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Deterministic soluble model of coarsening

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We investigate a three-phase deterministic one-dimensional phase ordering model in which interfaces move ballistically and annihilate upon colliding. We determine analytically the autocorrelation function $A(t)$. This is done by computing generalized first-passage-type probabilities $P_n(t)$, which measure the fraction of space crossed by exactly n interfaces during the time interval $(0,t)$, and then expressing the autocorrelation function via P_n's. We further reveal the spatial structure of the system by analyzing the domain size distribution. [S1063-651X(97)08201-9]

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I. INTRODUCTION AND THE MODEL

We examine phase ordering dynamics in a one-dimensional system with three equilibrium states. In our model, interfaces between dissimilar domains undergo ballistic motion and annihilate upon colliding. The process is thus deterministic, although randomness is hidden in the initial conditions. Given an appealing simplicity of the rules governing the dynamics, it is not surprising that this process and its generalizations naturally arise in different contexts ranging from ballistic annihilation [1–5] to growth processes [6–9] and dynamics of interacting populations [10–12]. Different viewpoints on the same model are very useful in that they suggest investigation of several correlation functions, some of them may be clearly interesting from one point of view, while they could hardly be thought of from another point of view. One such correlation function, namely, the autocorrelation function to be determined below, naturally appears in the context of population dynamics [12]; from other viewpoints, e.g., in the original framework of ballistic annihilation [1], it is not clear how to define the autocorrelation function.

We start by describing the two-velocity ballistic annihilation model and recalling its known basic properties [1,4]. The model assumes that interfaces may have two different velocities ± 1 without loss of generality and the densities of both populations of interfaces are equal to each other (otherwise the minority population quickly disappears). The interfaces are initially randomly distributed according to a Poisson distribution. The model exhibits a two-length spatial structure, with length scale $l(t) \sim \sqrt{t}$ describing the average distance between neighboring interfaces moving in the same direction and the length scale $\mathcal{L}(t) \sim t$ describing the typical distance between neighboring interfaces moving in the opposite directions. As we shall see below, however, the growth law for $l(t)$ cannot fully characterize the spatial structure: other natural measures of the spacing between similar neighboring interfaces behave differently, e.g., the rms separation $l_2(t) = \sqrt{\langle x^2 \rangle}$ grows as $t^{3/4}$. We shall argue below that all these length scales can be understood as the outcome of the competition between the length scale $O(1)$ characterizing initial data and the ballistic length scale $\mathcal{L}(t) \sim t$.

On the language of phase ordering dynamics, the two-velocity ballistic annihilation model may be treated as the three-phase, or three-color, process with deterministic nonconservative dynamics. Indeed, imagine that the one-dimensional line is drawn in three colors, say red, green, and blue. Suppose that the interface between red and green domains always moves inside the green one, the interface between green and blue domains moves inside the blue one, and the interface between blue and red domains moves inside the red one. Then the autocorrelation function $A(t)$ is defined as the probability that at a given point and at time t the color is identical to the initial color. In the dynamics of interacting populations, this model mimics a three-species cyclic food chain [12].

The rest of this paper is organized as follows. Generalized first-passage probabilities are determined in Sec. II. Section III contains a calculation of the autocorrelation function. The domain size distribution is analyzed in Sec. IV. Section V provides a summary and an outlook.

II. GENERALIZED FIRST-PASSAGE PROBABILITIES

Our first goal is to compute $P_n(t)$, which measures the fraction of space crossed by exactly n interfaces during the time interval $(0,t)$. Equivalently, $P_n(t)$ is the probability that a point has undergone exactly n changes of color. Clearly, the color of an arbitrary point changes cyclically with period 3, so the autocorrelation function is found from the relation

$$A(t) = \sum_{n=0}^{\infty} P_{3n}(t). \tag{1}$$

To determine $P_n(t)$, it proves convenient to consider an auxiliary one-sided problem with a finite number of interfaces on one side of a target point. Namely, imagine that we have N interfaces to the right of the origin (the target point). What is the probability $Q_n(N)$ that exactly n interfaces will cross the origin? To solve for $Q_n(N)$, we construct the following discrete random walk: Let $S_0 = 0$ and S_i are defined recursively via $S_i = S_{i-1} + v_i, i = 1, \ldots, N$, where $v_i = \pm 1$ is the velocity of the ith interface. Thus we indeed have a random walk (i, S_i) starting from the origin, with i being a timelike variable and S_i a displacement. The crucial point is that the number of interfaces that will cross the origin is given by the absolute value of the minimum of the random walk. Thus we identify $Q_n(N)$ with probability that an

