Coarsening in a driven Ising chain with conserved dynamics

V. Spirin, P. L. Krapivsky, and S. Redner
Center for BioDynamics, Center for Polymer Studies, and Department of Physics, Boston University, Boston, Massachusetts 02215
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We study the low-temperature coarsening of an Ising chain subject to spin-exchange dynamics and a small driving force. This dynamical system reduces to a domain diffusion process, in which entire domains undergo nearest-neighbor hopping, except for the shortest domains—dimers—which undergo long-range hopping. This system exhibits anomalous ordering dynamics due to the existence of *two* characteristic length scales: the average domain length $L(t) \sim t^{1/2}$ and the average dimer hopping distance $\ell(t) \sim \sqrt{L(t)} \sim t^{1/4}$. As a consequence of these two scales, the density of short domains decays as $t^{-5/4}$, instead of the $t^{-3/2}$ decay that would arise from pure domain diffusion. [S1063-651X(99)08109-X]

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I. INTRODUCTION

The approach to equilibrium in isotropic systems, which are quenched from a high-temperature homogeneous phase to a low-temperature two-phase region, is now relatively well understood [1,2]. The basic feature of such systems is that they typically organize into a coarsening mosaic of single-phase regions, with a characteristic length scale that grows as a power law in time. For driven systems, on the other hand, considerably less progress has been made in understanding the coarsening dynamics, although the stationary properties have been thoroughly investigated [3]. In the presence of driving, the physically relevant coarsening mechanisms are those with conserved order-parameter dynamics. This would be appropriate, for example, for treating the phase separation of binary liquids or binary alloys under the influence of gravity [4].

In this spirit, Cornell and Bray [5] recently studied the coarsening dynamics of a driven Ising (DI) chain that is endowed with conserved spin-exchange Kawasaki dynamics and which is also subjected to a driving field which favors transport of up spins to the right and down spins to the left. They argue that in the limit of low temperature and weak field, the spin dynamics of this DI chain reduces to a domain diffusion (DD) process [5] in which up domains hop rigidly by one lattice spacing to the right, and down domains hop by one lattice spacing to the left. Due to this nearest-neighbor hopping, small domains are progressively ''squeezed out'' and the adjacent neighboring domains coalesce. This random-walk mechanism leads both to a reduction in the number of domains and an increase in their average length, $L(t) \sim t^{1/2}$. Numerical evidence was also presented that the density of domains of length k obeys the scaling form $C_k(t) \sim (k/L^3)\exp(-k^2/L^2)$ [5]. This further implies a $t^{-3/2}$ asymptotic decay for the density of domains of fixed length.

The goal of this paper is to show that there is a subtle but crucial difference between the dynamics of individual spins in this DI chain and the DD process. The fundamental point is that for the shortest domains—dimers—the spin-level DI chain dynamics results in *long-range* dimer hopping, with their average jump length growing as $\sqrt{L}$. In contrast, for the DD process, dimers necessarily jump to the next domain boundary. As a result, dimers, and indeed all domains of length $\leqslant \sqrt{L}$, disappear more rapidly in the DD process than in the DI chain.

As we shall argue, the DI chain is thus characterized by two length scales: (a) the average domain length $L(t)$, which is still proportional to $t^{1/2}$, as in the DD process, and (b) the average dimer hopping distance, which is proportional to $t^{1/4}$. As a result of the two length scales, the density of domains of fixed length asymptotically decays as $t^{-5/4}$, instead of the $t^{-3/2}$ decay of the DD process. Correspondingly, the domain length distributions in the DI chain and in the DD model exhibit different small-length behaviors.

In Sec. II, we define the spin dynamics precisely, describe the correspondence between the DI chain and the DD process, and address their essential differences. Simulation results, which support our basic arguments, are presented in Sec. III. In Sec. IV, we outline a perturbative approach, based on a matched asymptotic expansion, which accounts for the observed breakdown of scaling in the domain length distribution for a vanishingly small minority fraction. Section V contains both a summary and a brief discussion of open issues.

