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LETTER TO THE EDITOR

Unconventional scaling theory for domain growth in the alternating bond Glauber–Ising chain

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Abstract. The domain growth after a quench is controlled by an exponent which generally has very broad universal properties. We investigate the alternating bond Ising chain with Glauber dynamics, and find that its growth exponent is universal, even though the dynamical critical exponent z is non-universal. We show that usual scaling theory can be reformulated to account for the above findings.

Much effort has been expended in recent years in attempting to explain the behaviour of a system initially in a high temperature equilibrium state and suddenly quenched in its ordered phase, below the coexistence curve [1].

Two types of phenomena can occur, depending on whether one quenches into a metastable state (homogeneous nucleation) or an unstable state (spinodal decomposition), although there is no sharp separation between the two cases [2]. Moreover, two time regimes should be distinguished: the early time one, and the late time one.

An interesting feature of this problem is that, in the late stage regime, this complicated non-equilibrium phenomenon exhibits simple scaling properties, both for nucleation and spinodal decomposition. This is clearly seen in the dynamical structure factor $S(q, t)$. The usual scaling theory asserts that after some transient time t_0 following the quench $S(q, t)$ behaves as

$$S(q, t) \simeq L(t)^d \Phi(qL(t); t/\tau) \tag{1}$$

where

$$L(t) \sim t^x \tag{2}$$

is the unique length characterizing the domain growth at time t, x is the growth exponent and τ a characteristic timescale. There are universality classes for x, whose characteristics have been made explicit by Bray [3]. Moreover, the dependence of the crossover function Φ on its second argument is very often negligible.

As noticed recently by Menyhárd [4], one-dimensional Ising systems with short range interactions have the property that the growth exponent x is related to the dynamical critical exponent z, which characterizes the relaxation time τ_c of the order parameter in the vicinity of a second-order phase transition. Namely,

$$\tau_c \sim \xi^z \tag{3}$$

where ξ is the correlation length.

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The explicit relation, which has been tested for different chains with homogeneous coupling constants and sequential or parallel dynamics [4], reads

$$z = 1/x. \tag{4}$$

Moreover, it has been shown [5, 6] that the critical exponent z is not always universal for one-dimensional Ising chains with nearest-neighbour interactions. Indeed for a chain with alternating ferromagnetic couplings $J_A > J_B$, one finds for Glauber dynamics that $z = 1 + J_A/J_B$ instead of 2 for homogeneous couplings.

One is then led to ask if the relation (4) is still valid, which would imply a non-universality for the growth exponent x, or if this one-length scaling theory described above should be corrected.

This is the question we are addressing in this letter, which is organized as follows. First we define the model; we then go on to compute analytically the structure factor and the kink density. Next, we report the results of numerical simulation. We end with a discussion of the scaling theory, and some conclusions.

The model we study is a one-dimensional Ising model, with Hamiltonian

$$\mathcal{H} = -\sum_i J_i \sigma_i \sigma_{i+1} \tag{5}$$

where $\sigma_i = \pm 1$, and the coupling constants assume alternately values J_A and J_B, i.e.

$$J_i = \begin{cases} J_A & i \text{ even} \\ J_B & i \text{ odd} \end{cases} \qquad J_A > J_B. \tag{6}$$

The system is in contact with a heat bath at temperature T, which causes the system state $\{\sigma\}$ to change by the flipping of single spins.

The probability per unit time W_i for the ith spin to flip is chosen to satisfy the condition of detailed balance, so that the system relaxes to equilibrium. We make the choice corresponding to that of Glauber [7]

$$W_i = \tfrac{1}{2}(1 - \sigma_i(\sigma_{i-1}\gamma_-^i + \sigma_{i+1}\gamma_+^i)) \tag{7}$$

with $\gamma_\pm^i \equiv \tfrac{1}{2}(\tanh(J_i + J_{i-1})/T \pm \tanh(J_i - J_{i-1})/T)$ in suitable time units.

