Domain scaling and glassy dynamics in a one-dimensional Kawasaki Ising model

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(Received 14 May 1991)

The one-dimensional spin-exchange kinetic Ising model is studied using approximations based on the motion of single spins. This model exhibits domain-scaling behavior after a deep quench to low temperatures, with the same scaling exponent ($\frac{1}{3}$) as in higher dimensions. Under slow cooling, the kink density of this system is predicted to freeze at a value proportional to $\tau^{-1/z}$, where τ is the inverse cooling rate and z is the dynamic critical exponent ($=5$) for "natural" cooling programs. The results of Monte Carlo simulations are found to compare favorably with these predictions. The residual temporal behavior in a frozen nonequilibrium state is studied in the short- and long-time regimes, approaching asymptotically a stretched-exponential form.

I. INTRODUCTION

There is much physical interest in the behavior of systems when not close to thermodynamic equilibrium. One example of such a situation is the domain scaling observed in many systems, such as binary fluids or magnetic systems, after rapid cooling, where a characteristic length scales with time to some exponent.[1] Another example is the departure from equilibrium and freezing of a nonequilibrium state when a liquid is cooled at a finite rate. The characteristics of the "glassy" state formed by such a process depend strongly on the history of the system, in particular upon the cooling rate, and exhibit anomalous behavior such as stretched-exponential (Kohlrausch-Williams-Watts) response functions and non-Arrhenius (Vogel-Tamman-Fulcher) divergence of relaxation times.[2] Very few analytic results exist in this area due to the technical difficulty in treating such liquid systems.

Just as the Ising model has helped our understanding of static critical behavior, studies of kinetic Ising models have been very fruitful in describing dynamic phenomena. However, while exact analytic results exist for the one-dimensional single-spin-flip (Glauber) (Ref. 3) model for domain scaling[4,5] and freezing,[6,7] as well as for dynamic critical behavior, the equations of motion may not be solved either for dimension $d \geq 2$, for a system in a magnetic field, or for the case of spin-exchange (Kawasaki) (Ref. 8) dynamics. No reliable approximation schemes exist in many cases, either, so the interest in Ising models has most recently been due to their suitability for Monte Carlo simulations.

In this paper, we consider domain scaling and glassy dynamics in the one-dimensional kinetic Ising model with Kawasaki dynamics. We use approximations based upon consideration of the most important physical processes, which were first used to reproduce the dynamic critical exponent,[9] and we compare the predictions with Monte Carlo simulations. This model corresponds to model B in the terminology of Hohenberg and Halperin.[10] The domain-scaling exponent of model B has recently been disputed, but a renormalization-group (RG) argument by Bray[11] has predicted a value of $\frac{1}{3}$. This argument assumes the existence of a scaling form and the validity of an underlying RG transformation. The value of $\frac{1}{3}$ for the scaling exponent is explained physically for $d \geq 2$ by surface dynamical arguments.[12,13] However, in one dimension, the inapplicability of such a physical picture and the lack of a finite-temperature critical fixed point means that different behavior might be expected.

The Kawasaki model is appropriate as a lattice model of a binary fluid. For ferromagnetic coupling values, it possesses an energy barrier at low temperatures, and so it might be expected to display some characteristics of a glass transition when cooled.

The structure of this paper is as follows. After defining the Hamiltonian and dynamics for the model, we develop an approximate equation of motion based on spin-motion arguments. We apply this equation to the case of an instantaneous quench and to slow cooling. We then compare the predictions with the results of Monte Carlo simulations. Finally, we consider the dynamical properties of a far-from-equilibrium state at low temperatures.

II. THE MODEL

The model system is a one-dimensional Ising chain with uniform nearest-neighbor coupling constants, described by the Hamiltonian

$$\mathcal{H} = -\sum_i J\sigma_i\sigma_{i+1} \,. \tag{1}$$

The system is subject to spin-exchange dynamics, where the only process that can occur is the exchange of two antiparallel nearest-neighbor spins. The order parameter of the system does not change under such conditions. Such dynamics is appropriate for the Ising system to be a model of lattice gases and binary alloys.

The master equation for the Kawasaki spin-exchange dynamics[8] is

$$\frac{dP(\{\sigma\},t)}{dt} = -\sum_i \tfrac{1}{2}(1-\sigma_i\sigma_{i+1})(1-\hat{p}_i\hat{p}_{i+1}) \times W_i(\{\sigma\},t)P(\{\sigma\},t) , \quad (2)$$

where P is the probability of the system being in state $\{\sigma\}$ at time t, $\hat{p}_i$ is the operator flipping the ith spin, and W_i is the probability per unit time for the ith spin to exchange with the $(i+1)$th. The factor $(1-\sigma_i\sigma_{i+1})$ ensures that the two spins are antiparallel.

The dynamics of this system is affected qualitatively by whether the couplings J are ferromagnetic or antiferromagnetic. If we perform a gauge transformation $\sigma_i \to \sigma_i' = (-1)^i\sigma_i$, the dynamics allows nearest-neighbor *parallel* pairs to flip, and so, in the antiferromagnetic case, the dynamics is no longer activated. An antiferromagnetic Kawasaki chain is in the same dynamic universality class as a Glauber chain.[14,15] In this paper, we shall consider the ferromagnetic case only.

The exchange rates W_i are constrained by detailed balance, through this is not sufficient to constrain the rates fully. We make the common choice

$$W_i = \frac{1}{2}\left[1 - \tanh\left[\frac{\beta\Delta}{2}\right]\right] , \quad (3)$$

for a process where energy changes by Δ, in natural time units.

Under these conditions, the equation of motion of the spin-spin correlation function, obtained by multiplying Eq. (2) by $\sigma_j\sigma_k$ and tracing over the spin configurations, contains four-spin-correlation functions, as well as two-spin functions. In general, the equation of motion for an nth order correlation function involves $(n+2)$th -order correlation functions, and so we have an infinite hierarchy of equations. This form occurs whatever choice is made for the functions W_i. For this reason, the model is not exactly solvable.

The origin of the higher-order correlation s is clear; the dynamics proceeds through the motion of free spins (three antiparallel spins), after evaporation (see below), and so four-spin-correlation functions are needed to describe the growth of correlations.

Nevertheless, the dynamic critical exponent z has been found by linear response[16] and real-space renormalization.[17] The conserved-order-parameter system obeys the conventional theory of critical slowing down,[10] although the kinetic coefficient diverges in an Arhennius-like way due to the activation energy, giving $z = 3(\text{conventional}) + 2(\text{Arrhenius}) = 5$.

III. SPIN-MOTION ARGUMENTS

Although the equation of motion for the correlation function cannot be solved exactly, the underlying physical processes are very simple (see Fig. 1). The first type of process is spin *evaporation* (E), where a spin with only one antiparallel nearest neighbor splits off from its domain. This requires an amount of energy $4J$. The reverse process is spin *condensation* (C). The other type of process is where a spin with two antiparallel nearest neighbors exchanges with a nearest neighbor, with no change in energy. This spin then performs a random walk until it condenses with another single spin or a domain wall. This we call spin diffusion (D).

