We study front propagation in the reversible reaction-diffusion system $A + A \leftrightarrow A$ on a 1-d lattice. Extending the idea of leading particle in studying the motion of the front we write a master equation in the stochastically moving frame attached to this particle. This approach provides a systematic way to improve on estimates of front speed obtained earlier. We also find that the leading particle performs a correlated random walk and this correlation needs to be taken into account to get correct value of the front diffusion coefficient.

### I. INTRODUCTION

Propagation of fronts into unstable states in reaction-diffusion systems has been an actively studied topic for a long time [1]. The dynamics of propagating fronts is of interest in various diverse physical situations [2]. Recently, there is renewed activity concerning connection between fronts in microscopic discrete stochastic models and macroscopic deterministic equations which are believed to be their mean-field limits [3]. In this paper we study front propagation in a system of reacting and diffusing particles on an infinite 1-d lattice (Fig.1). Initially, left half of the lattice is filled with a certain density of particles with the right half being completely empty, resulting in a sharp boundary between the two halves. As the system evolves, the particles move to the right resulting in a propagating front. After an initial transient, the front moves with an asymptotic speed $v$. Further, due to the inherent stochastic nature of the dynamics, the ensemble averaged front profile undergoes diffusive broadening (1a) with an associated diffusion coefficient $D_f$.

![FIG. 1. Schematic picture of the development of front in the reaction-diffusion system. (a): The ensemble averaged front propagates with a unique asymptotic speed $v$ and spreads diffusively with a coefficient $D_f$. (b) If the ensemble average is taken in a frame moving with the leading particle in each realization, the profile obtained is a time-invariant profile. The three profiles shown for different values of the parameters of the microscopic model discussed later in the text.](image)

There are a number of alternative definitions of the position of the front in any given realization of the process but it is found that all of them lead to the same values of $v$ and $D_f$. The simplest choice, which is also the easiest to implement numerically, is to take the position of the rightmost particle at any time to be the location of the front [5–7]. Thus, the dynamics of the front is reduced, in an approximate way, to the dynamics of a single particle - the leading particle. Treating the motion of this particle as a biased random walk, simple approximate expressions for the speed $v$ and diffusion coefficient $D_f$ have been derived [7,6]. However, in these approaches it is hard to find a systematic way to improve estimates for $v$ and $D_f$. In the present paper we show that by writing the front dynamics in a frame moving with the leading particle one can get numerically better estimates of the front speed and diffusion coefficient. We also show that the motion of the leading particle is correlated in time and thus the front diffusion coefficient differs from that obtained from a simple random walk approximation.

### II. MODEL AND RESULTS FOR $V$ AND $D_F$

We consider a 1-d lattice ($-\infty < i < \infty$) in which each site can hold atmost one particle ('hard-core exclusion'). The particles (denoted by A) undergo three basic microscopic processes: (i) Birth/creation: a particle can generate a new one on a neighbouring empty site with rate $\epsilon$, (ii) Death/annihilation: one of the two neighboring particles gets annihilated with rate $W$, and (iii) Diffusion: A particle diffuses to a neighbouring empty site with rate $D$ (see Fig.2). Initially, at $t = 0$, the left half of the lattice ($i \leq 0$) is filled with particles at a density $\rho = \overline{\rho}$, where $\overline{\rho} = \epsilon/(\epsilon + W)$ is the density of the equilibrium phase obtained if the process is allowed to occur in a finite system [8]. There are only two independent parameters in the system as one of the three rates $\epsilon, D, W$ can be scaled away by choosing the time scale appropriately. In all our simulations $\epsilon = 0.25$ and the two ratios $D/\epsilon$ and $W/\epsilon$ are of the order of unity. As was noted in [7], this choice is fairly generic for the diffusion limited fluctuation dominated regime we would like to focus on.
In the mean-field description, which is expected to be valid in the limit $D \to \infty$ and the evolution of the front is described by the F-KPP equation [9] $\partial_t \rho = D \partial^2_x \rho + \epsilon \rho - (\epsilon + W) \rho^2$, where $\rho$ is the coarse grained density of A particles. The front speed is then given by $v_0 = 2\sqrt{\epsilon D}$.