N-step random walk starting at the origin has a minimum at $-n$. This probability is simply found to be [13]

$$Q_n(N)=\widetilde{Q}_n(N)+\widetilde{Q}_{n+1}(N), \tag{2}$$

with

$$\widetilde{Q}_n(N)=\frac{1}{2^N}\frac{N!}{\left(\frac{N+n}{2}\right)!\left(\frac{N-n}{2}\right)!} \tag{3}$$

if n and N have the same parity; otherwise, $\widetilde{Q}_n(N)=0$.

Before returning to the original two-sided problem we consider the one-sided problem with an *infinite* number of interfaces initially placed to the right of the origin at random with density one. During the time interval $(0,t)$ interfaces initially located at distances $x\leqslant t$ could cross the origin. Clearly, the probability $Q_n(t)$ that exactly n interfaces cross the origin up to time t is

$$Q_n(t)=\sum_{N=n}^{\infty} Q_n(N)\frac{t^N e^{-t}}{N!}. \tag{4}$$

Substituting Eqs. (2) and (3) into Eq. (4) yields

$$Q_n(t)=e^{-t}[I_n(t)+I_{n+1}(t)], \tag{5}$$

where I_n denotes the modified Bessel function of order n. If the origin has not been crossed by a right-moving interface up to time t, an interface starting from the origin and moving with $+1$ velocity will survive up to time $t/2$. Thus the surviving probability $S(t)$ of an interface is given by

$$S(t)=Q_0(2t)=e^{-2t}[I_0(2t)+I_1(2t)]. \tag{6}$$

First-passage probabilities $P_n(t)$ corresponding to the two-sided problem are readily expressed via one-sided probabilities $Q_n(t)$ after realizing that in a configuration with n interfaces crossing the origin in the right-sided version and k interfaces crossing the origin in the left-sided version, the total crossing number in the two-sided version is equal to $\max(k,n)$. Thus we arrive at the relationship

$$P_n(t)=2Q_n(t)\sum_{k=0}^{n} Q_k(t)-Q_n(t)^2, \tag{7}$$

with the factor 2 accounting for the fact that a smaller number k of crossing interfaces can come from both the left and right. We have subtracted the last quantity $Q_n(t)^2$, which has been counted twice in the summation. As a useful check of self-consistency we verify that the normalization condition

$$\sum_{n=0}^{\infty} P_n(t)=1 \tag{8}$$

is satisfied. Indeed, Eq. (7) implies $\Sigma P_n=(\Sigma Q_n)^2$, and the latter sum is shown to be equal to one by using Eq. (5) and the identity $I_0(t)+2\Sigma_{j\geqslant 1}I_j(t)=e^t$ [14].

Note that P_n's, and especially the first ''persistence'' probability $P_0(t)$, recently have attracted considerable interest; see, e.g., [15–20]. These quantities can be thought of as first-passage time probabilities in the interacting particle systems [21]. Given the importance of the first-passage-type quantities in the classical probability theory [13], one can envision numerous applications of P_n's in the interacting particle systems. However, apart from a few findings in the framework of a mean-field approach (more precisely, for interacting particle systems on a complete graph) [12,19] and a limiting analytical solution for the one-dimensional voter model [19], no exact results are available. The model we consider here is an exception in that the complete analytical solution for P_n's exists; see Eqs. (5)–(7). In particular, we have $P_0(t)=Q_0^2(t)\simeq 2(\pi t)^{-1}$.