The dynamic critical behaviour of this system has been studied [5, 6], and the critical exponent z, defined by $\tau \sim \xi^z$, where ξ is the correlation length and τ a characteristic relaxation time, is found to be $1 + J_A/J_B$. This non-universal form is explained by the requirement of a non-universal activation energy for domain wall random-walk processes, and is therefore only present since the critical temperature is absolute zero.

We shall study two properties of the system, the kink density K and the structure factor $S(q, t)$. Both of these are related to the spin-spin correlation function $\langle \sigma_i \sigma_j \rangle$ (where $\langle \ldots \rangle$ represents an ensemble average). The equation of motion of the correlation function is

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \sigma_i \sigma_j \rangle = 2(2\langle \sigma_i \sigma_j \rangle - \gamma_+^i \langle \sigma_{i+1}\sigma_j \rangle - \gamma_-^i \langle \sigma_{i-1}\sigma_j \rangle - \gamma_+^j \langle \sigma_i \sigma_{j+1} \rangle - \gamma_-^j \langle \sigma_i \sigma_{j-1} \rangle. \tag{8}$$

By virtue of (6), this function is translationally invariant over even multiples of the lattice parameter only. The correlation function is therefore dependent not only on the distance $x = j - i$, but also on whether i, j are odd or even. We therefore have four distinct correlation functions, two of which are only defined for x even and two defined for x odd only. We eliminate the odd-even and even-odd correlation functions to

obtain an equation for the even-even function f_x (which is always equal to the odd-odd function when starting from thermal equilibrium):

$$\left(1+\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\right)^2 f_x = (\gamma_A^2+\gamma_B^2)f_x + \gamma_A\gamma_B(f_{x+2}+f_{x+2}) \tag{9}$$

where x assumes only even values, and

$$\begin{aligned}\gamma_A &= \tfrac{1}{2}(\tanh(J_A+J_B)/T+\tanh(J_A-J_B)/T)\\ \gamma_B &= \tfrac{1}{2}(\tanh(J_A+J_B)/T-\tanh(J_A-J_B)/T).\end{aligned} \tag{10}$$

Equation (9) differs from that obtained for the uniform system studied by Bray [8] in the temperature-dependent prefactors (corresponding to energy barriers) and the presence of second-order derivatives with respect to time.

We now calculate the structure factor $S(q, t)$ after a deep quench from infinite temperature to a low, finite temperature where the correlation length is $\xi \equiv 1/\kappa$. We first change the length scale by $x \to x' \equiv x/2$ so that it assumes all integer values. Such rescaling will not, of course, affect the exponent we shall obtain. We follow the method of integral transforms, as used by Bray [8]. Define the Fourier transforms

$$S(q, t) = \sum_x \exp(\mathrm{i}qx) f_x \qquad f_x = \frac{1}{2\pi}\int_0^{2\pi} S(q, t)\exp(-\mathrm{i}qx)\,\mathrm{d}q \tag{11}$$

and Laplace transforms

$$\tilde{S}(q, s) = \omega \int_0^\infty \exp(-s\omega t) S(q, t)\,\mathrm{d}t \tag{12}$$

where $\omega \equiv 4\gamma_A\gamma_B$ reduces to an Arrhenius factor $4\exp(-2(J_A-J_B)/T)$ at low temperatures. Equation (9) is not valid at $x = 0$, where instead we have

$$1 = f_0 = \frac{s}{2\pi}\int_0^{2\pi} \tilde{S}(q, s)\,\mathrm{d}q. \tag{13}$$

Starting from equilibrium at infinite temperature, i.e. a totally uncorrelated state, we have $f_x(0) = \delta_{x,0}$, and therefore through (8) we have $\dot{f}(0) = 0$.

Equation (9) yields an equation of motion for $\tilde{S}$, which contains an integral term coupling all modes. Substituting for $\tilde{S}$, we find that with the above choice of initial conditions we can evaluate the integral in equation (13) and eliminate the mode-coupling term in the equation of motion for $\tilde{S}$. Finally, we find

$$\tilde{S}(q, s) = \frac{[(4s+\omega s^2+2\cosh\kappa)^2-4]^{1/2}}{s(4s+\omega s^2+\lambda_q)} \tag{14}$$

where $\lambda_q = 2(\cosh\kappa - \cos q)$.

