Two-site self-consistent method for front propagation in reaction-diffusion systems

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We study front propagation in the reaction-diffusion process $A \leftrightarrow 2A$ on a one-dimensional lattice with hard core interaction between the particles. We propose a two-site self-consistent method to make analytic estimates for the front velocity that are in good agreement with the simulation results for all parameter regimes. We expect that the simplicity of the method will allow one to use this technique for estimating the front velocity in other reaction diffusion processes as well.

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Front propagation in reaction-diffusion systems is an important field of study in nonequilibrium physics. In many natural phenomena we often encounter propagating fronts separating different phases [1]. In this paper, we study front dynamics in the reaction-diffusion system $A \leftrightarrow 2A$, whose mean field description is given by the following Fisher-Kolmogorov equation [2] for the local density of A particles $\rho(x,t)$: $\partial\rho/\partial t = D(\partial^2\rho/\partial x^2) + k_1\rho - k_2\rho^2$. Here, D is the bare diffusion coefficient of A particles while k_1 and k_2 are the rates of creation and annihilation, respectively. This equation arises in the macroscopic description of many processes in natural science and serves as a generic description of front propagation in a system undergoing transition from unstable to stable state. The homogeneous steady states of this equation are $\rho=(k_1/k_2)$ (stable) and $\rho=0$ (unstable). Hence, starting with an initial condition in which both the states coexist, the stable state invades the unstable one with speed V as a traveling wave of the form $\rho=\rho(x-Vt)$. Such fronts are referred to as *pulled* in the sense that the leading edge, where $\rho \ll 1$, plays an important role in describing the front dynamics. Such leading edge analysis gives $V \geqslant V_0 = 2\sqrt{k_1 D}$. For steep enough initial conditions the minimum velocity V_0 is selected [3].

In discrete realizations of the process in low dimensions, with maximum occupancy per site restricted to N, the continuum description fails to capture the internal fluctuations of the system and thus the dynamical properties of the front are much different from that predicted by the continuum equation [4,5]. However, the mean field results are recovered for $N \to \infty$. In this paper, we study the one-dimensional system for $N=1$ which displays the largest deviation from the continuum mean field results.

Motivated by the velocity selection principle, in which the leading edge plays an important role, we propose a *two-site self-consistent method* (TSSCM). In this method, we describe the front dynamics by considering the evolution of occupancy at only two sites: The front site and the site just behind it. In other words, in the frame moving with the front we study evolution of occupancy at a site just behind it. By applying a self-consistent approach (explained later), we obtain analytic estimates for the front velocity which are in good agreement with the simulation results for all parameter regimes. In our simulation we consider a one-dimensional lattice composed of sites $i=1,2,\ldots,L$. Each site can either be empty or occupied by at most one particle, i.e., hard core exclusion is taken into account. Initially, we start with the left half of the lattice filled with A particles while keeping the right half empty. We update the system random sequentially where L attempts constitute one Monte Carlo step. During each update we select a site and one of its neighboring sites randomly and if the chosen site is occupied the particle at the site undergoes one of the following microscopic moves: (i) It diffuses to the neighboring site if the latter is empty with rate D, (ii) it gives birth to a particle at the neighboring site, if empty, with rate ϵ, or (3) it gets annihilated with rate W, if the neighboring site is occupied. Due to these microscopic processes the rightmost A particle, which is identified with the front, moves stochastically and we are interested in finding its asymptotic speed. Visualizing the leading particle as a random walker its velocity is given by [6]

$$V = \epsilon - \rho_1(W - D). \tag{1}$$

With ρ_1 denoting the density at the site just behind the leading particle, the latter moves forward with a rate $\epsilon+D$ and with rate $W\rho_1 + D(1-\rho_1)$ in the backward direction.

There is no systematic method to find ρ_1 exactly, however, several approximations have been proposed. For example, in [6], ρ_1 was taken as the bulk density $\bar{\rho}=\epsilon/(\epsilon+W)$ in the stable phase. This approximation is exact for $W=D$ and shows reasonable agreement for small values of $|W-D|$ [7]. However, for larger $|W-D|$, significant systematic deviation is observable (Fig. 1).