To make the results more transparent, it is useful to express solutions in the scaling limit

$$n\to\infty, \quad t\to\infty \tag{9}$$

for $z=n/\sqrt{2t}$ finite. Making use of the scaling behavior of the modified Bessel functions [14] $I_n(t) \simeq(2\pi t)^{-1/2}\exp(t-n^2/2t)$, we find

$$Q_n(t)\simeq\sqrt{\frac{2}{\pi t}}e^{-z^2} \tag{10}$$

for the one-sided probabilities and

$$P_n(t)\simeq\sqrt{\frac{8}{\pi t}}e^{-z^2}\mathrm{erf}(z) \tag{11}$$

for the two-sided probabilities.

III. AUTOCORRELATION FUNCTION

The scaling expression of Eq. (11) does not allow one to obtain the nontrivial long-time behavior of the autocorrelation function. Indeed, substituting Eq. (11) into Eq. (1) yields $A(t)\simeq 1/3$. We should therefore return to exact relations (5)–(7). We also extract the trivial $A(\infty)=1/3$ factor and consider three autocorrelation functions

$$A_\alpha(t)=\sum_{n=0}^{\infty} P_{3n+\alpha}(t)-\frac{1}{3}, \tag{12}$$

describing three possible color outcomes at time t, the same (say, red) color that initially corresponds to $\alpha=0$, $A_0(t)\equiv A(t)-1/3$; the ''next'' blue color corresponds to $\alpha=1$; finally, the green color corresponds to $\alpha=2$.

All three autocorrelation functions $A_\alpha(t)$ exhibit similar asymptotic behavior; additionally, they are related by the identity $A_0(t)+A_1(t)+A_2(t)\equiv 0$. Combining Eqs. (12) and (8), we obtain

$$\begin{aligned}3A_0(t)&=3\sum_{n=0}^{\infty} P_{3n}(t)-1\\&=\sum_{n=0}^{\infty}[(P_{3n}-P_{3n-1})+(P_{3n}-P_{3n+1})],\end{aligned} \tag{13}$$

where $P_{-1}\equiv 0$. Equation (7) allows us to express P_n's via Q_n's. Thus we get

$$P_{3n}-P_{3n-1}=Q_{3n}^2+Q_{3n-1}^2+2(Q_{3n}-Q_{3n-1})\sum_{k=0}^{3n-1}Q_k \tag{14}$$

and

$$P_{3n}-P_{3n+1}=Q_{3n}^2-2Q_{3n}Q_{3n+1}-Q_{3n+1}^2+2(Q_{3n}-Q_{3n+1})\sum_{k=0}^{3n-1}Q_k. \tag{15}$$

Substituting Eqs. (14) and (15) into Eq. (13) yields

$$3A_0(t)=\sum_{n=0}^{\infty}(Q_{3n}-Q_{3n+1})^2+\sum_{n=0}^{\infty}(Q_{3n-1}^2+Q_{3n}^2-2Q_{3n+1}^2)+2\sum_{n=0}^{\infty}(2Q_{3n}-Q_{3n-1}-Q_{3n+1})\sum_{k=0}^{3n-1}Q_k. \tag{16}$$

In the following calculations we use the exact solution (5), the asymptotic relation $I_n(t)\simeq(2\pi t)^{-1/2}\exp(t-n^2/2t)$, and the identity [14]

$$I_{n-1}(t)-I_{n+1}(t)=\frac{2n}{t}I_n(t). \tag{17}$$

The first sum on the right-hand side of Eq. (16) behaves as

$$\sum_{n=0}^{\infty}(Q_{3n}-Q_{3n+1})^2\simeq\frac{t^{-3/2}}{6\sqrt{\pi}}. \tag{18}$$