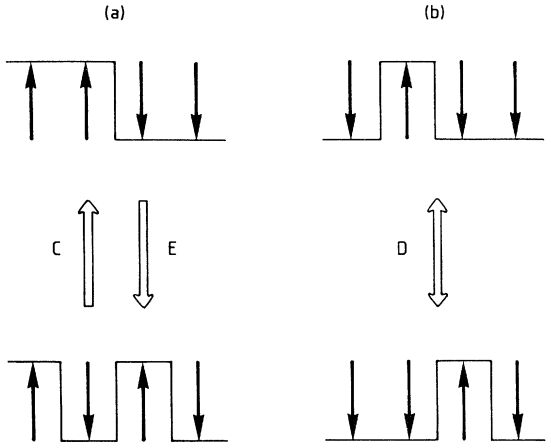

FIG. 1. (a) Condensation or evaporation and (b) spin diffusion for a Kawasaki chain.

We describe the relaxation towards equilibrium in terms of these processes; in particular, we treat the motion of single spins as interacting random walkers.[18] Such arguments were used to reproduce successfully the value of the dynamic critical exponent for the Kawasaki chain by Cordery *et al.*[9] In principle, the arguments were thought to give a lower bound to the critical exponent, although, in fact, in the case of the Glauber spin-flip system, they reproduce the exact value in numerous cases.[19] However, in the case of a Kawasaki chain with spatially modulated coupling constants, the domain-wall arguments[19] obtain an exponent *higher* than the result obtained by other methods.[14,15] Thus, the validity of such arguments as approximations might be called into question. The use of these arguments in our context is a useful test of their validity.

We choose to characterize the system by its kink density, which is a measure of the average inverse domain size. In the thermodynamic limit, the constraint that the magnetization be constant does not affect the static equilibrium behavior, and so the equilibrium kink density at low temperatures is

$$K_{\text{eq}} = \tfrac{1}{2}(1 - \langle \sigma_i\sigma_{i+1} \rangle) \approx \exp(-2\beta J) . \quad (4)$$

When the spin-motion arguments were applied to critical dynamics,[9] processes were considered that led to destruction of domains only. Since we are interested in the slow departure of the system from equilibrium under slow cooling, we need to know about the processes that lead to domain creation as well. At low temperatures, the system is in a state consisting of long domains. The dynamics is mediated by single spins evaporating from a domain wall and then performing a random walk. The

density of such single spins at equilibrium is

$$\langle(1-\sigma_i\sigma_{i+1})(1-\sigma_{i+1}\sigma_{i+2})\rangle \approx \xi^{-2} ,$$

while the domains are of length ξ, so there is an average of $1/\xi$ such single spins per domain. Most of the spins that evaporate simply return to their original domain wall. Some will reach the next domain wall, however, and this leads to the original domain moving through one lattice spacing. Although the net kink density does not change in one such process, as a result of many of these processes, the domain performs a random walk until it meets and annihilates with a neighboring domain wall. This process is the one considered in Ref. 9. On the other hand, a single spin may meet and annihilate with another single spin. The result of this is to create a new stable domain.

We shall now calculate the rates for these two types of process. Then we shall use these rates to derive an approximate equation of motion for the kink density, which we may then solve under a slow quench to obtain the freezing behavior.

A. Domain annihilation

If a spin splits off from a domain wall, let the probability that it first reaches a site L lattice spacings away before returning to the origin (and recondensing) be p_L. If the spin reaches $(L-1)$ before returning to the origin, it may either move next onto L (with probability $\frac{1}{2}$ or onto $(L-2)$ (also with probability $\frac{1}{2}$). If the latter occurs, there is a probability $(1-p_{L-1})$ that it returns to $(L-1)$ before returning to the origin, and the process repeats. The probability that the spin arrives at L is obtained from the total number of walks where the spin reaches the $(L-1)$th site 1,2,3,. . . times before returning to the origin, and then hops onto L:[9]

$$p_L = \sum_{n=0}^{\infty} \tfrac{1}{2} p_{L-1} \left[\frac{1-p_{L-1}}{2} \right]^n = \frac{p_{L-1}}{p_{L-1}+1} . \tag{5}$$

The solution to this equation with boundary condition $p_1 = 1$ is

$$p_L = \frac{1}{L} . \tag{6}$$

Thus, for long domains, the spin rarely reaches the next domain wall.

If the spin reaches the next domain wall before returning to its original wall, the domain has then moved through one lattice unit. On the basis of the central limit theorem, as $L \to \infty$, a total of order L^2 such processes must occur before the domain reaches and annihilates with the next domain wall, if this is a distance L away. Assuming each domain decays independently, and putting the average domain length $L \sim 1/K$, the rate of decay of kink density is therefore

$$\left. \frac{dK}{dt} \right|_{\text{annihilation}} = -A\omega K^3 \cdot K , \tag{7}$$

where $\omega = \exp(-4\beta J)$ is the Arrhenius factor associated with thermally creating a single spin. A is a number of order unity, which is expected to vary slowly with the probability distribution of domain sizes.

B. Domain nucleation

If a spin walks from one domain wall and then meets another domain, the kink density does not change on time scales coarse grained over the single-spin lifetime. The only way that new, stable domains can form is if two single spins collide and coalesce. The colliding spins may have been emitted from the same, or from neighboring domain walls. Since the spins rarely travel very far from their place of origin, however, it is clear that the contribution from the former is greater than from the latter by a factor $\sim 1/L$.

To obtain the probability of such a process happening, we consider a single spin performing a random walk on a lattice, starting at position 1, with an absorbing wall at the origin. A second spin will then be introduced at time $t' \sim \omega^{-1}$. Since the first spin has only a small chance of reaching the far domain wall, the approximation that the domain is of infinite size will not substantially affect the result. If the probability of the spin being at site l at time t is $p_l(t)$, the equations of motion are

$$\frac{dp_l}{dt} = \begin{cases} p_{l-1}+p_{l+1}-2p_l & \text{for } l \geq 1 \\ 0 & \text{for } l = 0 \end{cases} . \tag{8}$$

The solution of this master equation with initial condition

$$p_l(0) = \delta_{l,1} \tag{9}$$

is

$$p_l(t) = 2\int_0^1 \sin(q\pi)\sin(ql\pi) \times \exp[-2(1-\cos q)t]\,dq . \tag{10}$$

For $t \gg 1$, $l \gg 1$, this solution approaches the form

$$p_l \approx \frac{1}{2}\left[\frac{\pi}{t^3}\right]^{1/2} l\pi^2 \exp\left[-\frac{l^2\pi^2}{4t}\right] . \tag{11}$$

A second spin is introduced at time t'. Since the probability of the second spin remaining is very small, the probability of the first spin interacting with it is very small, and can be treated by perturbation theory. The second spin will then perform a random walk similar to the above, and will survive for a time $\ll t'$. The spin will also penetrate only a small distance into the lattice. The probability of the second spin interacting with the first is then simply proportional to something of the form

$$\sum_l f_l p_l(t') \propto (t')^{-3/2} , \tag{12}$$

where f_l represents the probability of the second spin reaching site l.