II. GEOMETRICAL PICTURE OF THE DYNAMICS

The microscopic system is a chain of Ising spins with nearest-neighbor ferromagnetic interaction J. The chain is subject to spin-exchange dynamics, where the only possible rearrangement process is the exchange of two antiparallel nearest-neighbor spins. Thus the magnetization is manifestly conserved (we use a magnetic terminology, although a system with conserved dynamics naturally applies to an alloy). The exchange occurs at a rate proportional to $e^{-\Delta/T}$, where Δ is the energy difference between the initial and final states, and T is the temperature (with Boltzmann constant set to unity). There is also a driving field E, which favors motion of up spins to the right and down spins to the left. The spin-flip events are

$$\begin{aligned}
&\text{(i)} && ++--\rightleftharpoons +-+- && \Delta = 4J - E,\\
&\text{(ii)} && --++\rightleftharpoons -+-+ && \Delta = 4J + E,\\
&\text{(iii)} && ++-+\rightleftharpoons +-++ && \Delta = -E,\\
&\text{(iv)} && -+--\rightleftharpoons --+- && \Delta = -E.
\end{aligned}$$

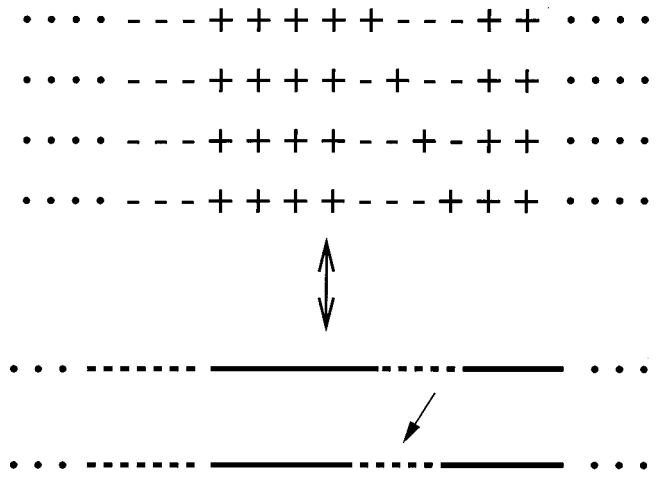

FIG. 1. Illustration of the detachment of an up spin from an up domain and its merging with the neighboring up domain to the right. In the upper part of the figure, each line represents the state of the system after a single spin-exchange event. This evolution is equivalent to rigid-body domain hopping, with a down domain hopping one lattice site to the left, as indicated in the lower portion.

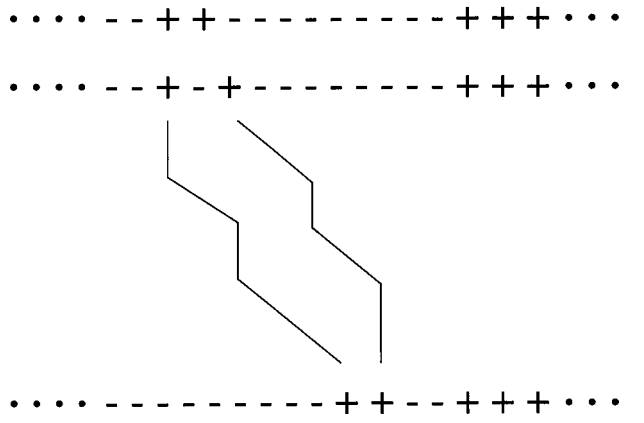

FIG. 2. Time evolution of an up dimer in a sea of down spins. When the dimer dissociates, the isolated spins independently hop to the right. Shown is the space-time trajectory of the dimer for the case where the dimer recombines and becomes stationary again before the next domain wall is reached.

The first two processes occur on domain boundaries, while the last two account for the motion of a single spin, which is inside a domain of the opposite sign. The ''forward'' processes involve the energy change Δ, while the ''backward'' processes have energy change $-\Delta$.

Interesting dynamics arises in the limit of low (but nonzero) temperature and weak driving field, that is, $0<T\ll E\ll J$. To appreciate the nature of the dynamics for this parameter range, notice that in one dimension the order-disorder transition occurs at $T_c=0$. At $T=0$, the spin-exchange dynamics traps the system in a metastable state, which consists of domains of lengths $\geqslant 2$ [6,7]. To avoid this ''freezing,'' the temperature must be nonzero. At low but nonzero temperature, the system will coarsen as long as the mean domain length is smaller than the correlation length $\xi\sim e^{J/T}\gg 1$.

