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

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We study front propagation in the reaction diffusion process $A \leftrightarrow 2A$ on one dimensional lattice with hard core interaction between the particles. We propose a two site self consistent method (TSSCM) to make analytic estimates for the front velocity and are in excellent 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 the reaction diffusion system is an important field of study in nonequilibrium physics. In many natural phenomena we often encounter propagating fronts separating different phases. Here, in this paper, we study the front dynamics in the reaction diffusion system $A \leftrightarrow 2A$ whose mean field description is given by the following Fisher-Kolmogorove equation \[ \frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2} + k_1 \rho - k_2 \rho^2. \] Here $D$ is the bare diffusion coefficient of $A$ particle 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 model to describe front propagation in a system undergoing transition from unstable to stable state. The homogeneous steady states of this equation are $\rho = \frac{1}{k_1}$ (stable) and $\rho = 0$ (unstable). Hence if we start with an initial condition where both the states coexist, the the stable phase invades the unstable one with speed $V$ as a travelling wave of the form $\rho = \rho(x - Vt)$.

Here, such fronts are referred to as pulled in which the leading edge where $\rho << 1$ plays important role in describing the front dynamics. Such leading edge analysis gives $V \geq V_0 = 2\sqrt{k_1D}$. However, for steep enough initial condition the minimum velocity $V_0$ is selected and it is known that convergence to $V_0$ takes place with a very slow power law $\rho \sim V_0 + \frac{1}{4} + O(t^{-2})$, where, $\epsilon < 0$.

In this paper, we study the microscopic realization of the process $A \leftrightarrow 2A$ on a lattice. The important feature to be noted here is that the Fisher equation fails to deal with internal fluctuations arising due to discrete nature of the reacting species, especially when occupancy per site $N$ is small $N \ll 1$. When $N \to \infty$, the mean field results are recovered.

Motivated by the velocity selection principle, in which the leading edge plays an important role, we propose a procedure called 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 first one is the front site while the other one is the site just behind it. In other words, in the frame moving with the front we study the evolution of occupancy at a site just behind it. By applying a self consistent approach (explained later) in this method we obtain the analytic estimates for the front velocity which are in excellent agreement with the simulation results for all parameter regimes. In our simulation we consider a one dimensional lattice composed of sites $i = 1, 2, ..L$, $L$ being the size of the lattice. Initially, we start with left half of the lattice filled with $A$ particles while keeping the remaining right half empty. Each site can either be empty or occupied by maximum one particle i.e. hard core exclusion is taken into account. We update the system random sequentially where $L$ microscopic moves correspond to one Monte Carlo step (MCS). During each update we randomly select a site and the particle at the site undergoes the following microscopic moves: (1) The particle can diffuse to the neighbouring empty site with rate $D$, (2) The particle can give birth of one particle at an empty neighbouring site with rate $\epsilon$, (3) The particle gets annihilated with rate $W$, if the neighbouring site is occupied. Due to these microscopic processes the rightmost $A$ particle, which is identified as a front, moves and we are interested in finding the velocity with which it moves, which is given by $V$:

$$V = \epsilon - \rho_1(W - D)$$

Here, $\rho_1$ is the density at the site just behind the front particle. The above expression for the front velocity can be understood by visualising the front particle as a random walker moving with rate $\epsilon + D$ in the forward direction and with rate $W\rho_1 + D(1 - \rho_1)$ in the backward direction.

From Eq. 1, it is obvious that we need to know $\rho_1$ in order to predict the front velocity $V$ and there is no systematic method to find this $\rho_1$ exactly. However, several approximations have been proposed, for example, in $\rho_1$ was taken as the bulk density $\bar{\rho} = \frac{N}{L}$. This approximation is exact for $W = D$ and shows reasonable agreement when $|W - D|$ is small but for larger $|W - D|$ we observe poor agreement, see Fig. 1. In order to make better estimate for $\rho_1$, especially when we are away from the special point $W = D$, in $\bar{\rho}_1$, we proposed a method which systematically improves analytic estimate to the desired degree of accuracy. Here we write a master equation in the frame moving with the front particle and study the evolution of one $l = 1$, two $l = 2$, three $l = 3$ sites behind the front. For example, for $l = 1$, we study the states $\{01, 11\}$ and for $l = 2$ we have the following set of states $\{001, 011, 101, 111\}$, with the rightmost ‘1’
from this, it uses the ansatz stricts its applicability for nonzero values of \( W \) between the first and second particle. This ansatz clearly representing the front. For larger value of \(|W − D|\), we need to study the states corresponding to larger values of \( l \) in order to get better analytic estimates but writing the transition matrix corresponding to the master equation becomes more difficult as its size increases as \( 2^l \times 2^l \). In order to make analytically tractable approximation for \( \rho_1 \) and hence the front velocity we have presented reduced three particle representation.

In \([3]\), Kerstein proposed a two particle representation for the reaction diffusion process \( A \rightarrow 2A \), where we study the evolution of following set of states: \([11, 101, 1001, 10001, \ldots]\), with rightmost ‘1’ representing the front. The important point that we note here is that this set of states is closed under the transition for \( W = 0 \) while for \( W \neq 0 \) it is not closed. This restricts its applicability for nonzero values of \( W \). Apart from this, it uses the ansatz \( p_j = p_0(1 − p_0)^j \), where \( p_j \) is the probability that there are \( j \) empty sites between the first and second particle. This ansatz clearly neglects the spatial density correlation which is, in general, not true, see Fig. \([2]\). In fact this correlation increases with \(|W − D|\) and vanishes for the special point \( W = 0 \). The ansatz also assumes the sites behind the front to be at the same density \( p_0 \), which is, of course, not true, Fig. \([1]\). This leads to a systematic error in the analytic estimates which increases gradually with increasing value of \(|W − D|\). However, one can get better and better results by studying the states having larger number of particles, for example in \([4]\), we presented mixed representation in which we study the following set of states \([011, 111, 0101, 1101, 01001, 11001, \ldots]\) with the rightmost ‘1’ representing the front and as expected we get better analytic estimates as compared to two particle representation. But writing the master equation gets complicated as we increase the number of particles in the states.