The probability of the second spin being introduced in the interval $t \to t+dt$ is $\omega \exp(-\omega t)dt$, so the total probability of any given spin colliding with a second is $\propto \omega^{3/2}$. The rate of domain nucleation is then

$$\left.\frac{dK}{dt}\right|_{\text{nucleation}} = B\omega\omega^{3/2}K \ , \tag{13}$$

where B is a number of order unity.

C. Equation of motion for the kink density

The two processes of nucleation and annihilation occur only rarely. We therefore expect them to occur independently, i.e., without interacting, to a good approximation. We make the assumption that there is just one relevant length scale in the problem, the average domain size, which we identify as $\propto 1/K$.

Combining the above two results, Eqs. (7) and (13), we expect the equation of motion for the kink density to be of the form

$$\frac{dK}{dt} = -A\omega K^4 + B\omega^{5/2}K \ . \tag{14}$$

The numbers A and B depend weakly on the distribution of domain sizes. At equilibrium, we have $K_{\text{eq}} = \omega^{1/2}$ $[= \exp(-2\beta J)]$, so we equate $A = B$. We also absorb the coefficient A into the units of time, and write

$$\frac{dK}{dt} = \omega(\omega^{3/2} - K^3)K \ . \tag{15}$$

Notice that, at low temperature, both of the terms on the right-hand side scale like $\omega^{5/2} \propto \xi^{-5}$, i.e., *both* terms give rise to equilibration with dynamic critical exponent $z = 5$. Although the unit of time is poorly defined, it is clearly of the same order as the attempt time for spin exchange.

Equation (15) contains the competing terms most significant at low temperatures. There are other processes which can occur, such as condensation of two spins emitted from two different domain walls, but these may be shown to be smaller than the ones described above by at least a factor $O(K)$. It is also important to point out that the central limit theorem has been used to obtain both terms, and at length scales not too great, we therefore expect further corrections, smaller by a factor $O(K)$.

It is worth noting that, in the arguments used above, it was assumed that whenever a spin arrives next to a domain wall it is always absorbed. In the Kawasaki dynamics, domain walls are not perfectly absorbing but the above arguments are expected to reproduce the correct scaling behavior at low temperatures.

The solution to (15) when ω is a function of time is

$$K(t) = \frac{\exp\int_0^t \omega^{5/2}(t')dt'}{\left[K^{-3}(0) + 3\int_0^t \omega(t')\exp\left[3\int_0^{t'} \omega^{5/2}(t'')dt''\right]dt'\right]^{1/3}} \ . \tag{16}$$

Three cases are interesting.

(i) For an instantaneous quench from equilibrium at high temperature to low, constant temperature, with $K(0) \gg \omega^{1/2}$,

$$K(t) = \frac{\exp(\omega^{5/2}t)}{\{K^{-3}(0) + \omega^{-3/2}[\exp(3\omega^{5/2}t) - 1]\}^{1/3}} \ . \tag{17}$$

Here ω is the Arrhenius factor at the final temperature. In the region $K^{-3}\omega^{3/2}(0) \ll \omega^{5/2}t \ll 1$, this gives

$$K \propto t^{-1/3} \ . \tag{18}$$

This is reminiscent of the domain scaling observed in a $d \geq 2$ conserved order parameter Ising systems[1] after a quench from the one-phase to the two-phase region. If a conserved-order-parameter system is subject to a deep critical quench to the two-phase region, the correlation function at separation x is found to be a function of the sclaing variable $(x/t^{1/3})$. In our system, however, we have not quenched through a phase transition; the equilibrium corresponds to very long domains, so the equilibration requires spins to flow through domains in a way reminiscent of phase separation in higher-dimensional systems. In $d \geq 2$, the exponent $\frac{1}{3}$ (Ref. 4) is interpreted physically by Huse,[13] after Lifshitz and Slyozov,[12] by arguments about the growth of droplets. In one dimension, it is explained by our spin-diffusion arguments.

(ii) If a low-temperature system is annealed at a higher temperature [but still with $J/kT \gg 1$, so as to ensure the validity of (15)], the solution predicts an initial domain *shrinkage* with

$$K \propto \exp(\omega^{5/2}t) \tag{19}$$

for the regime $3\omega^{5/2}t \ll \ln_{10}[K^{-3}(0)\omega^{3/2}]$. This law expresses the initial nucleation of domains. However, the "kink density" in the above equation describes stable domain walls only; in this region, we expect the population of single spins to be large in comparison to the kink density, and the thermal creation of these spins will mask the contribution to the kink density from stable-domain nucleation. This behavior does not last very long, and for $t \to \infty$,

$$K(t) = \omega^{1/2} + O(\exp(-\omega^{5/2}t)) \ . \tag{20}$$

(iii) For a slow, continuous quench to zero temperature, the system may freeze. By using an effective time

$$u \equiv \int_0^t \omega(t')dt' \ , \tag{21}$$

it is possible to show, in general, using (15) or (16) that the system freezes [in the sense that $K(t)$ does not evolve to zero] if and only if the effective time remains finite as $t \to \infty$.

We choose a "linear" cooling program so that the Arrhenius factors which control the system behave exponentially in time:

$$\omega(t) = \omega_0 \exp\left[-\frac{t}{\tau}\right] \ . \tag{22}$$

Under these conditions, the cooling "rate" is constant in time, $u(\infty)$ is finite, and the system freezes.

The full solution to (15) in this case is

$$K=\left[\omega_0^{-3/2}\exp(-\tfrac{6}{5}\tau[\omega_0^{5/2}-\omega^{5/2}]) +3\tau\int_{\omega}^{\omega_0}\exp\{\tfrac{6}{5}\tau[\omega^{5/2}-(\omega')^{5/2}]\}d\omega'\right]^{-1/3}. \quad (23)$$

The term corresponding to the memory of the initial condition quickly decays, and, for $t\gg\tau$, the solution may be written in the following form:

$$K\approx\tau^{-1/5}\left[3(\tfrac{5}{6})^{2/5}\int_{\omega\tau^{2/5}}^{\infty}\exp(\omega^{5/2}\tau-x^{5/2})dx\right]^{-1/3} \quad (24)$$

$$=\tau^{-1/5}f(\tau\xi^{-5}), \quad (25)$$

where ξ is the instantaneous value of the equilibrium correlation length, and

$$f(x)\sim\begin{cases}\text{const} & \text{as } x\to 0,\\ x^{1/5} & \text{as } x\to\infty.\end{cases} \quad (26)$$

The kink density therefore freezes like $\tau^{-1/5}$. Note that the parameter ξ changes in time. The same scaling form would not occur if a cooling program were used where ω does not vary exponentially in time. In Fig. 2 the above form for the kink density is plotted as a function of temperature. These plots are, in fact, for values of τ where the long lengths, low-temperature approximation breaks down, but serve as qualitative predictions for the freezing behavior in this region. The freezing exponent $\frac{1}{5}=1/z$ is what would be expected from simple arguments, where the system is assumed to freeze at the point where the equilibriation rate $r_e=\xi^{-5}$ equals the cooling rate $r_c=d\ln/dt$. As observed in a Glauber chain with spatially modulated coupling strengths,[20] the freezing relation may be altered by different choices of the cooling program, where r_c becomes a function of time.