In order to make a better estimate for ρ_1, especially away from the special point $W=D$, a method was proposed in [8] which may be used to systematically improve analytic estimate to the desired degree of accuracy. In this method, evolution of l sites behind the leading particle is written down. For example, for $l=1$, we study the states {01, 11} and for $l=2$ one has to deal with states {001, 011, 101, 111} with the rightmost "1" representing the front particle. Assuming the $l+1$ site is occupied with probability equal to the bulk density, a master equation for evolution of the 2^l states was written down and the steady state solution yielded the required ρ_1. For larger values of $|W-D|$, we need to include more states (i.e., larger l) in order to get better analytic estimates, but writing the transition matrix corresponding to the master equation becomes more difficult since its size increases as $2^l \times 2^l$. In order to make an analytically tractable

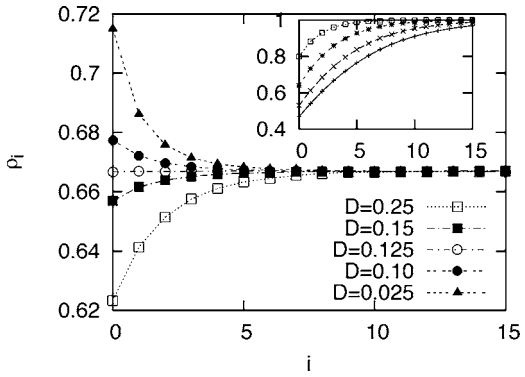

FIG. 1. Simulation results for the density profile behind the front for $\epsilon=0.25$, $W=0.125$ for different values of D. Inset: Density profile for $\epsilon=0.05$, $W=0$ for $D=0.05, 0.15, 0.30, 0.45$ from top to bottom. We note that the difference between ρ_1 or ρ_2 with bulk density increases with increasing $|W-D|$ and for $W=D$ all the sites have bulk density.

approximation for ρ_1 and hence the front velocity, a reduced three particle representation was presented in [8].

In [9], Kerstein proposed a two-particle representation for the reaction-diffusion process $A \to 2A$, and studied the evolution of the following infinite set of states: {11, 101, 1001, 10001, $\cdots$} with the rightmost "1" representing the front. The important point that we note here is that this set of states is closed under the transitions only if $W=0$ and thus is not applicable for $W>0$. Further, a product ansatz $p_j=p_0(1-p_0)^j$ was used, where p_j is the probability of the jth state with j zeros between the front particle and the next. This ansatz *a priori* excludes any spatial density correlations which is not true in general (Fig. 2). In fact, this correlation increases with $|W-D|$ and vanishes for the special point $W=D$. The ansatz also assumes that the sites behind the front are at the same density p_0, which is, of course, not true (Fig. 1). This leads to systematic error in the analytic estimates which increases gradually with an increasing value of $|W-D|$. However, one can get better results by studying the states having a larger number of particles but the computational complexity increases exponentially with the number of particles [10].

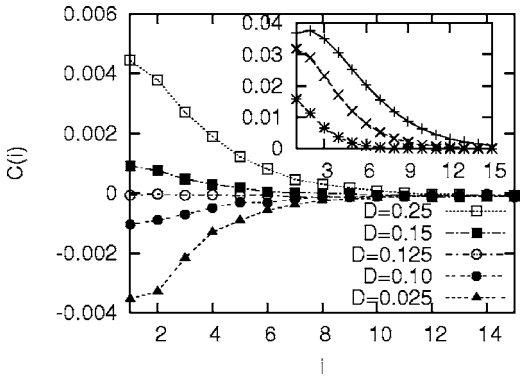

FIG. 2. Simulation results for the spatial density correlation between a pair of successive sites, $C(i)=\langle n(i)n(i+1)\rangle - \langle n(i)\rangle\langle n(i+1)\rangle$, for $\epsilon=0.25$, $W=0.125$ for different values of D. Inset: $C(i)$ versus i for $\epsilon=0.05$, $W=0$ for $D=0.30, 0.15, 0.05$ from top to bottom. Here we note that the range and magnitude of correlation increase as $|W-D|$ increases.

In this paper, we present a simple analytic esimate for ρ_1 and hence of the front velocity which is in good agreement with the simulation results. We use a self-consistent two-site scheme, where we write a master equation in the frame moving with the front particle (as in [8]) for the evolution of two states $\{0A, AA\}$. Here the rightmost A represents the front particle. In this truncated representation these two states make a transition between each other due to the microscopic processes and thus form a closed set under such transitions. For example, $0A \to AA$ if the leading particle gives birth to its left empty site. Diffusion of the front particle to its left changes the state $0A \to AA$, provided the second site $(F-2)$ behind the front particle is occupied and leaves it unchanged if $F-2$ is empty. If the probability of occupancy at $F-2$ is denoted as ρ_2 then the transition $0A \to AA$ occurs with rate $D\rho_2$. Similarly, if the leading particle in the realization AA gets annihilated, the state changes to $0A$ if $F-2$ is empty with rate $W(1-\rho_2)$, while it remains unchanged if $F-2$ is occupied. Considering all such transitions one can write the master equation for the state probabilities P_{0A} and P_{AA} as

$$\dot{P}_{0A} = (2D - D\rho_2 + 2W)P_{AA} - (2D\rho_2 + 2\epsilon + \epsilon\rho_2)P_{0A},$$

$$\dot{P}_{AA} = (2D\rho_2 + 2\epsilon + \epsilon\rho_2)P_{0A} - (2D - D\rho_2 + 2W)P_{AA}. \quad (2)$$