The second sum on the right-hand side of Eq. (16) is determined by treating $Q_{n-1}^2(t)-2Q_n^2(t)+Q_{n+1}^2(t)$ as the second derivative $\partial^2Q_n^2/\partial n^2$, which is asymptotically correct. Using the scaling expression (10) for $Q_n(t)$, this sum is shown to decay as t^{-2} in the scaling limit. Similarly, the computation of the third line on the right-hand side of Eq. (16) is simplified by the approximation $Q_{n-1}(t)-2Q_n(t)+Q_{n+1}(t)\simeq\partial^2Q_n/\partial n^2$. After some algebra, this third term is found to decay as $-(2/3\pi)t^{-1}$ and thus provides a dominant contribution. The corresponding values for $A_1(t)$ and $A_2(t)$ follow from the same kind of computation. Thus we finally arrive at the following asymptotic behavior of the autocorrelation functions:

$$A_0(t)\simeq-\frac{2}{9\pi t},\quad A_1(t)\simeq\frac{4}{9\pi t},\quad A_2(t)\simeq-\frac{2}{9\pi t}. \tag{19}$$

It is surprising that in the long-time limit A_0 and A_2 exhibit similar behaviors, while the amplitude of the A_1 has the opposite sign and is twice as large.

In the general context of coarsening [22], the autocorrelation function is known to decay as $\mathcal{L}^{-\lambda}$. It has been argued that the exponent λ satisfies $d/2\leqslant\lambda\leqslant d$ in d dimensions [23]. Our model implies $A(\mathcal{L})\sim\mathcal{L}^{-1}$ ($\lambda=1$) and thus coincides with the upper bound as it happens in a few other models, e.g., in the voter model [19]. Most other studies [24] also found values of the autocorrelation exponent satisfying $d/2\leqslant\lambda\leqslant d$ (see, however, Ref. [25], which reports a violation of the upper bound for the conserved dynamics).

IV. SPATIAL STRUCTURE

Turn now to the spatial structure formed as the ballistic annihilation process proceeds. Among several quantities characterizing the spatial distribution we choose the domain size distribution function for which some analytical results are already available [4]. Let us denote by $\mu_{+-}(x,t)$ the probability density that at time t the right nearest neighbor of a + interface is a − interface located at distance x apart. Similarly, we introduce $\mu_{++}(x,t)\equiv\mu_{--}(x,t)$ and $\mu_{-+}(x,t)$. The Laplace transform $\hat{\mu}(z,t)=\int_0^\infty dx e^{-xz}\mu(x,t)$ of these quantities has been computed exactly [4]:

$$\hat{\mu}_{++}(z,t)=\frac{1}{1+J+2z}, \tag{20}$$

$$\hat{\mu}_{-+}(z,t)=\frac{S(t)e^{-2zt}}{1+J+2z}, \tag{21}$$

$$\hat{\mu}_{+-}(z,t)=\frac{e^{2zt}}{S(t)}\,\frac{J^2+2z(J-1)}{1+J+2z}, \tag{22}$$

where $S(t)$, the probability for the interface to survive up to time t, is given by Eq. (6) and

$$J\equiv J(z,t)=e^{-2zt}S(t)+2z\int_0^t d\tau e^{-2z\tau}S(\tau). \tag{23}$$

The solution of Eqs. (20)–(22) has been originally derived in an alternative analytical approach to simpler previous ones [1,6]; this approach of Ref. [4] has an advantage of being applicable to more difficult ballistic annihilation processes such as the three-velocity ballistic annihilation [5]. However, the actual spatial characteristics have not been extracted from Eqs. (20)–(22).

As a first step, we compute the average length scale

$$\langle x\rangle=\frac{\int_0^\infty dx\,x\,\mu(x,t)}{\int_0^\infty dx\,\mu(x,t)}=-\frac{1}{\hat{\mu}(0,t)}\left.\frac{\partial\hat{\mu}(z,t)}{\partial z}\right|_{z=0}. \tag{24}$$

After straightforward calculations we find the average size of a domain with boundaries moving in the same direction,

$$\langle x\rangle_{++}=\frac{2}{1+S(t)}\left[\int_0^t d\tau S(\tau)-tS(t)+1\right]. \tag{25}$$

Similarly, we find the average domain size in two other situations

$$\langle x\rangle_{-+}=2t+\langle x\rangle_{++} \tag{26}$$

and

$$\langle x\rangle_{+-}=2\frac{1-S(t)}{S^2(t)}+2t-\frac{4}{S(t)}\int_0^t d\tau S(\tau)+\frac{2}{1+S(t)}\left[\int_0^t d\tau S(\tau)-tS(t)+1\right]. \quad (27)$$