IV. MONTE CARLO SIMULATION

Extensive Monte Carlo simulations were carried out to verify the above behavior. The system relaxes very slowly in time due to the rapid decay of the activation factor, $\exp(-4\beta J)$. A vectorized routine was used, exploiting the fact that the lattice may be split into three independent sublattices of bonds. The probability per sweep of a spin exchange was taken to be equal to W_i of Eq. (3). In principle, such a routine introduces artificial correlations between the motions of single spins, but these correlations should be of order $(\frac{1}{2})^l$, where l is the separation of the two spins. This was found not to be significant by checking that the results of two quenches using the above rates matched those using probabilities scaled down by some factor α and a factor $1/\alpha$ more sweeps.

The size of the system (3072 spins), using periodic boundary conditions, was judged to be sufficient for no finite-size effects to be important, since the longest domain size obtained was about 50 lattice units.

A. Domain growth scaling

The spin-diffusion arguments presented above predict that, after a deep quench and a short transient time, the domain size scales like $t^{1/3}$. This was simulated by starting with an entirely random configuration (but with total

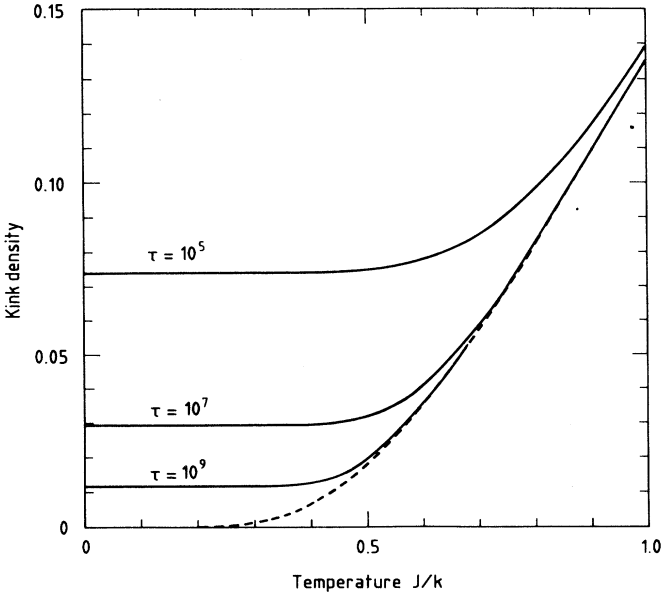

FIG. 2. Kink density as a function of temperature for three values of the cooling rate, evaluated from expression (24) (solid lines) and equilibrium value (dashed line).

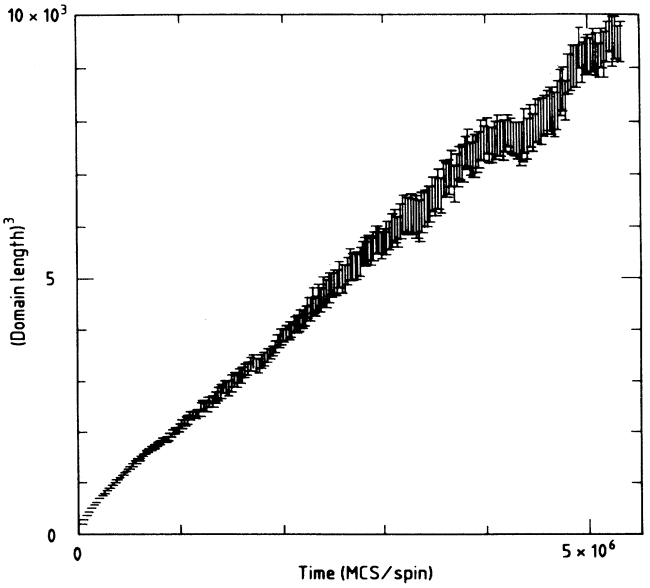

FIG. 3. (Domain length)^3 as a function of time, from a simulation of a deep quench to a low temperature.

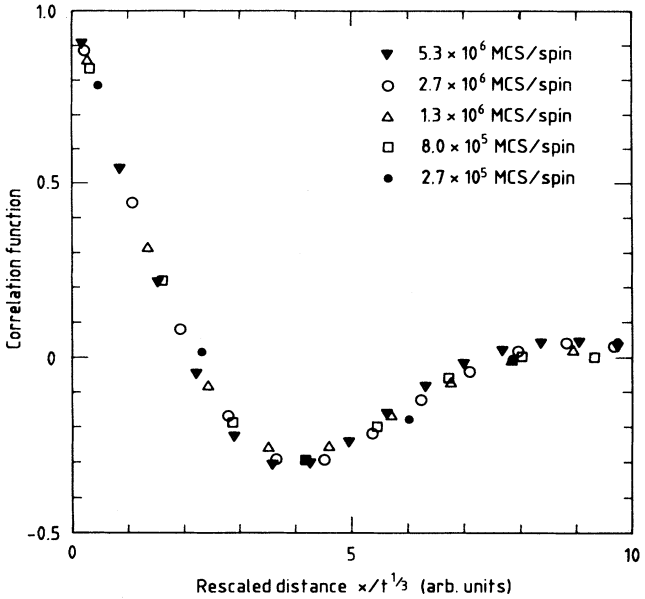

FIG. 4. Spin-spin-correlation function as a function of reduced distance $x/t^{1/3}$ at five different times following a deep quench.

magnetization zero, as the low-temperature behavior may be affected in off-critical simulations[21]), and then allowing the system to evolve at some low temperature.

Observing this behavior in one dimension is, in fact, more difficult than in $d \geq 2$ because the upper limit of the scaling region is bounded by the value of the correlation length [$\sim \exp(2\beta J)$], while in spinodal decomposition,[1] the system has an infinite relaxation time. If the correlation length is taken to be large, the Arrhenius factor $\exp(-4\beta J)$ becomes very small indeed, and so a very large number of time steps is necessary to obtain a wide scaling region. In two dimensions for instance, it is typical to take $\beta J \approx 2\beta_c J \approx 0.9$, whereas, in this simulation, it was necessary to take $\beta J = 2.05$, giving equilibrium domain length of about 60. A total of 2×10^7 sweeps were performed for ten independent initial conditions and seeds for the random number generator. This required 120 h of CPU time on a Stardent Titan minisupercomputer.

The domain-length cubed is plotted as a function of time in Fig. 3. The linearity of the plot (to within the error bars) is striking, in confirmation of the above prediction. The error bars were estimated from the statistics of the ten independent runs.

In Fig. 4 the spin-spin-correlation function is plotted as a function of scaled distance $x/t^{1/3}$. The full correlation function shows the same scaling behavior as the kink density, just as is observed in higher dimensions.[1] The scaling form is seen to be valid over a factor of 20 in time. Although the above arguments are formulated for the kink mode only, they are verified for all domain sizes.

B. Freezing

The behavior under continuous cooling was investigated by starting with an initially random configuration with magnetization zero, corresponding to $T = \infty$, and changing $\omega = \exp(-4\beta J)$ in discrete steps. After each step, a number n_s (in the range of $250-5 \times 10^6$) of sweeps was allowed at the new temperature, and then ω was changed by a factor of 0.9. The entire simulation required several hundred hours of CPU time.