The limit where the driving field satisfies $T\ll E\ll J$ leads to an *approximate* equivalence with the DD process [5]. To understand this correspondence, consider the situation after domains have coarsened to a relatively large length. By process (i$\rightharpoonup$), an up spin may detach from the right edge of an up domain with rate $e^{-(4J-E)/T}$, or equivalently, a down spin may detach from the left edge of a down domain. Similarly, an up spin may also detach from the left edge of an up domain (or a down spin may detach from the right edge of a down domain) by step (ii$\rightharpoonup$). However, this process occurs at a rate which is a factor $e^{-2E/T}$ smaller than step (i$\rightharpoonup$). Moreover, even if step (ii$\rightharpoonup$) occurs, the detached spin quickly recombines with the same domain by the reverse process (ii$\leftharpoondown$), since the motion of the detached spin away from the domain is energetically unfavorable.

Once step (i$\rightharpoonup$) occurs, the system evolves further either by step (iv$\rightharpoonup$), which corresponds to the up spin moving to the right and eventually joining the next up domain, or by step (iii$\rightharpoonup$), where a down spin moves to the left and joins the next down domain. The former process is illustrated in Fig. 1. As a result of these processes, an up domain hops rigidly by one lattice spacing to the right or a down domain hops one spacing to the left. If we measure the time in units of $e^{(4J-E)/T}$, then both these hopping steps occur at unit rate, *independent* of the domain length.

An essential feature of the low-temperature weak-field limit $T\ll E\ll J$ is that all other processes are asymptotically negligible in the intermediate-time range where coarsening is occurring. Thus in this time range the system consists of the contiguous array of alternating up and down domains, and the dynamics proceeds by taking an up (down) domain and moving it one lattice site to the right (left). Whenever a domain shrinks to zero size, its two adjacent neighbors coalesce. This description is the basis of the correspondence to the DD model. It is also worth noting that in the absence of a driving field, the dynamics again reduces to a DD process, but with a length-dependent hopping rate that is proportional to the inverse domain length [7,8].

A crucial feature of the mapping between the spin and the domain dynamics, which is not apparent from the above description, is the evolution of dimers (see Fig. 2). Consider an up dimer. If the rightmost spin of the dimer detaches, the dimer is converted into two isolated up spins in a sea of down spins. According to the spin dynamics, each isolated spin independently and freely hops to the right. Consequently, their separation undergoes a simple random walk. The motion of spins antiparallel to the field can be neglected, since this motion is inhibited by a factor $e^{-2E/T}$. The hopping of this pair of separated spins terminates in one of two ways: (i) The rightmost up spin reaches the next domain boundary and subsequently the other up spin hits this same boundary. This corresponds to the coalescence of the two adjacent down domains and is part of the DD picture. (ii) The dimer recombines *before* the next domain boundary is reached (Fig. 2).

Dimer recombination is the crucial new feature which was not included in the DD process. This recombination plays an essential asymptotic role because the average dimer jump distance ℓ is much smaller than the average domain length L in the long-time limit. Consequently, recombination of a dimer is much more probable than domain coalescence. To verify this assertion let us estimate ℓ. The dimer recombines if the separation between the two spins shrinks to zero before

the rightmost spin reaches the next domain boundary. This is a classic first-passage process, and the probability that this separation first equals zero at $2l$ steps is given by [9]

$$\mathcal{P}(l)=\frac{1}{2^{2l-1}}\frac{(2l-2)!}{(l-1)!l!}. \tag{1}$$

For large l, this expression simplifies to $\mathcal{P}(l)\sim\pi^{-1/2}l^{-3/2}$. The average dimer jump distance ℓ may now be estimated as $\ell=\Sigma_{l\leq L}l\mathcal{P}(l)\sim\sqrt{L}$. Thus asymptotically $\ell\ll L$.

We now use this picture to estimate the overall time dependence of small-length domains. The crucial feature is that a domain can disappear only if a dimer first dissociates and then does not recombine before its constituent spins reach the next domain boundary. From the analogy with the first-passage process, the probability $R(t)$ that the dissociated dimer does not recombine before the next domain boundary is given by

$$R\sim\sum_{l=L}^{\infty}\mathcal{P}(l)\sim\sum_{l=L}^{\infty}l^{-3/2}\sim L^{-1/2}. \tag{2}$$

Since the disappearance of a dimer leads to domain coalescence, the total number of domains $N(t)$ obeys the rate equation

$$\frac{dN}{dt}=-RC_2\sim-\frac{C_2}{\sqrt{L}}. \tag{3}$$

On the other hand, the dynamics of large domains should still be governed by the gain and loss of single spins at the boundary, as outlined in Fig. 1. Since these gain and loss processes occur at the same rate, the domain length undergoes an isotropic random walk, so that $L(t)$ should grow as $t^{1/2}$. Correspondingly, the number of domains $N(t)$ decays as $t^{-1/2}$, the inverse of the average domain length. Substituting these two expectations into Eq. (3), we immediately obtain

$$C_2(t)\sim t^{-5/4}. \tag{4}$$

This should be compared with the prediction $C_2(t)\sim t^{-3/2}$, which arises from the DD process. This latter time dependence would be obtained from Eq. (3) if the rate of dimer disappearance were unity, rather than proportional to $L^{-1/2}$.