Making use of the asymptotic relation $S(t)\simeq(\pi t)^{-1/2}$, we arrive at the long-time behaviors

$$\langle x\rangle_{++}\simeq\sqrt{\frac{4t}{\pi}},\quad \langle x\rangle_{-+}\simeq 2t,\quad \langle x\rangle_{+-}\simeq 2(\pi-3)t. \quad (28)$$

It is instructive to proceed by computing $\langle x^n\rangle^{1/n}$ for an arbitrary positive integer index n. One readily expresses $\langle x^n\rangle^{1/n}$ via $\hat{\mu}(z,t)$, e.g., $\langle x^2\rangle=[\hat{\mu}(0,t)]^{-1}[\partial^2\hat{\mu}(z,t)/\partial z^2]|_{z=0}$. Any of these quantities can be used to characterize the length scale. For domains with dissimilar boundary interfaces one finds $\langle x^n\rangle_{+-}^{1/n}\sim\langle x^n\rangle_{-+}^{1/n}\sim t$, implying that all these distances are characterized by the single ballistic length scale $\mathcal{L}(t)\sim t$. In contrast, for similar interfaces we get anomalous asymptotic behaviors $\langle x^2\rangle^{1/2}\simeq(9\pi)^{-1/4}t^{3/4}$ and generally $\langle x^n\rangle_{++}^{1/n}\sim t^{1-1/2n}$ for integer n. This odd feature indicates that the length scale characterizing the average separation of the nearest similar moving interfaces $l(t)=\langle x\rangle_{++}\sim\sqrt{t}$ is just one of the hierarchy of length scales $l_n(t)=\langle x^n\rangle_{++}^{1/n}$ All these scales are better thought of as effective scales resulting from the competition between the two basic scales in the problem: the scale of order one forced by initial conditions and the ballistic scale of order t.

This two-scale spatial structure clearly appears in the form of the nearest-neighbor distributions $\mu(x,t)$. To determine these distributions, we compute the inverse Laplace transform of Eqs. (20)–(22). We first note that $J(z,t)$ can be rewritten as

$$J(z,t)=2z\int_0^\infty d\tau e^{-2z\tau}S(\tau)-\int_t^\infty d\tau e^{-2z\tau}S'(\tau)$$
$$=-z+\sqrt{z^2+2z}+\int_{2t}^\infty d\tau e^{-z\tau}\frac{e^{-\tau}I_1(\tau)}{\tau}, \quad (29)$$

where we have computed the Laplace transform $\hat{S}(2z)$ and the derivative of $S(t)$. We then expand $\hat{\mu}_{++}$ to find

$$\hat{\mu}_{++}(z,t)=\hat{a}(z)-\hat{a}(z)^2\hat{b}(z,t)+\hat{a}(z)^3\hat{b}(z,t)^2+\cdots, \quad (30)$$

where

$$\hat{a}(z)=z+1-\sqrt{(z+1)^2-1} \quad (31)$$

and

$$\hat{b}(z,t)=\int_{2t}^\infty d\tau e^{-z\tau}\frac{e^{-\tau}I_1(\tau)}{\tau}. \quad (32)$$

Performing the inverse Laplace transform of $\hat{a}(z)$ and $\hat{b}(z,t)$, we get

$$a(x)=\frac{e^{-x}I_1(x)}{x},\quad b(x,t)=\frac{e^{-x}I_1(x)}{x}\Theta(x-2t). \quad (33)$$

Combining Eqs. (30) and (33) we finally obtain

$$\mu_{++}(x,t)=a-a^{*2}*b+a^{*3}*b^{*2}-a^{*4}*b^{*3}+\cdots, \quad (34)$$

where $f*g=\int_0^x dy f(y)g(x-y)$ is the convolution of f and g, $f^{*2}=f*f$, $f^{*3}=f*f*f$, etc.