For the case $W = 0$, which arises naturally in the context of turbulent flame front propagation [5], the existence and uniqueness of an asymptotic front solution were established rigorously in [10] and it was shown that the 'mean-field' limit is obtained as $D \to \infty$. For finite values of $D$, a 'two particle' representation was used in [6] to get an approximate value of the front speed which works quite well for $D/\epsilon \sim O(1)$. In [4], using the inter-particle distribution functions an exact solution was obtained for the special case $W = D$. In this case, it was shown that in each realization of the front evolution, the leading particle performs a biased random walk and the particles behind it are distributed exactly in equilibrium with density $\rho = \overline{\rho}$. The speed and the diffusion coefficient were found to be $v = \epsilon$ and $D_f = \epsilon + D$ respectively.

If $W \neq D$, the method used in [4] does not work and an exact solution is no longer possible. Also, the two particle representation of [6] does not close if particle annihilation is introduced, i.e, $W > 0$. In [7], an approach based explicitly on the motion of the leading particle as a biased random walker was introduced and the following approximate expressions for speed and diffusion coefficient were obtained.

$$v = \epsilon - \rho_1(W - D); 2D_f = 2D + \epsilon - \rho_1(W - D),$$ (1)

where $\rho_1$ is the probability of occupation of the site just behind the leading particle. Expression (1) above may be written down by noting that the front moves right with rate $P = \epsilon + D$ (i.e. whenever a particle is created to the right of the leading particle or the later makes a diffusive move to the right). The leading particle takes a negative step when it gets annihilated by the particle on the left (with rate $W \rho_1$) or if it makes a diffusive move to an empty left site (with rate $D(1 - \rho_1)$), where $\rho_1$ is the occupation probability of the site immediately to the left of the leading particle. For $W = D$, these results reduce to those obtained exactly in [4]. In order to get more accurate values of $v$ and $D_f$ one needs to find better estimates of $\rho_1$ (the bulk value $\rho_1 = \overline{\rho}$ was used in [7]). While (1) works quite well (with $\rho_1 = \overline{\rho}$) for $W$ close to $D$, there are significant deviations as one moves away from this special point.

In order to get successively better estimates for $\rho_1$, we look at the invariant profile of the front as observed from the leading particle. Starting from an ensemble of $\mathcal{N}$ realizations this invariant profile is obtained, after an initial transient time, by aligning the leading particle of each member of the ensemble (Fig. 1b). From the definition of $\rho_1$ it then follows that out of the $\mathcal{N}$ realizations $\rho_1 \mathcal{N}$ have a particle in the site to the left of the leading particle and the rest $(1 - \rho_1)\mathcal{N}$ have an empty site next to it. In the steady state (which is asymptotically reached after transients) it thus follows that there is a kinetic balance between the two types of realizations: those with 11 or 01 as the occupancy of the rightmost pair of sites (where the second 1 denotes the leading particle). Thus, the two states 01 and 11 may be thought of as a truncated representation of the full lattice. Due to the microscopic moves there are transitions between these two 'states'. For example, in a realization in the 11 state the leading particle makes a diffusive move to the right, the state of realization changes to 01 [11]. Considering all such transitions one can write a master equation for the probabilities $p_{11}$ and $p_{01}$ in this truncated state space [12]

$$\dot{p}_{01} = (2D - D\rho_b + 2W)p_{11} - (2D\rho_b + 2\epsilon + \epsilon\rho_b)p_{01},$$

$$\dot{p}_{11} = (2D\rho_b + 2\epsilon + \epsilon\rho_b)p_{01} - (2D - D\rho_b + 2W)p_{11}. \quad (2)$$

