Deterministic Soluble Model of Coarsening

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We investigate a 3-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.

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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 of growing interfaces moving in the same direction, and the length scale \( \ell \) characterizing initial data and the ballistic length scale \( b \) describing the average distance between neighboring interfaces moving in the same direction, and the length scale \( L \) describing the typical distance between terminating interfaces moving in the opposite directions. As we shall see below, however, the growth law for \( \ell(t) \) cannot fully characterize the spatial structure – other natural measures of the spacing between similar neighboring interfaces behave differently, e.g., the rms separation \( \ell_2(t) = \sqrt{\langle x^2 \rangle} \) 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 \( L(t) \sim t \).

On the language of phase ordering dynamics, the two-velocity ballistic annihilation model may be treated as the 3-phase, or 3-color, process with deterministic non-conservative dynamics. Indeed, imagine that the one-dimensional line is drawn in three colors, say red, green, and blue. Let 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 domain 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 3-species cyclic food chain [12].

The rest of this paper is organized as follows. Generalized first-passage probabilities are determined in section II. Section III contains a calculation of the autocorrelation function. The domain size distribution is analyzed in section IV. The last 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 arbitrary point changes cyclically with period 3, so the autocorrelation function is found from 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 
\[ S_i = S_{i-1} + v_i, \quad i = 1, \ldots, N, \]
where \( v_i = \pm 1 \) is the velocity of the \( i \)th interface. Thus we indeed have a random walk \((i, S_i)\) starting from the origin, with \( i \) being a time-like variable and \( S_i \) a displacement. The crucial point is that the number of interfaces which 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

\[ Q_n(N) = \hat{Q}_n(N) + \hat{Q}_{n+1}(N), \tag{2} \]

with

\[ \hat{Q}_n(N) = \frac{1}{2^N} \binom{N}{\frac{N}{2}} \frac{N!}{(\frac{N}{2}!)^2} \tag{3} \]

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

Before returning to the original two-sided problem we consider the one-sided problem with 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 \( x \leq t \) 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 (2) and (3) into (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 is not 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 \( \text{max}(k, n) \), as illustrated in Fig. 1. 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 factor 2 accounting for the fact that smaller number \( k \) of crossing interfaces can come both from 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 \( \sum P_n = (\sum Q_n)^2 \), and the latter sum is shown to be equal to one by using Eq. (3) and identity \( I_0(t) + 2 \sum_{j \geq 1} I_j(t) = e^t \).

Note that \( P_n \)'s, and especially the first “persistence” probability \( P_0(t) \), have attracted a considerable recent interest, see e.g. [14–20]. These quantities can be thought as first-passage time probabilities in the interacting particle systems [22]. 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 mean-field approach (more precisely, for interacting particle systems on a complete graph) [22,44] and a limiting analytical solution for the 1D voter model [13], 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 [3]–[7]. In particular, we have \( P_0(t) = Q_0^2(t) \zeta 2(\pi t)^{-1} \).

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

\[ n \to \infty, \quad t \to \infty, \quad z = \frac{n}{\sqrt{2t}} = \text{finite}. \tag{9} \]

Making use of the scaling behavior of the modified Bessel functions [14], \( I_n(t) \zeta 2(\pi t)^{-n/2} \exp(t - n^2/2t) \), we find

\[ Q_n(t) \zeta \sqrt{\frac{2}{\pi t}} e^{-z^2} \tag{10} \]

for the one-sided probabilities and

\[ P_n(t) \zeta \sqrt{\frac{8}{\pi t}} e^{-z^2} \operatorname{Erf}(z) \tag{11} \]

for the two-sided probabilities.

### III. THE AUTOCORRELATION FUNCTION

The scaling expression of Eq. (11) does not allow to obtain non trivial long-time behavior of the autocorrelation function. Indeed, substituting (11) into (4) yields \( A(t) \zeta 1/3 \). We should therefore return to exact relations (3)–(5). 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 as initially corresponds to \( \alpha = 0 \),
$A_0(t) \equiv A(t) - 1/3$; the “next” blue color corresponds to $\alpha = 1$; and finally the green color corresponds to $\alpha = 2$.