Noting that $a^{*k}(x)=ke^{-x}I_k(x)/x$ [27], the convolution in the second term on the right-hand side of Eq. (34) can be calculated in the long-time limit to yield

$$a*a*b\simeq\frac{\Theta(\xi)}{\sqrt{2\pi x^3}}\{1-e^{-\xi}[I_0(\xi)+2I_1(\xi)+I_2(\xi)]\}, \quad (35)$$

where $\xi=x-2t$. The following terms in Eq. (34) give corrections for $x\geqslant 4t,6t,\ldots$.

The only contribution to $\mu_{++}(x,t)$ for $x<2t$ is the first time-independent term $a(x)$. For large x, it scales as $x^{-3/2}$. According to the mapping of Sec. II, it is analogous to the probability that a random walker starting at the origin first returns to the origin after x steps. A singularity in the second derivative arises at $x=2t$ and weaker and weaker singularities appear for x being an integer multiple of $2t$. It should be noted that the scale $l\sim\sqrt{t}$ does *not* appear in this distribution. The only arising scales are the scale $O(1)$ characterizing the time-independent contribution $a(x)$ and the ballistic scale $O(t)$ characterizing the following terms. The origin of other length scales can be traced to the power-law tail of the time-independent part $a(x)$ of $\mu_{++}(x,t)$. Indeed, $l_n(t)=\langle x^n\rangle_{++}^{1/n}\sim[\int_0^{2t}dx x^n a(x)]^{1/n}\sim t^{1-1/2n}$. This behavior should be contrasted with systems presenting multiscaling [26], where an infinite number of length scales are present.

Using properties of the Laplace transform [27], the distributions $\mu_{+-}(x,t)$ and $\mu_{-+}(x,t)$ can be expressed via $\mu_{++}(x,t)$,

$$\mu_{+-}(x,t)=S(t)\mu_{++}(x-2t,t)\Theta(x-2t),$$
$$\mu_{-+}(x,t)=\frac{\mu_{++}(x+2t)}{S(t)}, \quad (36)$$

thus providing a comprehensive description of the interfaces distribution in this problem.

V. SUMMARY AND OUTLOOK

We have shown that the two-velocity ballistic annihilation process may be thought of as the three-phase deterministic model of coarsening. This is one of the simplest models of coarsening ever known and we have derived exact solutions for the generalized first-passage probabilities $P_n(t)$ and for the autocorrelation function.

We have revealed a rich spatial structure arising as the phase-separation process develops. In particular, the moments of the domain size distribution $l_n(t)=\langle x^n\rangle_{++}^{1/n}$ exhibit a variety of scales from the time-independent one to the scale linearly growing with time:

$$l_n(t)\sim\begin{cases}1 & \text{when } n<1/2\\ t^{1-1/2n} & \text{when } n>1/2.\end{cases} \quad (37)$$

We have argued that only the two extreme scales, the ballistic one and the scale $O(1)$ characterizing the initial distribution, are important, while the others are effective in that they arise as the result of competition between the extreme scales. The distribution of nearest neighbors has shown a nontrivial behavior with singularities at each x being an integer multiple of $2t$.

Using the mapping on a random walk problem introduced in Sec. II, it should be possible to compute the two-point equal-time correlation function $G(x,t)$ and even the most general two-point correlation function $C(x,t|0,t')$, which contains both the equal-time correlation function $G(x,t)\equiv C(x,t|0,t)$ and the autocorrelation function $A(t)\equiv C(0,t|0,0)$. We were able to solve for $G(x,t)$ for $x\geqslant 2t$, but the solution is very cumbersome, so we could not derive clear scaling results. Numerical simulations, however, reveal an interesting oscillatory behavior of $G(x,t)$.

Another interesting question concerns the extension of the three-phase deterministic model to higher dimensions. It is very simple to define a three-color cyclic *lattice* model in arbitrary dimension [10,12]. The problem is that the system does *not* exhibit coarsening when $d\geqslant 2$ and instead approaches a reactive state with the average number of color changes growing linearly with time. However, one can hope that a proper higher-dimensional extension still exists.

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