We are unable to evaluate the inverse Laplace transform in this general case, but we make the following observations.

(i) The terms ωs^2 that arise due to the second-order derivative in (9) are insignificant when $s \ll \omega^{-1}$, and therefore do not contribute for times $t \gg 1$.

(ii) For $s \ll 1$, $q \ll 1$, $\kappa \ll 1$,

$$\tilde{S} \approx \frac{(\kappa^2+4s)^{1/2}}{s(\kappa^2+q^2+4s)} \tag{15}$$

yielding

$$S(q,t)=2\left(\frac{\theta}{\pi}\right)^{1/2}\frac{\exp(-\kappa^2\theta)}{q^2+\kappa^2}$$
$$\times\int_1^\infty \mathrm{d}y(y+1)^{-1/2}[\kappa^2\exp(-\kappa^2\theta y)+q^2\exp(-(q^2+\kappa^2)\theta+q^2\theta y)] \qquad (16)$$

with $\theta=\gamma_A\gamma_B t$, which is result (21) of Bray [8]. The domain length therefore scales like $t^{1/2}$ in the region $\omega^{-1}\ll t\ll\omega^{-1}\xi^2$. From (i), the presence of the second derivative in the equation of motion is irrelevant in this regime.

We can therefore see that, in the scaling region, the presence of the alternating bonds merely changes the timescale by an Arrhenius factor.

Similar results can be obtained for the density of kinks on weak or strong bonds (K_B and K_A respectively) [9, 10]. The result is of the scaling form

$$K_{A/B}(t)-K_{A/B}(\infty)=t^{-1/2}\exp(-\theta\kappa^2)g(\theta\kappa^2) \qquad (17)$$

where g is slowly varying in the scaling region. The limits on the scaling region are the same as for the structure factor.

The above results assumed an initially uncorrelated state. If the initial state has correlations of range l, these will be destroyed after a time $\sim l^2\omega^{-1}$, and the above scaling form is then valid for $t\gg l^2\omega^{-1}$ [9, 10].

The approximations made in the above analytical approach can be compared with the results of numerical simulation. The dynamic evolution of a chain of size 1000 spins was simulated by the Monte Carlo method. This length is sufficient for finite-size effects to be negligible, since the correlation length never exceeded a value of about 30. The ratio $A/B=2$ was chosen, corresponding to $z=3$. 'Checkerboard' updating was used, with the lattice split into two interlocking sublattices, largely to circumvent the need for generating too many random numbers. The random number generator used was based on that of Kirkpatrick and Stoll [11]. A random initial condition was chosen, and the temperature chosen so that the final correlation length was 33.3 lattice units. The system was allowed to evolve over 5000 MCS/spin. We therefore expect domain scaling in the region $30\ll t\ll 30\,000$, where time is measured in units of MCS/spin. The results were averaged over 4000 independent runs.

The kink densities K_A and K_B are plotted in figure 1, together with the inverse Bragg peak $1/S(0,t)$, on a log-log scale. Following equation (16), the final equilibrium values for the kink densities have been substracted from the results, and we have corrected the overall exponential decay factor, in order to give a better fit. The scaling behaviour is seen for $100<t<3000$. The kink densities at the latest times are about twice their equilibrium values, with the Bragg peak half of its equilibrium value. The results clearly support the scaling form with exponent $\frac{1}{2}$, rather than $1/z=\frac{1}{3}$.

A lower final temperature would give a wider scaling region, but the divergence of the Arrhenius factor associated with domain wall diffusion processes would mean that computing time would be greatly increased.