This slower decay of dimers is one of the primary features of the DI chain dynamics and it has fundamental implications for the density of domains of length k, $C_k(t)$. Let us suppose that this density obeys the single-length scaling hypothesis

$$C_k(t)\sim\frac{1}{L^2}F\left(\frac{k}{L}\right), \tag{5}$$

where the prefactor L^{-2} follows from the length normalization condition $\Sigma kC_k(t)=1$. If $C_2(t)\sim t^{-5/4}$, then either $F(z)\sim\sqrt{z}$ as $z\to 0$, or $C_k(t)$ does not obey scaling for small k. We shall present evidence from both simulations and an analytical approach that strongly favors the latter alternative.

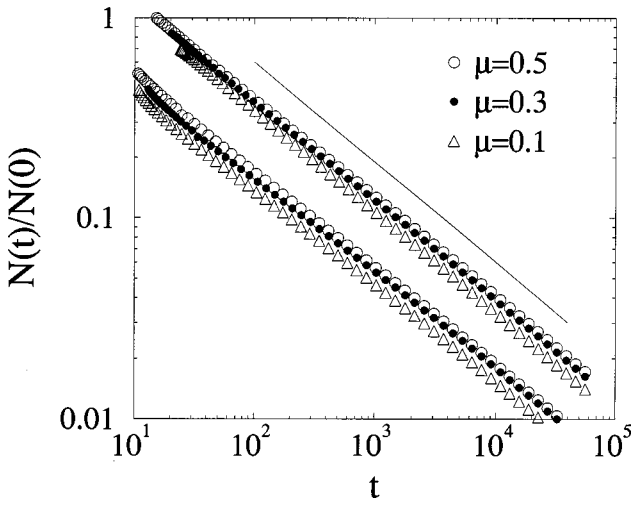

FIG. 3. Time dependence of the domain density for various minority spin fractions μ. Upper set of points, DI chain; lower set, DD model. The DD data are divided by 2 to separate the two sets. As a guide to the eye, the solid line has a slope $-1/2$.

III. SIMULATION RESULTS

In our simulations, we first initialize an array of alternating up and down domains of random lengths. For minority phase density μ, we choose the average length of minority domains to be $L=10$, and L/μ for the majority phase. The time evolution involves the following steps: (i) Pick a domain at random. (ii) Move an up (down) domain of length >2 to the right (left). (iii) If the domain is a dimer, choose its jump distance l from the probability distribution $\mathcal{P}(l)$ given by Eq. (1). If l exceeds the length of the neighboring domain, remove the dimer and merge the surrounding domains. (iv) Update the time by 1/(number of domains). Simulations were performed on a chain of 4×10^6 domains for times up to 5×10^5, and averaged over 16 samples. This is of the same order of data as the simulations of Cornell and Bray [5].

A. Average time-dependent properties

In Fig. 3, we plot $N(t)$ for various minority fractions μ.

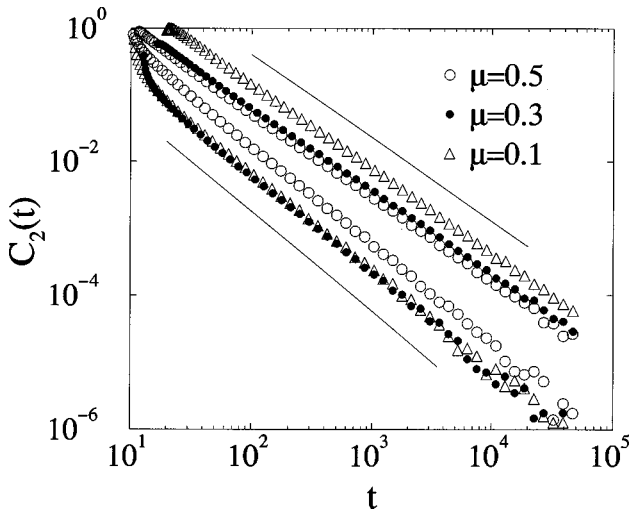

FIG. 4. The density of dimers as a function of time. Upper points, DI chain; lower points, DD model. As a guide to the eye, the solid lines have slopes $-5/4$ (upper) and $-3/2$ (lower).