In Fig. 5 the kink density is plotted as a function of temperature for nine different values of n_s. It is interesting to note that the kink density lags behind its equilibrium value for most of the cooling process, even well before the freezing occurs. This lag is greater for faster cooling. The freezing is still fairly abrupt at slow cooling. The error bars are estimated from the statistics of the independent runs.

The values of the frozen kink density are plotted as a function of τ on a log-log scale in Fig. 6. The points do not lie clearly on a straight line. The straight line is one of gradient $-1/z = -0.2$ (predicted by the analysis), and is a guide to the eye only. The best fit to the data gives a gradient -0.182 ± 0.02. The reason for this discrepancy is that the lengths are not sufficiently long for the central limit theorem results to be exactly applicable; we expect systematic corrections of $O(K)$. It is straightforward to check that the deviations of the points in Fig. 6 from the line are of this order. Ideally, results would be obtained for slower cooling, but this is simply not feasible given the CPU times that would be required (approximately 500 h for a value of K lower by $4^{-1/5}$).

The same data is plotted in the form K versus $\tau^{-1/5}$ in Fig. 7. This data approaches a straight line through the

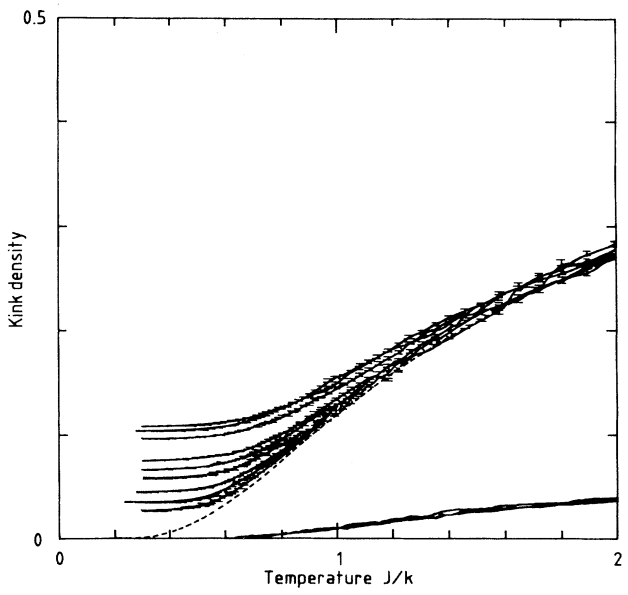

FIG. 5. Kink density as a function of temperature during simulations of nine different cooling rates. The dashed curve corresponds to thermal equilibrium. The lower curve is the density for single spins during the cooling.

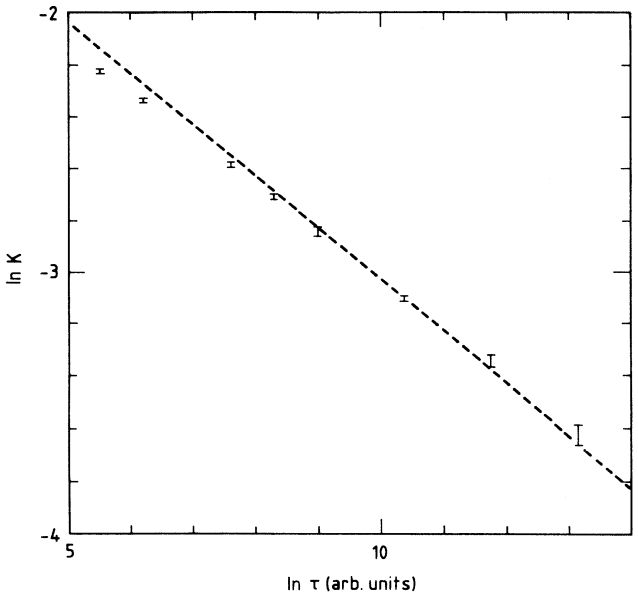

FIG. 6. ln(frozen kink density) as a function of $\ln(\tau)$ for the cooling processes shown in Fig. 5. The dotted curve is a guide to the eye only with the gradient -0.2 predicted for asymptotically large τ.

origin as the origin is approached, verifying the asymptotic form.

Figure 8 shows a comparison of the simulation data with the form in (24) for the three slowest cooling programs. This curve has been fitted to the final value of the kink density and has also been corrected to allow for the fact that, for the temperatures shown, the equilibrium value $\frac{1}{2}(1-\tanh\beta J)$ differs from the approximate vlaue $\exp(-2\beta J)$ in (24). The data shows a slower crossover from equilibrium to the frozen value than the approximation. Data for much slower cooling rates (and much lower temperatures) would be necessary for a more searching comparison to be made. Given the significant deviations from the asymptotic long-length and low-temperature regime of this data, an explicit fit to a scaling form such as (25) was not attempted.

V. SHORT-TIME AND LONG-TIME RELAXATION AT ZERO TEMPERATURE

The Kawasaki system is qualitatively different from the activated Glauber systems considered elsewhere[6,7] in that the system is still capable of relaxing at zero temperature. The asymptotically long-time behavior of this system at zero temperature is most easily simulated when the structure still contains a large number of single spins. We treat instantaneous cooling as the limiting case of rapid cooling, where the system will fall out of equilibrium at high temperature. The case of a two-dimensional Kawasaki system quenched to zero temperature was studied briefly by Sadiq and Binder,[22] though they did not discuss the properties of this state beyond stating that its domain size was about ten lattice units.

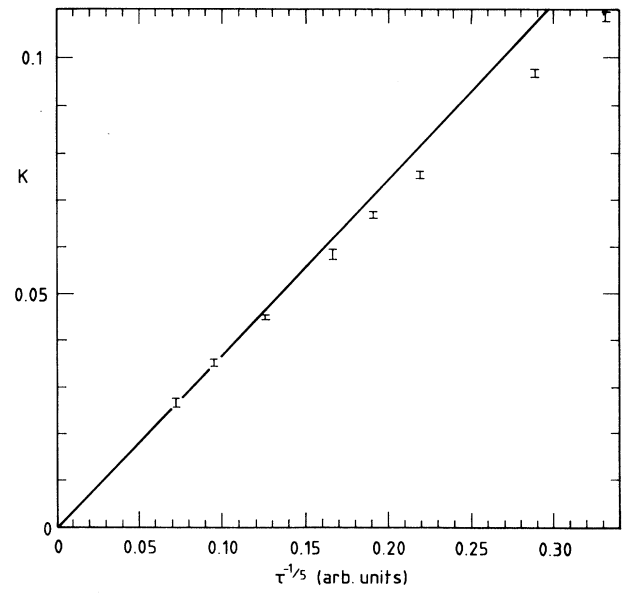

FIG. 7. The same data as in Fig. 6, plotted as a function of $\tau^{-1/5}$.