Thus we need to know ρ_2 in order to find the steady state probabilities P_{0A} and P_{AA}. We note that as $\epsilon \to 0$, ρ_2 as well as P_{AA} vanish, and hence we may write the former as a truncated polynomial of the latter (in steady state):

$$\rho_2 = aP_{AA} + bP_{AA}^2. \quad (3)$$

Thus the steady state value of P_{AA} is determined by ρ_2 which in turn is related to the former through Eq. (3) and the method is *self-consistent*. To determine the coefficients a and b we note that for $W=D$ all sites behind the front particle are at bulk density, i.e., $\rho_2=P_{AA}=\bar{\rho}=\epsilon/(\epsilon+D)$ and we rewrite Eq. (3) as

$$\rho_2 = \left(1 - \frac{b\epsilon}{\epsilon + D}\right)P_{AA} + bP_{AA}^2. \quad (4)$$

Using this value of ρ_2 in Eq. (2) along with normalization condition $P_{0A}+P_{AA}=1$, we obtain the following equation:

$$\alpha P_{AA}^3 + \beta P_{AA}^2 + \gamma P_{AA} - \delta = 0, \quad (5)$$

with

$$\alpha = 2b\epsilon D + bD^2 + b\epsilon^2,$$

$$\beta = D^2 + \epsilon^2 + 2\epsilon D - 4b\epsilon D - 2bD^2 - 2b\epsilon^2,$$

$$\gamma = 2b\epsilon D + \epsilon D + \epsilon^2 b + \epsilon^2 + 2\epsilon W + 2WD,$$

$$\delta = 2\epsilon^2 + 2\epsilon D. \quad (6)$$

Equation (5) is in terms of two unknowns b and P_{AA} and hence we must fix b in order to find P_{AA}. It is known that in the limit $D \to \infty$, the front moves with Fisher velocity

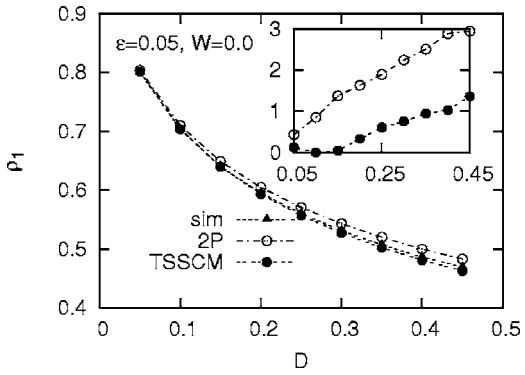

FIG. 3. Comparison between simulation and analytic results for ρ_1 for $\epsilon=0.05$, $W=0.0$, and for different values of D. The open circle corresponds to Kerstein two-particle representation while the closed circle is the result from the present work. We note that the results of TSSCM are essentially coincident with the simulation results. Inset: Percentage relative error in ρ_1 as a function of D.

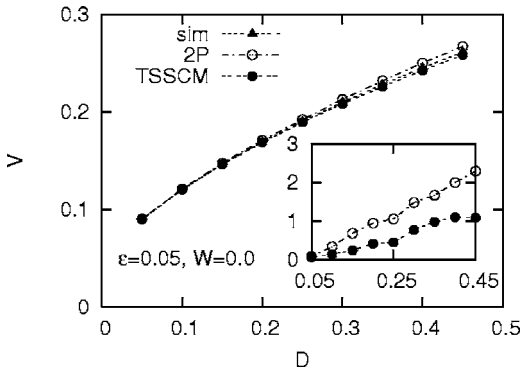

FIG. 5. Comparison between simulation and analytic results for front velocity V for $\epsilon=0.05$, $W=0$ and for different values of D. Open circles correspond to Kerstein's two-particle representation while closed circles are the result from the present work. We note that the results of TSSCM are closer to the simulation results. Inset: Percentage relative error in V as a function of D.