We can now interpret the results in terms of a scaling theory. The analytical solution (16) shows that, in the low temperature limit, two timescales enter in the scaling form of $S(0,t)$, namely $\tau_1=\xi^{(z-2)}$ and $\tau=\xi^z$. For $t\gg\tau_1$, $S(t,0)$ is of the form

$$S(0,t)=\left(\frac{t}{\tau_1}\right)^{\bar{x}}\Phi\left(\frac{t}{\tau}\right) \qquad (18)$$

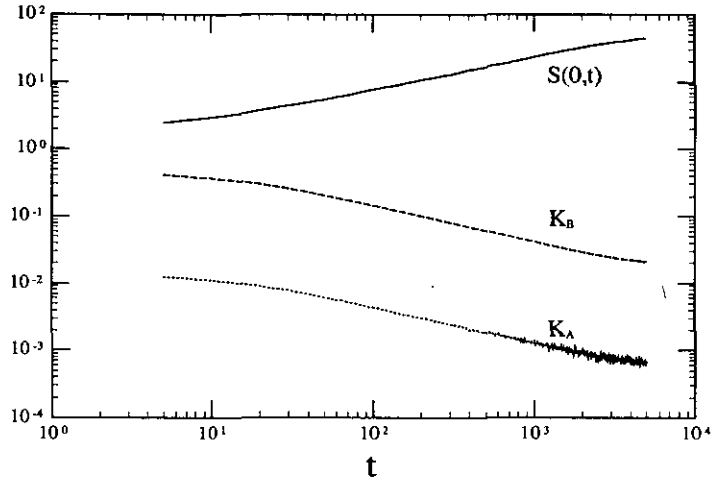

Figure 1. The Bragg peak $S(0, t)$ and corrected kink densities K_A and K_B as a function of time, on log-log axes. The gradients in the scaling region are 0.49, −0.518, −0.508 for $S(0, t)$, K_B, K_A respectively.

with $\bar{x} = \frac{1}{2}$. Thus, one sees that the usual scaling form is recovered providing the variable t by a rescaled one $\bar{t}$ defined as:

$$\bar{t} = t \exp\left(-\frac{\Delta}{T}\right) \tag{19}$$

where

$$\Delta = 2(J_A - J_B). \tag{20}$$

Then one can write

$$S(0, t) = \bar{t}^{\bar{x}} \bar{\psi}\left(\frac{\bar{t}}{\bar{\tau}}\right) \tag{21}$$

with $\bar{\psi}(y) \to$ (constant) when $y \to 0$ and $\bar{\tau} = \xi^{1/x}$.

The rescaling of t in $\bar{t}$, expresses the fact that the inhomogeneous couplings $J_A > J_B$, introduce activation energy barriers into the problem. This is an explicit example of a dangerous irrelevant variable described by Bray [3].

On the other hand, in the region of validity of this scaling form we would expect there to be only one important relaxation time, namely τ. We would then expect $S(0, t)$ to be of the scaling form

$$S(0, t) = t^x \Psi\left(\frac{t}{\tau}\right) \tag{22}$$

where $S(0, \infty) = \xi = \tau^{1/z}$ implies that $x = 1/z$.

In order to be consistent with the result that $S(0, t) \sim t^{\bar{x}}$ for $t/\tau \ll 1$, we require that Ψ assumes the *unusual* form

$$\Psi(y) \sim y^a \psi(y) \tag{23}$$

where

$$a = \bar{x} - \frac{1}{z} \tag{24}$$

and $\psi(0) = (\text{constant})$. This is consistent with (21) since

$$z = \frac{\Delta}{2J_B} + \frac{1}{\bar{x}} \tag{25}$$

provided $\bar{\psi} = \psi$. We therefore see that the two pictures (conventional theory with rescaled time or unusual scaling theory with non-universal critical exponent) are completely equivalent.

The above simple model shows explicitly that dynamical scaling theory may be applied provided some care is taken when activated processes are present. The usual scaling theory is recovered if time is rescaled with an Arrhenius factor.

A similar problem is encountered in the case of a uniform Ising chain under Kawasaki dynamics [12]. Here the growth exponent is $\bar{x} = \frac{1}{3}$, as in higher dimensions [9] and the energy barrier is $\Delta = 4J$. This is consistent with equation (25) since $z = 5$ [13]. However, in case of alternating bond the energy barrier is $\Delta = 4J_A$, which is consistent with $z = 3 + 2J_A/J_B$ (as obtained in [5]) rather than the more accepted result of [14]. Either the scaling theory for this system is more complex, or the growth exponent is non-universal.

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