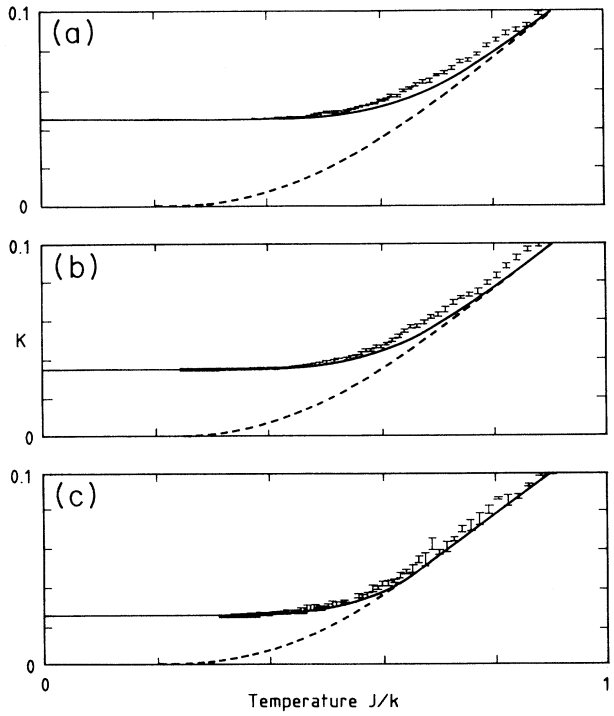

FIG. 8. Fit of the approximate form (24) to the data for the three slowest cooling procedures in Fig. 5 (solid line). The dashed curve corresponds to thermal equilibrium.

If the system undergoes a deep quench to a very low temperature, the behavior may be split up into four successive distinct regions: (i) unstable decay of clusters of three or more kinks (energy reducing), (ii) diffusion and condensation of the free single spins present, (iii) thermal evaporation of new single spins, and (iv) domain growth and approach to equilibrium.

If the quench is to sufficiently low temperature, (iii) and (iv) (dealt with earlier in this paper) may be separated arbitrarily in time from (i) and (ii). For the conventional Kawasaki flip rates (3), (i) and (ii) occur on similar time scales and are usually described as the "transient region." However, we are at liberty to choose the relative rates of D and of C/E processes independently, so that, by a different choice, (i) and (ii) may be made to occur on different timescales.

In this section, we first investigate the early-time behavior (i). Secondly, we investigate the relaxation of the structure (ii) due to the surviving single-spin density. The results for (ii) are valid for slow as well as instantaneous cooling.

A. Initial behavior after instantaneous quench to absolute zero

After an initial quench from high temperature to absolute zero, or a sufficiently rapid one where the system departs from equilibrium at a high temperature, the structure contains a relatively high density of kinks. Since a significant fraction of these will be nearest neighbors, many different decay processes may occur. We define a *cluster of kinks* (henceforth just cluster) of size l as a chain of l and not more nearest-neighbor kinks, so that an l cluster is not part of an $(l+1)$ cluster (see Fig. 9). Such a cluster (for $l \geq 3$) may decay by spin exchange at the mth bond (say) in the chain where $2 \leq +m \leq (l-1)$. When this happens, the $(m-1)$th and $(m+1)$th kinks disappear, and so the cluster has decayed into three clusters, of sizes $(m-2)$, 1, and $(l-m-1)$. (See Fig. 9.)

The equations of motion for the densities n_l of clusters of size l are

$$\frac{dn_1}{dt} = n_3 + \sum_{s=4}^{\infty} s n_s \ , \tag{27}$$

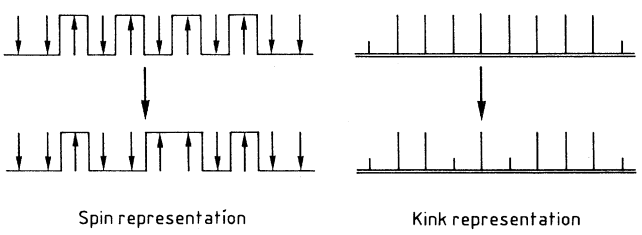

FIG. 9. A cluster of eight kinks decaying by condensation to three clusters, of two, one, and three kinks, respectively. The kink representation denotes a kink by a long line and an unbroken bond by a short line.

$$\frac{dn_s}{dt} = -(s-2)n_s + 2 \sum_{i=s+3}^{\infty} n_i, \quad s \geq 2 \ . \tag{28}$$

Using the vector notation

$$\mathbf{n} = \begin{bmatrix} n_2 \\ n_3 \\ \vdots \end{bmatrix} \ , \tag{29}$$

the equation becomes

$$\frac{d\mathbf{n}}{dt} = \underline{M}\mathbf{n} \ , \tag{30}$$

where the matrix $\underline{M}$ is

$$\underline{M} = \begin{bmatrix} 0 & 0 & 0 & 2 & 2 & 2 & 2 & \vdots \\ 0 & -1 & 0 & 0 & 2 & 2 & 2 & \vdots \\ 0 & 0 & -2 & 0 & 0 & 2 & 2 & \vdots \\ 0 & 0 & 0 & -3 & 0 & 0 & 2 & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \tag{31}$$

The eigenvalues of $\underline{M}$ are just the diagonal elements $0, -1, -2, \ldots$, since M has no elements below the diagonal. The left and right eigenvectors $\mathbf{q}_-^l$ and $\mathbf{q}_+^l$ corresponding to eigenvalue $(-l)$ are of the form

$$\mathbf{q}_-^l = (0, \ldots \{l \text{ zeros}\} \ldots 0, a_0^-, a_1^-, a_2^-, \ldots) \ , \tag{32}$$

$$\mathbf{q}_+^l = \begin{bmatrix} a_{l-1}^+ \\ a_{l-2}^+ \\ \vdots \\ a_1^+ \\ a_0^+ \\ 0 \\ 0 \\ \vdots \end{bmatrix} \ , \tag{33}$$

where the $\{a_j^{\pm}\}$ form a set that is independent of l, satisfying

$$n a_n^{\pm} = a_{n-1}^{\pm} \mp 2 a_{n-3}^{\pm} \ , \tag{34}$$

$$a_n^{\pm} = 0 \quad \text{for } n \leq -1 \ . \tag{35}$$

If we define the generating function

$$g_{\pm}(t) = \sum_{i=0}^{\infty} a_i^{\pm} t^i \ , \tag{36}$$

then $g_{\pm}$ satisfies

$$(1-t)\frac{dg_{\pm}}{dt} = \mp 2t^2 g \ , \tag{37}$$

whose solution is

$$g_{\pm} = A(1-t)^{\pm 2} \exp[\pm 2(t + t^2/2)] \ , \tag{38}$$

where A is a constant, which we will set equal to unity (it is trivial to prove *a posteriori* that this definition leads to

correctly normalized eigenvectors).

