuss the domains of '±' in the absence of '0'. This is exactly the same as the pure Ising case, and has been discussed for for the case of domain growth by Cornell *et al* [6] after arguments originally by Cordery *et al* [11]. A single spin is nucleated from a domain wall (activation energy $4J$), and then performs a random walk until it either returns to the original domain wall or it meets another domain of the same type (with probability $1/L$, where L is the characteristic size of domains). The domain needs a number proportional to L^2 of the latter type of process to be annihilated; the typical decay time for such a domain is therefore $\sim L^3$. The *density* of domains ($\sim 1/L$) therefore decays like $t^{-1/3}$, and so the domain size scales like

$$L \sim t^{1/3}. \tag{8}$$

The BEG model is complicated by the fact that we will in general have domains of '0' as well as '±'. The domain walls between '+' and '−' domains typically have a greater activation energy than those between '0' and '±'. Therefore, the domains of '0' will grow much more rapidly than the domains of '±1'. Moreover, the processes that lead to annihilation of domains of type '±' are affected by the presence of domains of '0' between them. However, in the scaling limit this merely leads to both types of domain having a length that scales according to (8), although with different (temperature-dependent) constants of proportionality. The x exponent is therefore equal to $\frac{1}{3}$, irrespective of the relative values of these energy barriers. These constants of proportionality will, however, affect the z exponent.

3.2. Critical z exponent

The arguments in the previous subsection may be extended to give the dynamic critical exponent by recognizing that characteristic equilibration processes are merely domain annihilation on a length scale of order ξ. In principle, near equilibrium we also have to take into account processes that lead to creation of domains, but these must in fact have the same scaling behaviour [6]. The characteristic relaxation time is therefore

$$\tau \sim \exp(\beta\Delta)\xi^3 \tag{9}$$

where Δ is the activation energy of the slowest process. ξ is the correlation length appropriate to the order parameter that becomes critical; in the BEG model there is only one correlation length that diverges at a given point in parameter space (on the tricritical line, both ξ_q and ξ_m diverge, but both diverge in the same way, so there is only one length scale).

In the case of the BEG model with three states, we have then three different kinds of domains, and in contrast to the case of the Ising model, we have to compare rates in different configurations, to identify the slower processes. Thus, looking to region I (see figure 1), three different subregions C1, C2 and C3 with different values of z appear, depending on the value of the rates and the correlation length. In subregion C1 ($D > 2K$) the correlation length behaves like $\xi \sim e^{2J+2K-D}$ at low temperatures and the large rates correspond to walls between domains of '+' and '−' spins so $\Delta = 4J$. Using result (9), we obtain the values for the z exponent quoted in table 1. In subregion C2 ($D < 2K$), $\xi \sim e^{2J}$, and the process that dominates is associated with the $++/--$ wall, so again $\Delta = 4J$. If $K < 3J$ we obtain $z = 5$ (table 1). In subregion C3 ($K > 3J$) the rates for domains involving zeros dominates, so $\Delta = (J + K)$ and we obtain the result for z, again plotted in table 1.

Table 1. Values of the critical z exponent obtained by the domain-wall method in different subregions of the phase space.

Region	Subregion	z exponent
I	A1	$3 + 4J/(2J + 2K - D)$
	A2	5
	A3	$3 + (J + K)/2J$
IV	B1	$3 + 8J/(J + K)$
	B2	$3 + (J + K)/2J$

In region IV, we obtain two different regions E1 and E2, corresponding respectively to $K < 3J$ ($\xi \sim e^{2J}$) and $K > 3J$ ($\xi \sim e^{(J+K)/2}$). Proceeding in the same way as before we obtain the results plotted in table 1 for the z exponent.

4. Monte Carlo simulations

4.1. Algorithm

The Monte Carlo simulations were carried out with two different algorithms. The first one was based on the conventional Monte Carlo algorithm, and is useful only for the cases of small correlation length and z exponent. In other cases (larger values of the correlation length and z exponent) the appropriate simulation method is the 'minimal process method' also called 'Gillespie algorithm' [14]. The system possesses large activation energies, and so it will spend long periods of time inactive. The Gillespie algorithm eliminates these dead periods of time in the simulation, and so under these conditions this algorithm will be much more efficient than the conventional one. This means that we can simulate the system at temperatures very close to zero, where the correlation length ξ becomes very large (but always smaller than the system size), and the CPU time does not increase greatly even for large values of z ($z \sim 6,7$).