Here, in this paper we present a simple analytic estimate for \( \rho_1 \) and hence the front velocity which are in excellent agreement with the simulation results. Here we propose a self consistent two-site representation, where we write master equation in the frame moving with the front particle(as in \([3]\)) for the evolution of two states \([0A, AA]\). Here the rightmost \( A \) represents the front particle. In this truncated representation these two states make transition between each other due to the microscopic processes of the model and form a closed set under such transitions. For example, \( 0A \rightarrow AA \) if the leading particle gives birth to its left empty site with rate \( \epsilon \). Diffusion of the leading particle to its left changes the state \( 0A \rightarrow AA \), provided the second site \( (F − 2) \) behind the leading particle is occupied and remains unchanged if it is empty. If the probability of occupancy at \( F − 2 \) is denoted as \( \rho_2 \) then the transition \( 0A \rightarrow AA \) occurs with rate \( D\rho_2 \). Similarly, when the leading particle in the realization \( AA \) gets annihilated the state of realization changes to \( 0A \) if \( F − 2 \) is empty with rate \( W(1 − \rho_2) \) while state \( AA \) 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,

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

\[
\dot{P}_{AA} = (2D\rho_2 + 2\epsilon + \epsilon\rho_2)P_{0A} − (2D − D\rho_2 + 2W)P_{AA}.
\]

(2)

From Eq. \([2]\), it is obvious that we need to know \( \rho_2 \) in order to find the steady state probabilities \( P_{0A} \) and \( P_{AA} \). In \([5]\), \( \rho_2 \) was approximated as \( \bar{\rho} \) = bulk density \( \frac{\rho}{1+W} \), which works reasonably well for smaller values.
for $|W - D|$ but shows poor agreement with the larger values of $|W - D|$. We note that $\rho_2$, in general, is a function of all the parameters ($\epsilon$, $D$, $W$) of the model. We express the dependence of $\rho_2$ on the parameters as follows:

$$\rho_2 = aP_{AA} + bP^2_{AA}$$

(3)

Here, the dependence of $\rho_2$ on the parameters is expressed implicitly by $P_{AA}$ whose solution is to be sought and hence we call the method self consistent. Now using the fact that when $W = D$, $\rho_2 = P_{AA} = \bar{\rho} = \epsilon/(\epsilon + D)$, we rewrite equation (3) as:

$$\rho_2 = (1 - \frac{b\epsilon}{\epsilon + D})P_{AA} + bP^2_{AA}$$

(4)

Using this value of $\rho_2$ in the master equation (2) and using the normalisation condition $P_{\bar{A}A} + P_{AA} = 1$, we obtain the following equation.

$$\alpha P^3_{AA} + \beta P^2_{AA} + \gamma P_{AA} - \delta = 0$$

(5)

with

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

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

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

$$\delta = 2\epsilon^2 + 2\epsilon D.$$

(6)

Now Eq. (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 the Fisher velocity $V_0 = 2\sqrt{\epsilon D}$. Also from equation (1), the front velocity is given as $V = D\rho_1 = DP_{AA}$, when $D$ is very large compared to $\epsilon$ and $W$. Equating this velocity with the Fisher velocity $V_0$, we get $P_{AA} = 2\sqrt{\text{AA}}$. Now substituting this value of $P_{AA}$ in Eq. (6), we have an equation which is linear in $b$ and which in the limit $D \to \infty$ gives $b = \frac{1}{4}$. Substituting this value of $b$ in the Eq. (6) we obtain the following cubic equation in $P_{AA}$.

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

(7)

One can easily solve the above cubic equation and the density at site just behind the front particle $\rho_1 = P_{AA}$ can be obtained. The results obtained have been shown in the Figs. 3 and 4 and are in excellent agreement with the simulation results. Here we have also shown the percentage relative error in $\rho_1$. i.e., $\frac{|\rho_1 - \rho_1^s|}{\rho_1^s} \times 100$, where $\rho_1^s$ and $\rho_1^t$ correspond to simulation and analytic results. Once we know this $\rho_1$, the front velocity is obtained from Eq. (1) and we have shown it in the Fig. (3) and (4). Here, we also observe very good agreement with the simulation results. In Figs. (3) and (4) we have compared the results with that of Kerstein two particle representation. The interesting thing that we notice here is that the results obtained from the present work is 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 $A \leftrightarrow 2A$ whose results are in excellent 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 work appears to have an advantage over Kerstein’s two-particle representation.
representation due to two key factors: firstly, TSSCM does not neglect the spatial density correlation which, indeed, is neglected in two particle representation by using the product measure ansatz, secondly, TSSCM forms a closed set of states under transitions due to the microscopic processes for all parameter regimes while the two-particle representation does not provide a closed set for $W \neq 0$. The simplicity of our analytic method provides a scope to study the velocity of propagating front in other reaction diffusion processes as well.

**FIG. 5**: Comparison between simulation and analytic results for front velocity $V$ 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 present work. We note that the results of TSSCM are essentially coincident with the simulation results. Inset: Percentage relative error in $V$.

**FIG. 6**: Comparison between simulation and analytic results for front velocity $V$ for $\epsilon = 0.25, W = 0.125$ and for different values of $D$. 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 $V$.

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