The initial condition corresponding to thermal equilibrium at temperature $T=1/(k_B\beta)$ is

$$n_s(0)=\tau^{s+2}\ , \tag{39}$$

where

$$\tau\equiv\tfrac{1}{2}[1-\tanh(\beta J)]\ . \tag{40}$$

so

$$\mathbf{n}(0)=\tau^4\begin{bmatrix}1\\ \tau\\ \tau^2\\ \vdots\end{bmatrix}\ . \tag{41}$$

Writing the matrices of eigenvectors $\underline{Q}^{\pm}$ and eigenvalues Λ,

$$\underline{Q}^{+}=\begin{bmatrix}a_0^+ & 0 & 0 & \cdots\\ a_1^+ & a_0^+ & 0 & \ddots\\ a_2^+ & a_1^+ & a_0^+ & \ddots\\ \vdots & \vdots & \vdots & \ddots\end{bmatrix}\ , \tag{42}$$

$$\underline{Q}^{-}=\begin{bmatrix}a_0^- & a_1^- & a_2^- & \cdots\\ 0 & a_0^- & a_1^- & \cdots\\ 0 & 0 & a_0^- & \cdots\\ \vdots & \ddots & \ddots & \ddots\end{bmatrix}\ , \tag{43}$$

$$\underline{\Lambda}=\begin{bmatrix}0 & 0 & 0 & \cdots\\ 0 & -1 & 0 & \ddots\\ 0 & 0 & -2 & \ddots\\ \vdots & \ddots & \ddots & \ddots\end{bmatrix}\ , \tag{44}$$

the solution to Eq. (30) is

$$\mathbf{n}(t)=\underline{Q}^{+}\exp(\underline{\Lambda}t)\underline{Q}^{-} \tag{45}$$

$$=\tau^4 g_-(\tau)g_+[\tau\exp(-t)]\begin{bmatrix}1\\ \tau\exp-t\\ \tau^2\exp-2t\\ \vdots\end{bmatrix}\ . \tag{46}$$

Thus, the dominant decay of n_s at long time goes like $\exp[-(s-2)t]$. The cluster densities from this formula are plotted in Fig. 10. The one-cluster density is obtained from integration of (27). Notice that all cluster densities except n_1 and n_2 decay to zero. Also plotted in Fig. 10 are Monte Carlo simulation results for a spin-exchange Ising model with the ratio τ_1/τ_2 of the time scale τ_1 of D processes to the time scale τ_2 of C/E processes equal to 0, 0.1, and 1. The last case corresponds to the conventional Kawasaki dynamics. The simulations were averaged over 1000 initial configurations, and all flip probabilities were renormalized by a factor of 0.01 so as to ensure accurate simulation of the master equation. We estimate the size of the error bars due to statistical fluctuations to be smaller than the thickness of bold lines in the diagram as drawn.

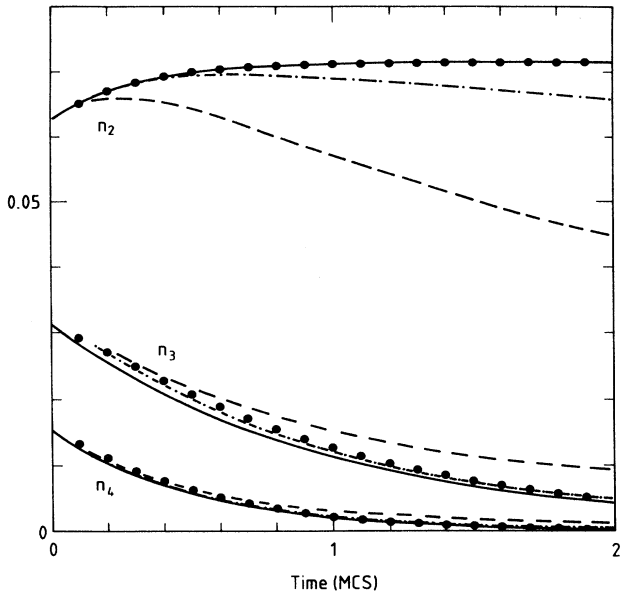

FIG. 10. Cluster densities n_1, n_2, n_3 after a deep quench to zero temperature. The solid curve is the exact solution in the absence of spin diffusion, and the points are a Monte Carlo simulation of this situation. The dashed and dot-dashed curves are simulations of spin-exchange dynamics with spin diffusion inhibited by factors 1 and 0.1 in comparison to the Kawasaki transition rates.

The curves follow the results of (46) for times up to 1 MCS or so. The two-cluster density then decays. This decay consists initially of collisions between spins, and also spins coalescing with stationary domain walls (one-clusters). The fraction of single spins which decay by the first process is shown by the simulation to be close to the fraction which decay by the latter mechanisms.

The decay of the spin (two-cluster) density is a complex problem because it involves nonlinear terms and depends sensitively upon the spatial structure. At long times, the two-cluster density is small, and the dominant relaxation is from single spins coalescing with domain walls. Under these conditions, the decay is dominated by free spins originally in long domains. This is the topic of the next section.

B. Late-time relaxation after cooling to absolute zero

At very late times after a quench to absolute zero, most of the free single spins will have diffused to the domain walls and coalesced. The only remaining spins will be those originally in long domains, which therefore had a much smaller probability of decay. Thus, the long-time behavior is dominated by the probability distribution of long domains, which, in turn, depends upon the temperature at which the system was last in thermal equilibrium, as the quench can only have affected the correlation func-

tion over a finite distance. The long-time behavior is dependent upon the initial equilibrium state only, and not on the type of cooling, so the results will also be valid for the continuous cooling considered in Sec. II.

Consider a single spin in a domain of otherwise parallel spins of length L, starting at site k. Since the long-time behavior is sharply dependent upon L, we consider only domains with single spins in them; ones with more than one will tend to have decayed earlier. The equation of motion of the probability $p_l(t)$ of being at site l at time t is

$$\frac{dp_l}{dt} = -2p_l + p_{l-1} + p_{l+1} , \tag{47}$$

$$p_0 = p_L = 0 , \tag{48}$$

which has solution

$$p_l(t) = \frac{2}{L}\sum_{m=1}^{L-1} \sin\left[\frac{ml\pi}{L}\right] \sin\left[\frac{km\pi}{L}\right] \times \exp\left[-2\left[1-\cos\frac{m\pi}{L}\right]t\right] . \tag{49}$$

In thermal equilibrium, the probability of the spin being at k is independent of k, and the effects of the quench will be to affect the distribution near the edges of the domain only. Summing over k and l, we find that the probability of a spin remaining in the domain after time t is

$$\rho_L = \frac{2}{L^2}\sum_{m=\text{odd}} \cot^2\left[\frac{m\pi}{L}\right] \times \exp\left[-2\left[1-\cos\frac{m\pi}{L}\right]t\right] . \tag{50}$$

The number of domains of size L containing one spin at thermal equilibrium is just proportional to L. Thus, since the density of domains of size L is proportional to $\exp(-L/\xi)$, the total single-spin density as $t \to \infty$ is

$$n_2(t) \propto \sum_L \exp(-L/\xi) L \rho_L . \tag{51}$$

From Eq. (50), we see that the most dominant contribution to n_2 comes from a value of $L \ll t^{1/2}$. The argument of the exponential in (50) can be Taylor expanded, since the only significant contributions are from low harmonics satisfying $m \ll L$. Then

$$n_2(t) \propto \sum_{m,L} \exp\left[-\frac{L}{\xi} - \frac{m^2\pi^2 t}{L^2}\right] . \tag{52}$$

The number of L terms which contribute to n_2 will be large, so the sum over L may be replaced by an integral, which may be evaluated by a saddle-point approximation. For $t \gg \xi^2$, the only important term is $m = 1$, yielding

$$n_2(t) \propto \exp\left[-3\left[\frac{\pi^2 t}{2\xi^2}\right]^{1/3}\right] . \tag{53}$$

The density of single spins therefore decays with a Kohlrausch form. Such behavior usually occurs in systems with frustration and/or randomness, such as spin glasses or the random-field Ising model. This is a very unusual example of such stretched-exponential decay in a system without frustration or any disorder implied by the Hamiltonian; there is, however, "quenched" disorder in the form of the distribution of domain sizes.