The principle behind the Gillespie algorithm is to determine the *next* process that will occur in a stochastic system, together with the waiting time. The probability that a given process will occur next is proportional to the transition rate $p(i)$ for that process, whereas the actual waiting time is exponentially distributed, with characteristic time equal to the inverse total transition rate. The book-keeping necessary to perform this updating procedure is much slower than the code necessary to test one given flip process in the conventional algorithm, and so the Gillespie algorithm is only more efficient if the probability per test of a spin flip is very small.

The algorithm consists of the following few steps.

Step 1 (initialization). At time $t = 0$, generate an initial configuration (in this particular case, randomly, with equal probability for the three states). Classify the possible 'processes' (in our case, nine) that can occur, where each 'process' is characterized by a given energy change. From the configuration, the $n(i)$ sites at which a process of type i may take place are stored.

Step 2. For each process type (i) we calculate the product of the number $n(i)$ of sites where a process of this type can occur and the probability per unit time $p(i)$ associated with this process type.

Step 3. Determine the time step Δt for the next transition at $t + \Delta t$. Δt is calculated in such way that is distributed with probability density

$$Pr(\Delta t) = \mathcal{R} e^{-(\mathcal{R}\Delta t)} \tag{10}$$

where

$$\mathcal{R} = \sum_{i=1}^{N_{\text{process}}} n(i)p(i). \tag{11}$$

We therefore determine Δt by

$$\Delta t = -\frac{1}{\mathcal{R}} \log(1 - r) \tag{12}$$

where r is a random number with equal probability in $0 \leqslant r\langle 1$.

Step 4. Choose the process type according the probability rates $[p(i)]$. This is implemented by choosing a second random number (r) uniformly distributed in $[0,1]$, and setting an auxiliary variable $\mathcal{A}$ to zero. Then, for all possible processes, while $\mathcal{A} < r$, then $\mathcal{A} \rightarrow \mathcal{A} + (n(i)p(i))/\mathcal{R}$. The process i is chosen when $\mathcal{A}$ is bigger than r. The specific site at which the process (of type i) takes place is chosen randomly from the $n(i)$ possibilities.

Step 5. Update the spins, and according to the new configuration update the lists of sites at which the processes can occur. After, return to step 2, unless the final time has been reached.

4.2. Scaling theory

We will assume that the correlation function $C(r,t) = \langle \sigma_0 \sigma_r \rangle$, after a transient time t_0, acquires the expected scaling form in the critical region:

$$C(r,t) = r^{-(d-2+\eta)} F\left(\frac{r}{\xi}, \frac{t}{\xi^z}\right). \tag{13}$$

In one dimension this reduces to $F(x,y)$, because $\eta = 1$. Here ξ is the correlation length and z is the dynamic critical exponent.

In the domain growth scaling region, $(t/\xi^z \ll 1)$, the correlation function is a function of one scaling variable $(r/L(\xi,t))$ only, where L is the characteristic domain length. This implies that $F(u,v) \xrightarrow{v \ll 1} G(u/\Phi(v))$. We define

$$\tilde{L} = (1 - C(1,t))^{-1} \tag{14}$$

which is a useful definition of domain length even out of the domain growth region. With this assumption and postulating that $(1-C(r,t)) \xrightarrow{(r/L)\rightarrow 0} r/L$, which is equivalent to Porod's law [15], one finds that $G(w) \xrightarrow{w \rightarrow 0} (1-w)$. Hence, substituting the form for C in terms of G in (14), we find, for $\tilde{L} \gg 1$,

$$\tilde{L}(\xi,t) = \xi \Phi\left(\frac{t}{\xi^z}\right). \tag{15}$$

This is our main result, because is from this relation that we obtain the dynamic critical z exponent. However, we observe that we have to add a correction term to the expression of $\tilde{L}(\xi,t)$, of the form

$$\tilde{L}(\xi,t) = \xi \Phi\left(\frac{t}{\xi^z}\right) + \xi A\left(\frac{1}{\xi}\right). \tag{16}$$

We obtain a good fit for Monte Carlo results. The correction term is a consequence of the fact that the asymptotic regime is constrained by $1 \ll L \ll \xi$, and so does not strictly exist at finite temperature. This is in contrast to the case $d \geqslant 2$, where average domain size has no upper bound, and so the scaling region is always obtained as $t \rightarrow \infty$. The scaling function takes the form $\Phi(v) = v^x$, where the domain growth exponent x takes the value $\frac{1}{3}$ according to the simulations. Figures 2 and 3 show part of the linear regime of $L(t)$ against t^x, with $x = \frac{1}{3}$. This value is confirmed by the linearity of the plot over more than two decades in time. The continuation of the straight line of the fit does not match in the origin, due to the correction term. A plot of the intersection point with the abscissae axis against $1/\xi$ gives a good fit, which confirms the form of the correction term. We also see from the results of figures 2 and 3, for two different values of z, and others not presented here, that the x exponent is universal, in contrast to the z exponent which we study next.