In the steady state $\dot{p}_{01} = 0 = \dot{p}_{11}$ and one obtains ($p_{11} = \rho_1$ in steady state)

$$\rho_1 = \frac{3\epsilon^2 + 2\epsilon(W + D)}{3\epsilon^2 + 2W^2 + 4\epsilon W + 3\epsilon D + 2WD} \quad (3)$$

where we have used $\rho_b = \overline{\rho}$, an approximation which becomes better as one includes more sites in the truncated representation. E.g. we have also computed $\rho_1$ by keeping $l = 3$ sites (i.e. 4 states: 111, 011, 101, 001), $l = 4$ sites (8 states) and the values obtained for $\rho_1$ are plotted in Fig. 3 and the corresponding front speed (using Eq.(1)) in Fig. 4. It is to be noted that expression (3) above reduces to $\rho_1 = \overline{\rho}$ for $W = D$ as it should. Further, in this approach it is also possible to obtain the spatial density correlation between site occupancies $\phi_{12} = \langle n_1n_2 \rangle - \rho_1\rho_2/\overline{\rho}^2$ (Fig. 5).
A. Reduced 3-particle representation

The drawback of the above approach is that it is not easy to write the transition matrix as the number of sites \( l \) is increased (number of states increases as \( 2^l \)). In the following we try to find an analytically tractable estimate for \( \rho_1 \) using an alternative reduced representation similar to Kerstein’s approach [6]. Instead of keeping a fixed number of sites to denote a state, Kerstein chose the following infinite set of two particle states: \( \{11, 101, 1001, 10001, \cdots \} \) where the ‘k’th state has \( k \) empty sites between the leading particle (denoted by the 1 on the right) and the next particle (denoted by the 1 on the left). If there is no annihilation process, i.e., \( W = 0 \), then these set of states is closed with respect to transitions between the states. However, as was pointed out in [7], this breaks down as soon as \( W > 0 \). To see this let us consider the 11 state and the microscopic process in which one of the two particles gets annihilated. The resulting state depends upon the location of the third particle in the initial configuration of the lattice. I.e., one needs to go to a 3-particle representation. However the same problem occurs while considering annihilation in the 111 state. Thus, to take care of this problem which arises due to the effective non-locality in transition rates by going to the moving frame attached to the leading particle one needs to make a reasonable truncation of the hierarchy. We extend the set of states by including the states \( \{111, 1101, 1011, \cdots \} \) where the rightmost 1 denotes the leading particle. Let us denote by \( p_k \) the probability of the two particle states \( 1\, 0 \ldots 0 \, 1 \) with \( k \) empty sites between the leading particle and the next and by \( q_k \) the probability of the three particle state \( 1\, 0 \ldots 0 \, 1 \, 1 \) with \( k \) empty sites between the second and the third particles. The transition rates within these states can be written down following the procedure as in the case of fixed number of sites representation discussed above and one obtains the following rate equations for the \( p_k \)’s.

\[
\begin{align*}
\dot{p}_k &= (2D - D\rho + W\rho)p_{k-1} + (2D + \epsilon)p_{k+1} \\
&\quad + (q_{k-1} + q_k)W - (4D - D\rho + 3\epsilon + W\rho)p_k; \quad k \geq 2, \\
\dot{p}_1 &= (2D - D\rho)p_0 + (2D + \epsilon)p_2 + (2q_0 + q_1)W \\
&\quad - (4D - D\rho + 3\epsilon + W\rho)p_1; \\
\dot{p}_0 &= (2D + \epsilon)p_1 + 2(1 - p_0) - (2D - D\rho - 2W)p_0,
\end{align*}
\]

where we made the approximation that \( \rho \) is the probability that the site next to the last particle in the two or three particle states is occupied independent of its distance from the leading particle. We do not write the
equations for $q_k$’s as it can be shown that they can be eliminated in the steady state. To obtain the steady state solution $p_k = 0$, following Kerstein, we make the ansatz $p_k = p_0 (1 - p_0)^k$ and write $\rho = A p_0 - B p_0^2$ to take care of the ignored correlations in the ansatz in a phenomenological way. The parameters $A$ and $B$ are fixed in the following way. We first note that for $D = W$, both the quantities $\rho$ and $p_0$ equal the bulk density, namely, $\rho = p_0 = \rho = \epsilon/(\epsilon + W)$ implying $A = 1 + \epsilon B/(\epsilon + W)$ and thus

$$\rho = (1 + \frac{\epsilon B}{\epsilon + W}) p_0 - B p_0^2$$  \hspace{1cm} (5)$$