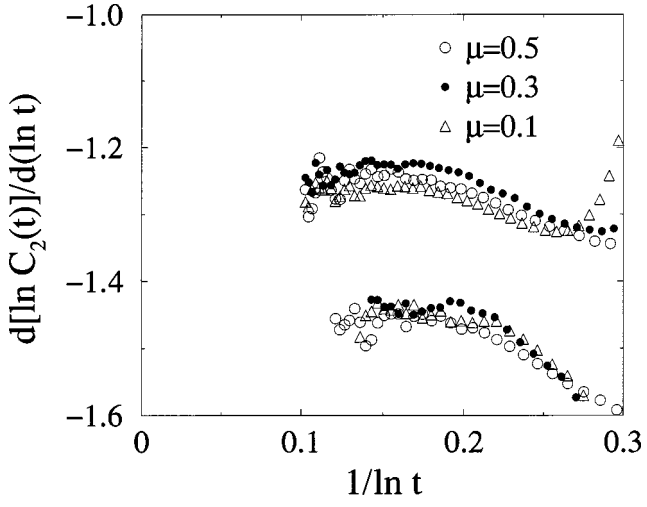

FIG. 5. Local exponents for the time dependence of the number of dimers. Upper points, DI chain; lower points, DD model.

Also shown are the corresponding results for the DD process. The linearity of the data suggests power-law behavior, and visually the asymptotic slopes are very close to the expected value of $-1/2$. The essential difference between the DI chain and the DD model is manifested by the behavior of the dimer density. Figure 4 shows that the dimer density indeed decays more slowly than in the DD model.

To highlight this difference, we plot the corresponding local exponents in Fig. 5. We define the local exponent at time t as the best-fit straight line to ten successive data points (equally spaced on a logarithmic scale) up to time t in the double logarithmic plot of $C_2(t)$ versus t. This definition significantly smooths statistical fluctuations while still revealing systematic trends in the data. As shown in Fig. 5, the local exponents of the DI chain and the DD model are clearly different. For the DD model, these exponents are close to the expected value $-3/2$ and also exhibit weak systematic time dependence. Thus, the natural conclusion is that the dimer density (as well as the density of domains of any fixed length) asymptotically decays as $t^{-3/2}$.

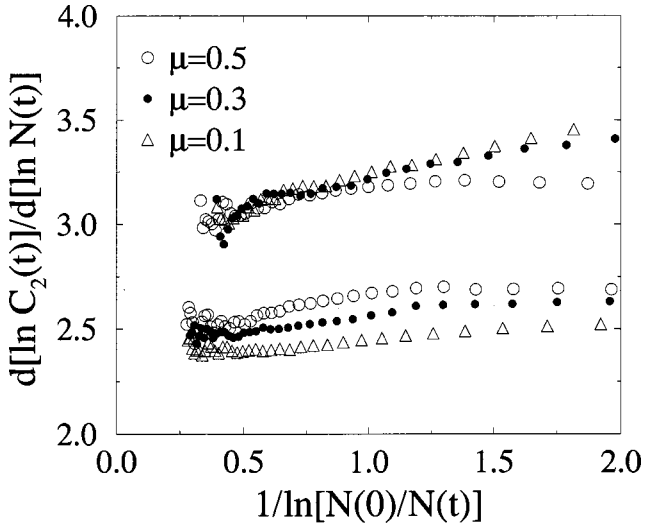

FIG. 6. Local exponents for the dependence of the number of dimers on the total number of domains. Lower points, DI chain; upper points, DD model.