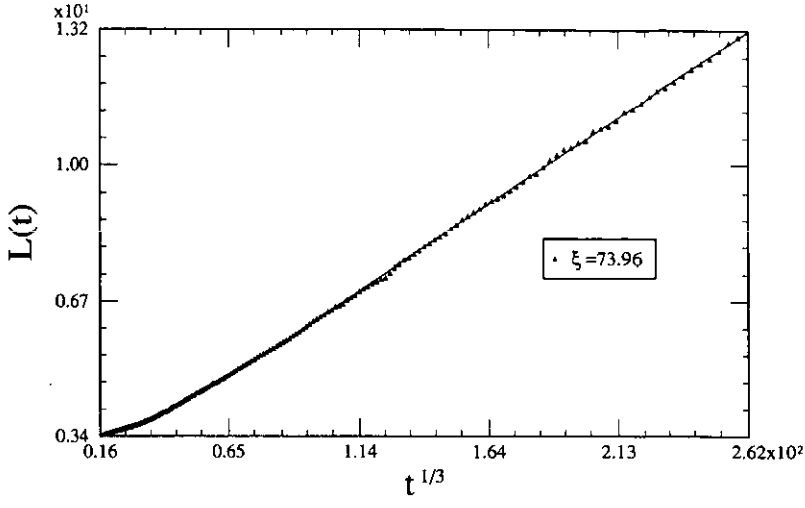

Figure 2. The average domain length $L(t)$ as a function of $t^{1/3}$, corresponding to the point B in the phase space. This corresponds to part of the scaling region.

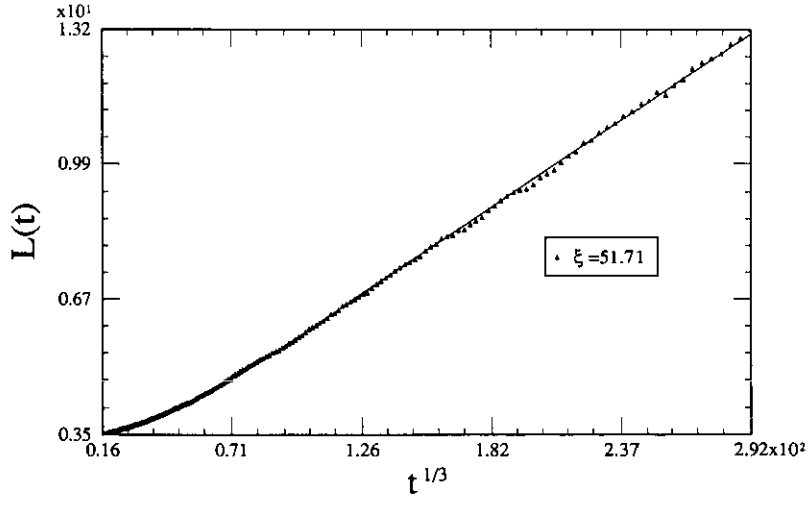

Figure 3. The average domain length $L(t)$ as a function of $t^{1/3}$, corresponding to the point F in the phase space. This corresponds to part of the scaling region.

4.3. Results for the z exponent

Monte Carlo simulations were performed for lattice size of between $N = 1024$ and $N = 16\,384$ spins, with periodic boundary conditions. The results are not significantly affected by finite-size effects, because the largest correlation lengths that were used never exceed 100 lattice units. The results are averaged over 100 independently generated initial configurations and seeds for the random number generator. The random number generator that we used was the well-known R250 of Kirkpatrick and Stoll [16]. The CPU time expended for all the simulations was several hundred hours on

Apollo Workstations 400 and 10000.

Different points in the phase diagram (figure 1) were simulated (A, B, D and F) and the corresponding values for the z exponent were calculated in the following way.

We simulated the system for different temperatures, where the the correlation length took the values between 30 and 90. From the simulations we obtained the value of domain size L as a function of t. We then plotted curves of $\tilde{L}(\xi, t)$ against $\xi(t/\xi^z)^{1/3}$ for several trial values of z, the correct value of z being the one for which the different curves match, by virtue of (15). This method of finding z is very accurate, since a single change of the order 0.1 in z put the curves out of scaling. The error bars in z are estimated from the subjective quality of fit for different trial values of z.