This form also ensures that $W = 0$ and $p_0 = 1$ imply $\rho = 1$. Using $\rho$ from Eq. (5) in Eqs. (4) (in steady state $p_k = 0$) we get the following cubic equation for $p_0$,

$$DB(\epsilon + W)p_0^3 + (\epsilon^2 + \epsilon W + \epsilon D + WD - DB\epsilon)p_0^2$$

$$+ (\epsilon^2 + 3\epsilon W + 2W^2)p_0 - 2\epsilon^2 - 2\epsilon W = 0$$  \hspace{1cm} (6)$$

In order to fix $B$ we note that for large $D$ we expect the front to approach the mean-field limit with the speed given by $v_0 = 2\sqrt{\epsilon D}$. Since, in terms of $p_0$, the velocity is given by (from eq. (1)) $v = \epsilon - (W - D)p_0 \sim Dp_0$ for $D >> W, \epsilon$, this implies, in this limit, $p_0 = 2\sqrt{2\epsilon D}$. Substituting this expression for $p_0$ in Eq. (6) we obtain $B = 3(\epsilon + W)/4\epsilon$. Using this expression for $B$ in Eq. (6) one obtains $p_0 = \rho_1$ implicitly through,

$$D = \frac{4\epsilon(2\epsilon - \rho_1^2 - \epsilon \rho_1 - 2\rho_0 W)}{(\epsilon + 3\epsilon \rho_1 + 3W \rho_1^2)}$$  \hspace{1cm} (7)$$

The result is shown in Fig. 3 (square symbols marked as 2P). We note that, although several ad-hoc assumptions were made in arriving at eq. (7), including using results that are strictly valid in the mean-field limit $D \rightarrow \infty$, the agreement with direct numerical results is remarkable even for the finite values of $D$ considered.

**B. Diffusion coefficient: $D_f$**

In Fig. 6, we plot the front diffusion coefficient $D_f$ as a function of $D$ ($W = 0$, $\epsilon = 0.05$). The lower curve is from direct simulation and the upper one is that obtained from Eq. (1) by using the most accurate estimate of $\rho_1$. We see marked deviation of the values obtained from the analytic expression which implies that the simple (uncorrelated) random walk picture of the leading particle in not quite correct. The motion of a correlated biased random walker is described by $x(t + 1) - x(t) = v + \eta(t)$ where the noise term $\eta$ is temporally correlated: $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\eta(t') \rangle = C(t - t') \neq 0$. The mean speed of the walker is $v$ and the asymptotic diffusion coefficient is given by

$$D_f = \sum_{t=0}^{\infty} \langle \eta(0)\eta(t) \rangle = \sum_{\tau=0}^{\infty} C(\tau).$$  \hspace{1cm} (8)$$

Indeed, for the front under study we find that there is long range correlation between the successive steps of the leading particle (Fig. 6, inset). This correlation is non-positive for all parameters (both $D > W$ as well as $D < W$) and vanishes for the special case of $D = W$. Once this correlation is taken into account the diffusion coefficient matches reasonably well with that obtained from direct simulations for the range of $D$ studied [13]. Preliminary fits indicate that the correlation function has the functional form $C(t) = A t^{-\alpha} \exp(-t/\tau)$.

**III. CONCLUSION**

We have illustrated the usefulness of the leading particle picture in describing the propagation of fronts in the $A + A \leftrightarrow A$ reaction-diffusion process in the diffusion controlled limit in one dimension. By writing the master equation in the moving frame attached to the leading particle we are able to obtain better numerical estimates for the density of the site behind the leading particle and thus the front speed. In addition, this approach, in principle allows one to compute the spatial density profile and density-density correlations away from the special point $D = W$.

Our numerical results show that the motion of the leading particle is correlated in time and this needs to be taken into account in order to get the correct diffusion coefficient. It is seen that this correction increases with increasing $D$ (the microscopic particle diffusion constant) and thus it might play an important role in determining how the mean-field limit is achieved as $D \rightarrow \infty$.

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[13] Values of $D_f$ obtained from eq. (1) is essentially $C(0) = \langle \eta^2(0) \rangle$. 