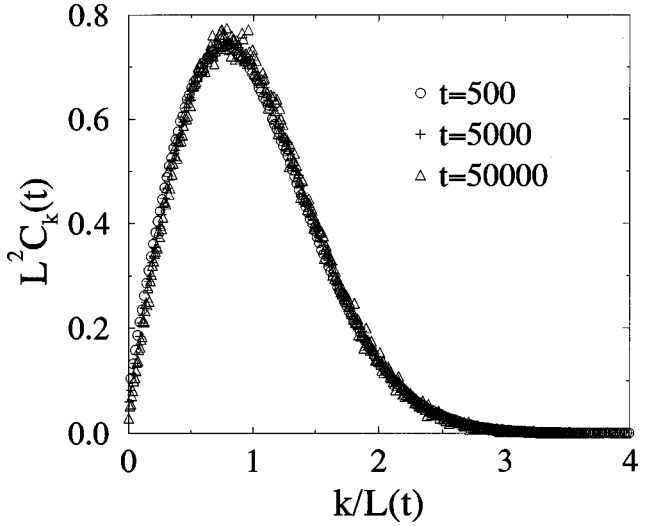

FIG. 7. Scaling plot for the domain length distribution for the DI chain with equal fractions of up and down spins. Notice that this distribution does not reach zero at $k/L=0$ (see Fig. 8).

For the DI chain, the situation is more subtle. The local exponents initially are increasing with time, but this time dependence slows when the effective exponent value is close to the anticipated value $-5/4$. However, the systematic ambiguities in the data make an extrapolation for the asymptotic value of the exponent uncertain. This uncertainty and the relatively small difference in the dimer exponent for the two models led us to consider $C_2(N)$ rather than $C_2(t)$. Indeed, since both $N(t)$ and $C_2(t)$ should be influenced by the same preasymptotic corrections, such corrections might cancel when C_2 is expressed as a function of N. From a scaling perspective, it is also natural to express dependences in terms

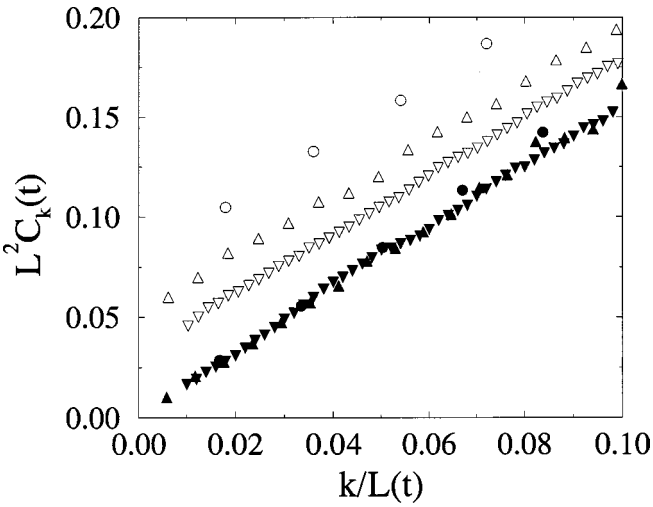

FIG. 8. Tail of the domain length distribution for the DI chain (open symbols) for equal fractions of up and down spins. Shown are data for $t=500(\bigcirc)$, $t=5000(\nabla)$, and $t=50\,000(\Delta)$. Notice the systematic time dependence with a nonzero intercept at $k=0$. For comparison the tail of the domain length distribution for the DD process at the same times is also shown (filled symbols). Data for $t=50\,000$ were smoothed over a 9-point range to reduce fluctuations.

of intrinsic variables, rather than in terms of the extrinsic time variable. Thus in Fig. 6, we plot the local exponents of $C_2(N)$ versus N and the results are now relatively straightforward to interpret. Since the variation in the local exponent for the DI chain is small over the entire range of N, the result $C_2(N)\sim N^{5/2}$ is strongly suggested. Similarly, the DD data suggests that $C_2(N)\sim N^3$, as is anticipated from $N(t)\sim t^{-1/2}$ and $C_2(t)\sim t^{-3/2}$. Coupled with the basic result $N(t)\sim t^{-1/2}$ that holds for both models, we conclude, now with considerable confidence, that $C_2(t)\sim t^{-5/4}$ for the DI chain.

B. Domain length distribution

The behavior of the domain length distribution is especially interesting in the small-length limit. This ultimately arises from the multistep dissociation and recombination processes that govern the disappearance of dimers. We first test the conventional scaling hypothesis for the domain length distribution, namely, $C_k(t)\sim L^{-2}F(k/L)$, by plotting $L^2C_k(t)$ versus k/L in Fig. 7.