$V_0=2\sqrt{\epsilon D}$. Also, from Eq. (1), the front velocity in terms of ρ_1 is given as $V\sim D\rho_1=DP_{AA}$, when D is very large compared to ϵ and W. Equating this with velocity V_0, we get $P_{AA}=2\sqrt{\epsilon/D}$. Substituting this value of P_{AA} in Eq. (5), we have an equation which is linear in b and which, in the limit $D\to\infty$, gives $b=1/4$. Substituting this value of b in Eq. (5) we obtain the following cubic equation in P_{AA}:

$$(\epsilon^2+D^2+2\epsilon D)P_{AA}^3+(2\epsilon^2+2D^2+4\epsilon D)P_{AA}^2+(5\epsilon^2+6\epsilon D+8\epsilon W+8WD)P_{AA}-8\epsilon^2-8\epsilon D=0. \quad (7)$$

Solving the above cubic equation, the density at the site just behind the front particle $\rho_1\equiv P_{AA}$ may be obtained. The results obtained have been shown in Figs. 3 and 4 and are in good agreement with the simulation results. We have also shown the percentage relative error in ρ_1, i.e., $|\rho_1^s-\rho_1^a|/\rho_1^s\times 100$, where ρ_1^s and ρ_1^a correspond to simulation and analytic results, respectively. Once we know ρ_1, the front velocity is obtained from Eq. (1) and shown in Figs. 5 and 6. Here, we also observe very good agreement with the simulation results. For $W=0$, we have compared the results with that of Kerstein's two-particle representation in Figs. 3 and 5. We notice the interesting fact that the results obtained from the present work are closer to the simulation results as compared to that obtained using two-particle representation.

To conclude, we have developed a two-site self-consistent method for the propagating fronts in the reaction-diffusion system $A\leftrightarrow 2A$. The analytic estimates obtained using this method are in good agreement with the simulation results for all parameter regimes. We observe that for $W=0$, the results obtained are better than that using Kerstein's two-particle representation. We also notice that the present method has an advantage over Kerstein's two-particle representation due to the following key factors. First, TSSCM does not neglect the spatial density correlation as in Kerstein's product measure ansatz. Secondly, TSSCM uses a set of states closed under transitions due to the microscopic processes for all parameter

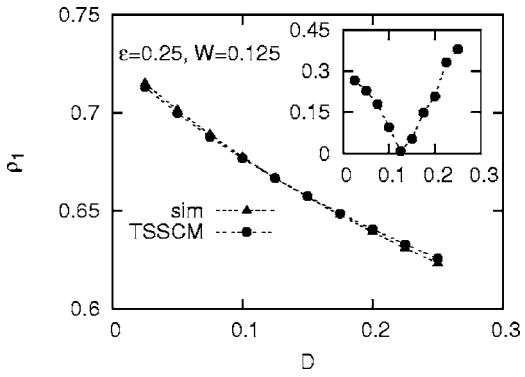

FIG. 4. Comparison between simulation and analytic results for ρ_1 for $\epsilon=0.25$, $W=0.125$ and for different values of D. The closed triangle corresponds to the simulation results while the closed circle is the results from the present work. We note that the analytic results are essentially coincident with the simulation results. Inset: Percentage relative error in ρ_1 as a function of D.

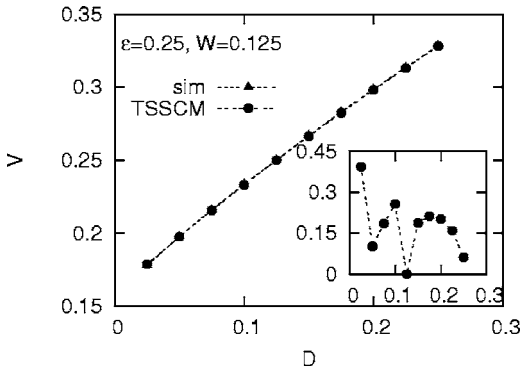

FIG. 6. Comparison between simulation and analytic results for front velocity V for $\epsilon=0.25$, $W=0.125$ and for different values of D. Closed triangles correspond to simulation results while the closed circles are the results using TSSCM. We note that the analytic results are essentially coincident with the simulation results. Inset: Percentage relative error in V as a function of D. Errors in each data are of the order of $\sim 0.2\%$.

regimes while the two-particle representation does not provide a closed set for $W \neq 0$. The simplicity of our analytic method provides the scope to study the velocity of a propagating front in other reaction-diffusion processes in discrete lattice models. Lastly, although we have demonstrated the method for pulled fronts, it should also work for *pushed* or nonlinear fronts as well provided the front speed for the corresponding continuum equation is known *a priori*.

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