All three autocorrelation functions $A_n(t)$ exhibit similar asymptotic behavior; additionally, they are related by identity $A_0(t) + A_1(t) + A_2(t) \equiv 0$. Combining (12) and (3) we obtain

$$3A_0(t) = \sum_{n=0}^{\infty} \left[ (P_{3n} - P_{3n-1}) + (P_{3n} - P_{3n+1}) \right]$$

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

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

and

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

Substituting (14) and (15) into (3) yields

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

$$+ \sum_{n=0}^{\infty} (Q_{3n-1}^2 + Q_{3n}^2 - 2Q_{3n+1}^2)$$

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

In the following calculations we use the exact solution (3), the asymptotic relation $I_n(t) \approx (2\pi t)^{-1/2} \exp(t - n^2/2t)$, and the identity (14)

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

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

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

The second sum in the right-hand side of Eq. (16) is undergone by treating $Q_{n-1}^2(t) - 2Q_n^2(t) + Q_{n+1}^2(t)$ as the second derivative, $\partial^2 Q_n^2/\partial n^2$, 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 in the right-hand side of Eq. (16) is simplified by the approximation $Q_{n-1} - 2Q_n(t) + Q_{n+1}(t) \approx \partial^2 Q_n/\partial n^2$. 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 $A_2(t)$ follows from the same kind of computation. Thus, we finally arrive at the following asymptotic behavior of the autocorrelation functions:

$$A_0(t) \sim -\frac{2}{9nt}, \quad A_1(t) \sim \frac{4}{9nt}, \quad A_2(t) \sim -\frac{2}{9nt}.$$ (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 twice bigger.

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

IV. THE 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 [5]. 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 $\mu_{+-}(x,t)$ and $\mu_{-+}(x,t)$. The Laplace transform, $\hat{\mu}(z,t) = \int_0^\infty dx e^{-zt} \mu(x,t)$, of these quantities has been computed exactly [5]:

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

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

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

where $S(t)$, the probability for the interface to survive up to time $t$, is given by Eq. (8), and

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

The solution of Eqs. (20)–(22) has been originally derived in an alternative analytical approach to simpler previous ones [1,5]; this approach of Ref. [4] has an advantage of
being applicable to more difficult ballistic annihilation processes like the three velocity ballistic annihilation \[3\]. However, the actual spatial characteristics have not been extracted from Eqs. (20,21,22).

As a first step, we compute the average length scale

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

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:

\[
\langle x \rangle_- = 2t + \langle x \rangle_+,
\]

and

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

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

\[
\langle x \rangle_+ \approx 2\frac{1-S(t)}{S^2(t)} + 2t - \frac{4}{S(t)} \int_0^t d\tau \ S(\tau) + \frac{2}{1+S(t)} \left[ \int_0^t d\tau \ S(\tau) - tS(t) + 1 \right]. \tag{28}
\]

The latter result is surprising, one might expect that \( \langle x \rangle_+ \) grows as \( \langle x \rangle_+ \) while in fact it grows much faster.

It is instructive to proceed by computing \( \langle x^n \rangle^{1/n} \) for arbitrary positive integer index \( n \). One readily expresses \( \langle x^n \rangle^{1/n} \) via \( \hat{\mu}(z,t) \), e.g., \( \langle x^2 \rangle = [\hat{\mu}(0,t)]^{-1} \frac{\partial^2 \hat{\mu}(z,t)}{\partial z^2} \bigg|_{z=0} \). Any of these quantities can be used to characterize the length scale. For domains with dissimiliar 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, \( L(t) \sim t \). In contrast, for similar interfaces we get anomalous asymptotic behaviors: \( \langle x^2 \rangle^{1/2} \approx (9\pi)^{-1/4} t^{3/4} \), and generally \( \langle x^n \rangle^{1/n}_+ \sim t^{1-1/n} \) for integer \( n \). This odd feature indicates the length scale characterizing the average separation of the nearest similar moving interfaces, \( \ell(t) = \langle x \rangle_+ \sim \sqrt{t} \), is just one of the hierarchy of length scales \( \ell_n(t) = \langle x^n \rangle^{1/n} \). All these scales are better thought 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 \( t \).