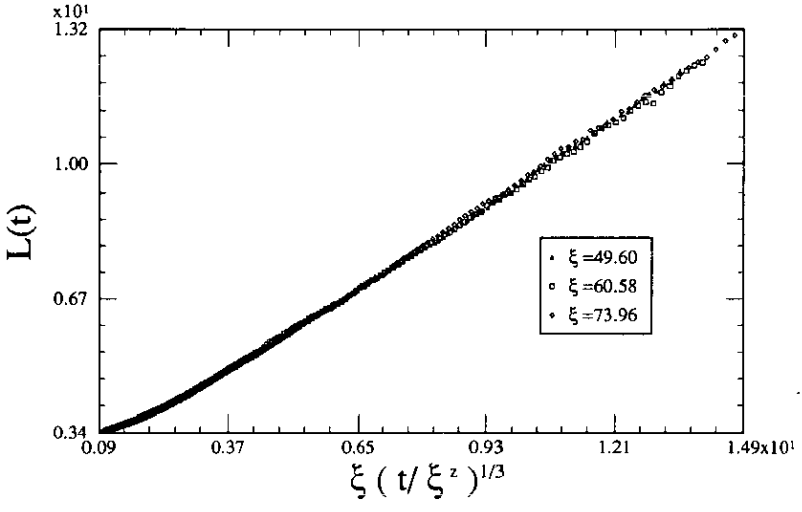

Figure 4. Scaling of different curves $L(t)$ against $\xi(\xi/t^z)^{1/3}$ corresponding to different values of the correlation length. The value of z here is 5.0 and corresponds to the point B in the phase space.

In figures 4 and 5 we plot $L(t)$ against $\xi(t/\xi^z)^{1/3}$ for three different values of ξ and $z = 5.0 \pm 0.1$ and 6.0 ± 0.1, respectively, corresponding in the phase space to the points B and D. The other points simulated were A and F and the values obtained were 4.95 ± 0.1 and 6.0 ± 0.1, respectively.

5. Conclusion

In this paper we have studied the one-dimensional BEG model with spin-exchange dynamics. This model presents a rich ground-state phase diagram as a function of the constant couplings of the Hamiltonian. We have studied the dependence of the domain growth and critical dynamics exponents on this phase space.

Physical domain-wall arguments predict the value $x = \frac{1}{3}$ for the domain growth exponent, which is the same as for the Ising model with order-parameter conserving dynamics. This result is in good agreement with the results of our Monte Carlo simulations. These arguments also predict non-universal values for the dynamic critical exponent. We have found that, within the framework of a scaling theory for this

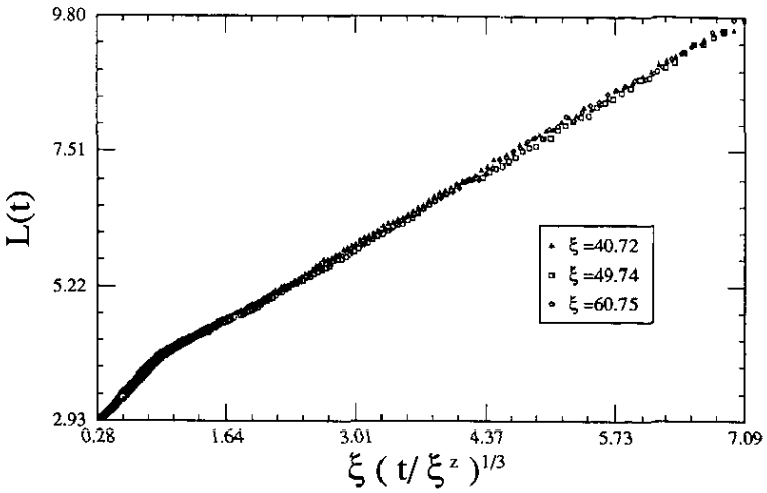

Figure 5. Scaling of different curves $L(t)$ against $\xi(\xi/t^z)^{1/3}$ corresponding to different values of the correlation length. The value of z here is 6.0 and corresponds to the point D in the phase space.

model, which assumes that there exists only one relevant characteristic time, these predictions appear to be correct. The presence of more than one divergent time in this model is therefore irrelevant at sufficiently long times.

An analogous scaling theory has previously been used to obtain the relationship between the growth exponent and dynamic critical exponent for the case of the Ising model with alternating coupling constants under Glauber dynamics [7]. In fact, a scaling theory of this type will always predict the same relation between exponents as the domain-wall arguments, since it assumes that the dynamics is controlled by only one energy barrier. The case of the alternating-bond Ising chain with Kawasaki dynamics is now being studied to clarify the discrepancy between the results of domain-wall arguments [10] and the real space renormalization group [17].

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