At the scale shown, this distribution appears to exhibit data collapse. In fact, at the resolution of this figure, the domain length distributions for the DI chain and for the DD process are virtually indistinguishable. However, for the scaling form to be compatible with $C_2(t)\sim t^{-5/4}$, the scaling function must vary as $F(z)\sim z^{1/2}$ as $z\to 0$, while the length distribution appears to be linear in k in the small-length limit. This linearity implies that the distribution cannot obey single-parameter scaling for all lengths. In fact, a closer examination of the small-k tail (Fig. 8) reveals a small but systematic deviation from data collapse. This deviation is manifested by the length distribution having a nonzero intercept with the $k=0$ axis, whose value is systematically decreasing with time.

IV. DOMAIN LENGTH DISTRIBUTION IN THE LIMIT $\mu\to 0$

To better understand the nature of the domain length distribution, we focus on the limit where the fraction of minority spins μ is vanishingly small. This leads to considerable simplification in the domain dynamics. Generally, the length of a domain can change by ± 1 due to diffusion of neighboring domains, or the length can change arbitrarily by domain coalescence. In the limit $\mu\to 0$, the diffusive ''shrinkage'' governs the disappearance of minority domains, while coalescence governs the disappearance majority domains. To verify this, let us estimate the characteristic times for the disappearance of the majority and minority domains by shrinkage. Let $L_-(L_+)$ denote the average length of minority (majority) domains. A majority domain can shrink to zero in a time t_+ of order L_+^2, while the shrinking and disappearance of a minority domain requires a time $t_-\sim L_-^2$. Thus

$$\frac{t_-}{t_+}\sim\left(\frac{L_-}{L_+}\right)^2=\mu^2. \tag{6}$$

Therefore in the minority limit, shrinkage of majority domains, or equivalently, coalescence of minority domains is negligible. Consequently, the minority domains are effectively noninteracting and they evolve only by the addition or loss of single spins as a result of the hopping of majority domains. Therefore, the density of minority domains $C_k(t)$ obeys the discrete diffusion equation

$$\frac{dC_k}{dt}=C_{k+1}-2C_k+C_{k-1},\quad k>2 \tag{7}$$

The density of dimers ($k=2$) obeys a separate, but similar equation. For dimers, there is no gain term due to processes that involve monomers, and the loss of dimers due to their dissociation into two monomers and ultimate domain coalescence occurs at a rate $R\sim L^{-1/2}$ (see Sec. II), since a dissociated dimer may recombine before the coalescence occurs. Therefore, the master equation for $C_2(t)$ is

$$\frac{dC_2}{dt}=C_3-C_2-\frac{C_2}{\sqrt{L}}. \tag{8}$$

In the continuum limit, Eq. (7) is equivalent to

$$\frac{\partial C_k(t)}{\partial t}=\frac{\partial^2 C_k(t)}{\partial k^2}, \tag{9}$$

while Eq. (8) provides the boundary condition. In this equation, the left-hand side scales as $t^{-1}C_2$, while the last term on the right-hand side scales as $L^{-1/2}C_2\sim t^{-1/4}C_2$. Thus in the long-time limit the left-hand side is negligible and Eq. (8) becomes

$$\left[\frac{\partial C_k(t)}{\partial k}-\frac{C_k(t)}{\sqrt{L}}\right]_{k\to 0}=0. \tag{10}$$

This radiation boundary condition [10] expresses the fact that a dimer does not necessarily disappear when it dissociates, but it may be reconstituted and then grow into a finite-size domain.

By dimensional analysis, Eq. (9) implies the existence of the usual diffusive length scale $L=\sqrt{t}$. By similar reasoning, Eq. (10) suggests the existence of an additional length scale $\ell=\sqrt{L}$. The competition between these two scales determines the asymptotic behavior. We therefore separately consider the ''inner'' region of small domains $k\ll L$ and the ''outer'' region of large domains $k\gg\ell$, and then match these limiting solutions in the overlap region $\ell\ll k\ll L$ [11].

In the inner region $k\ll L$, the diffusion equation simplifies to $\partial^2 C/\partial k^2=0$, whose solution is $C_k(t)=A(t)+B(t)k$. Employing the boundary condition Eq. (10) we obtain

$$C_k(t)^{\text{inner}}=A(t)\left(1+\frac{k}{\sqrt{L}}\right). \tag{11}$$

In the outer region $k\gg\ell$, the system is governed by the original diffusion equation (9), while Eq. (10) reduces to the absorbing boundary condition. The solution in this region thus becomes

$$C_k(t)^{\text{outer}}=\frac{k}{t^{3/2}}\exp\left(-\frac{k^2}{4t}\right). \tag{12}$$