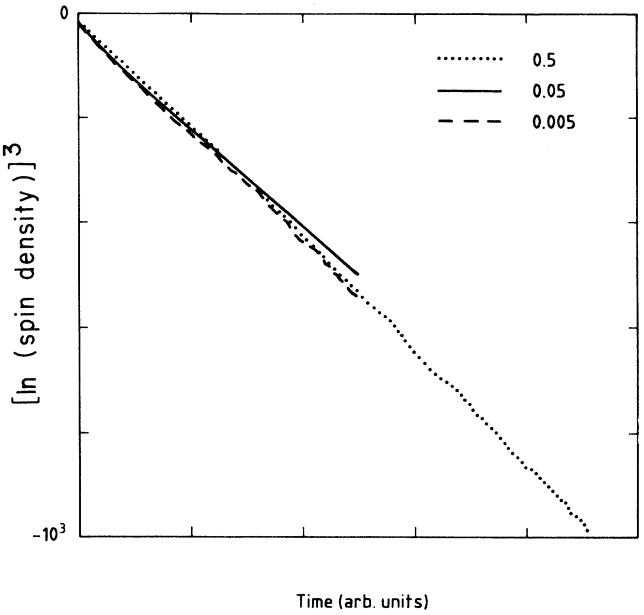

FIG. 11. Plot of [ln(spin density)] as a function of time for simulations at zero temperature after an infinite quench, for different values of the ratio τ_1/τ_2 of time scales for spin diffusion and condensation.

Figure 11 shows a plot of [ln(single-spin density)]^3 versus time for a Kawasaki chain after an instantaneous quench from $T = \infty$ to 0. The three different curves correspond to spin-diffusion rates reduced relative to Kawasaki dynamics by a factor of 0.01, 0.1, and 1 respectively. The validity of the straight-line fit shows that the "absorbing-wall" assumptions used above do indeed predict the correct scaling behavior. The straight-line fit is very striking; a slight deviation points to a small time-dependent prefactor to Eq. (53). The statistics on the simulation are very good as the results are averaged over 1000 independent runs.

It must be stressed that the Kohlrausch form (53) is quite general for a one-dimensional Kawasaki system at $T = 0$, at times when the spin density is small. It will, in general, be difficult to detect in simulations, however, by virtue of the very small amplitude involved; we have been able to do so by virtue of very high run-time statistics.

VI. CONCLUSIONS

In this paper, we have studied the Kawasaki chain under both slow and instantaneously rapid cooling to absolute zero temperature. Under rapid cooling, we observe the same domain scaling as observed in higher dimen-

sions, with the scaling exponent $\frac{1}{3}$. Just as for the spin-exchange case, the exponent is the same as in higher dimensions. This happens even though there is no finite-temperature critical point through which to quench, and the physical origins are different. For the one-dimensional spin-exchange model, our spin motion arguments surplant those of Lifshitz and Slyozov in higher dimension. Our simple physical pictures are insufficient to reproduce the full correlation function. The presence of an energy barrier leads to temperature being a dangerously irrelevant variable, and, as discussed elsewhere,[23] the full scaling theory is expected to be more subtle than in other activated systems.

After completion of this work, we discovered that Layvraz and Jan[24] had discussed the domain scaling in this system. They used arguments similar to those presented in this paper to predict the domain-scaling behavior when the domain size is much smaller than the equilibrium correlation length, although they were, in fact, interested specifically in the dynamic critical behavior. They also reported simulations, obtaining a scaling exponent $1/(3.05\pm0.1)$. However, they did not discuss the competing processes that must be present when the system is close to equilibrium, nor did their simulations verify the full scaling form for the correlation function.

Under slow cooling, arguments based on spin motion predict that the kink density scales with cooling time like $K \propto \tau^{-1/z}$, where $z=5$ is the dynamic critical exponent. This relationship is similar to that which had previously been obtained for the one-dimensional Glauber model,[20] with the appropriate (different) value for z. The simulations are consistent with a slow approach to this law, with corrections smaller by a factor $O(K)$. To obtain results well into the asymptotic region requires impractically high run times, so this method is a very inefficient way of measuring the critical exponent.

The success of the spin-motion arguments in describing the scaling behavior under domain growth, as well as the apparent agreement with freezing behavior, suggests that they are indeed valid descriptions of the Kawasaki chain. This should motivate further investigation into the disputed critical exponent for the alternating bond Kawasaki chain.[19,14,15]

Under an instantaneous quench to absolute zero, the transient behavior due to an unstable decay of clusters of kinks has been studied exactly in the limit that the time scale for spin diffusion is much longer than that for condensation. Simulations of different values of the ratio of these two time scales show that the exact solution is valid for these for only about one time step, but the final structure is only weakly dependent on this ratio.

In contrast to activated Glauber models,[20] the Kawasaki chain has nontrivial temporal behavior at zero temperature, since single spins may move unhindered. The exponential distribution of domain sizes for large distances gives rise to a Kohlrausch form for the relaxation function. This form will describe the residual decay of the system independently of the details of the cooling program.

It is important to note that this behavior is a property of the far-from-equilibrium state only, since at any finite temperature the long-time behavior will be dominated by thermally activated processes at the domain walls. It would be possible to observe the Kohlrausch form as a response function to some impulse whose effect is to inject a small number of spins randomly into the system (e.g., if the system is, say, a gas adsorbed on a substrate, then exposing the system briefly to the vapor will allow spins to be introduced evenly over the lattice).

The frozen Kawasaki chain therefore displays some of the features of a glass. The system freezes into a random domain structure, stabilized by an energy barrier, which is not describable as an equilibrium state at some effective temperature. Kohlrausch forms obtain for relaxation functions, which are specific to the frozen state (in contrast to the artificial kinetic Ising models of Palmer *et al.*[25] and Frederickson and Anderson[26]). However, all relaxation times are of Arrhenius form, in contrast to behavior in true glasses; we would expect that frustration (e.g., from competing further-neighbor interactions) and/or higher dimensions would be required for such behavior to occur.

We have characterized the system before, during, and after cooling by one or two parameters, but it would be desirable to describe the system more fully, e.g., by the full correlation function. However, it is unlikely that this may be obtained analytically to any good approximation because of the mathematical difficulties in treating this system.

The Kawasaki model in two or higher dimensions is a still more complex problem. As mentioned before, Sadiq and Binder[22] considered this system very briefly. This system will clearly freeze as zero temperature is approached, and the long-time behavior will again be dominated by remnant single spins in large domains. Simple arguments analogous to those used in this paper suggest that a Kohlrausch form would be observed for long-time relaxation at zero temperature even in dimensions greater than one, although it is often the case that stretched exponential forms observed in one dimension do not appear in three.[27] This question is currently under investigation, as are other questions relating to freezing in the Kawasaki model in dimension greater than one.

ACKNOWLEDGMENTS

S.J.C. acknowledges partial support from SERC for the duration of this work. We would like to thank Stardent U.K. and Oxford Molecular for access to their computer facilities.

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