To clarify these results, we compute the inverse Laplace transform of Eqs. (21,22,23). We first note that \( J(z,t) \) can be rewritten as

\[
J(z,t) = 2z \int_0^\infty d\tau e^{-2\pi z S(\tau)} - \int_{\infty}^\infty d\tau e^{-2\pi z S'(\tau)}
\]

\[
= -z + \sqrt{z^2 + 2z} + \int_{\infty}^\infty d\tau e^{-\pi z} I_1(\tau) \tag{29}
\]

where we have computed the Laplace transform \( \hat{S}(2z) \) and the derivative of \( S(t) \). We then expand \( \hat{\mu}_{++}(z,t) = \hat{a}(z) - \hat{a}(z)^2 \hat{b}(z,t) + \hat{a}(z)^3 \hat{b}(z,t)^2 + \ldots \) \( \tag{30} \)

where

\[
\hat{a}(z) = z + 1 - \sqrt{(z+1)^2 - 1} \tag{31}
\]

and

\[
\hat{b}(z,t) = \int_{2t}^\infty d\tau e^{-\pi \tau} e^{-\pi t} I_1(\tau). \tag{32}
\]

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

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

Combining (22) and (23) we finally obtain

\[
\mu_{++}(x,t) = a - a^2 b + a^3 b^2 - a^4 b^3 + \ldots \tag{34}
\]

where \( f \ast f = \int_0^x dy f(y)g(x-y) \) is the convolution of \( f \) and \( g \).

Noting that \( a^k(x) = ke^{-x} I_k(x)/x \) \( \tag{34} \)

the convolution in the second term of the right-hand side of Eq. (34) can be calculated in the long time limit to yield:

\[
a \ast a \ast b \approx \frac{\Theta(\xi)}{\sqrt{2\pi x^3}} \times \left[ 1 - e^{-\xi} \left[ I_0(\xi) + 2I_1(\xi) + I_2(\xi) \right] \right]. \tag{35}
\]

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

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 Section II, it is analogous to the probability that a random walker starting at the origin first returns back 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 integer multiple of \( 2t \). It should be noted that the scale \( t \sim \sqrt{t} \) does not appear in this distribution. The only scales appearing are the scale \( \mathcal{O}(1) \) characterizing the time-independent contribution \( a(x) \), and the ballistic scale \( \mathcal{O}(t) \) characterizing next terms. The asymptotic average distance \( \langle x \rangle_+ \approx \sqrt{4t/\pi} \) of Eq. (23) is readily obtained by the integration \( \int_{0}^{2t} dx x \mu_{++}(x,t) = \int_{0}^{2t} dx x \mu_{++}(x,t) \), following terms give corrections \( \mathcal{O}(1) \).

Using properties of Laplace transform \( \mathcal{L} \), the distributions \( \mu_{--}(x,t) \) and \( \mu_{--}(x,t) \) can be expressed via \( \mu_{++}(x,t) \),
\[
\begin{align*}
\mu_{+}(x, t) &= S(t) \mu_{++}(x - 2t, t) \Theta(x - 2t) \\
\mu_{-}(x, t) &= \frac{\mu_{++}(x + 2t)}{S(t)},
\end{align*}
\]

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 as the 3-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, \( \ell_n(t) = (x^n)^{1/n} \), exhibit a variety of scales from the time-independent one and the ballistic one and the scale \( \ell_{0}(t) \equiv \langle x^0 \rangle \) (the autocorrelation function).

We have argued that only the two extreme scales, the ballistic one and the scale \( \ell_{0}(t) \), 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 non-trivial behavior with singularities at each \( x \) being an integer multiple of 2.

Using the mapping on a random walk problem introduces in Section 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 \( x \geq 2t \), 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 3-phase deterministic model to higher dimensions. It is very simple to define a 3-color cyclic lattice model in arbitrary dimension. The problem is the system does not exhibit coarsening when \( d \geq 2 \) 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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\[ \begin{align*}
\mu_{+}(x, t) &= S(t) \mu_{++}(x - 2t, t) \Theta(x - 2t) \\
\mu_{-}(x, t) &= \frac{\mu_{++}(x + 2t)}{S(t)},
\end{align*} \]

\[ \ell_n(t) \sim \begin{cases} 
1 & \text{when } n < 1/2, \\
t^{-1-2n} & \text{when } n > 1/2.
\end{cases} \]

\[ (37) \]

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