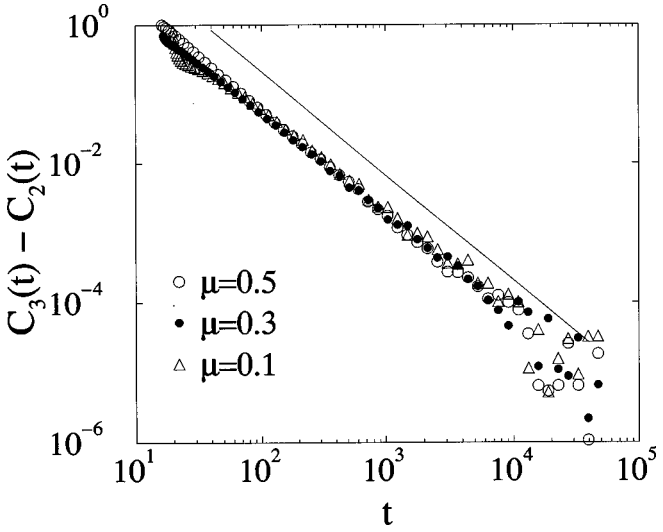

FIG. 9. Plot of $C_3(t)-C_2(t)$ versus time. As a guide to the eye, a straight line of slope $-3/2$ is shown.

The inner and outer solutions should match in the overlapping region $\ell \ll k \ll L$. This determines the amplitude $A(t)$ in Eq. (11) to be proportional to $t^{-5/4}$. The inner solution now becomes

$$C_k(t)^{\text{inner}} = \frac{\gamma}{t^{5/4}} + \frac{k}{t^{3/2}} \tag{13}$$

with γ a constant.

These two limiting forms for $C_k(t)$ match smoothly in the overlap region $\ell \ll k \ll L$. This further suggests that the domain length distribution for the entire length range can be accounted for by the composite form

$$C_k(t) = \left(\frac{\gamma}{t^{5/4}} + \frac{k}{t^{3/2}} \right) \exp\left(-\frac{k^2}{4t} \right). \tag{14}$$

To determine the validity of this hypotheses, we test for the existence of the $k/t^{3/2}$ correction term, since the leading $t^{-5/4}$ time dependence has already been established. For this purpose, consider $C_3(t)-C_2(t)$ versus t. This difference eliminates the leading $t^{-5/4}$ behavior and thus isolates the $k/t^{3/2}$ correction term (Fig. 9). As seen in the figure, the data for C_3-C_2 is consistent with a $t^{-3/2}$ time dependence. This test also supports the correctness of the composite form of Eq. (14) for the domain length distribution. Finally, our numerical data suggests that this same dependence holds for all values of μ.

V. SUMMARY AND DISCUSSION

We investigated the low-temperature coarsening of an Ising chain subject to spin-exchange dynamics and a weak driving force. The spin dynamics of this DI chain was reduced to a domain diffusion process together with long-range dimer hopping. From this picture, we established the existence of *two* growing characteristic length scales; one is the fundamental diffusion length $t^{1/2}$, that provides the average domain size, and the other, $\ell \sim t^{1/4}$, is the average dimer hopping distance. The competition between these two scales leads to an unusual small-length tail of the domain length distribution. As a consequence, the density of fixed-length domains decays as $t^{-5/4}$ as $t \to \infty$. A key step to verify this latter result was to study the dependence of C_k on N, rather than the dependence on t.

For the one-dimensional system, several basic unresolved issues remain. Thus far, an analytical solution for the length distribution of minority domains only has been obtained in the extreme minority limit. It would be worthwhile to study analytically the case of an arbitrary minority fraction. One approach is to treat domains as statistically independent. Such an approximation is exact in the extreme minority limit and also works well for the coarsening of the undriven Ising chain for both spin-flip and spin-exchange dynamics [12–14]. Under the assumption of statistical independence, it is possible to solve the rate equations for $C_k(t)$. This solution reproduces the correct dynamical exponent, as well as the linear small-length tail for the domain length distribution [15]. This approach further predicts an exponential decay for the the large-length limit of the domain length distribution, for any nonzero fraction of minority spins. However, our numerical simulations at zero magnetization suggest that this large-length tail has the leading behavior $\exp(-(k/L)^{\nu})$, with ν greater than 1 and less than 2. This puzzling feature, neither an exponential nor a Gaussian decay for the large-length tail of the distribution, deserves more careful attention.

ACKNOWLEDGMENTS

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