Velocity of front propagation in the epidemic model $A + B \rightarrow 2A$.

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We study front propagation in the irreversible epidemic model $A + B \rightarrow 2A$ in one dimension. Here, we allow the particles $A$ and $B$ to diffuse with rates $D_A$ and $D_B$, which, in general, may be different. We find analytic estimates for the front velocity by writing truncated master equation in a frame moving with the rightmost $A$ particle. The results obtained are in reasonable agreement with the simulation results and are amenable to systematic improvement. We also observe a crossover from the linear dependence of front velocity $V$ on $D_A$ for smaller values of $D_A$ to $V \propto \sqrt{D_A}$ for larger $D_A$, but numerically still significantly different from the mean field value. The deviations reflect the role of internal fluctuations which is neglected in the mean field description.

I. INTRODUCTION

In many natural phenomena we encounter propagating fronts separating different phases [2]. In this paper we study the autocatalytic reaction $A + B \rightarrow 2A$ in a one dimensional lattice. Models of this type have been studied actively because of several interesting features of the process [3] [4] [5]. We can think of this reaction as a model for various spreading phenomena such as an epidemic: particle $A$ is an infectious agent which infects a healthy particle $B$ on contact. We are interested in finding the velocity of propagation of this infection. The macroscopic description for this process is given by the following mean field equation [1].

$$\frac{\partial \rho_A}{\partial t} = D_A \Delta \rho_A + \epsilon \rho_A \rho_B = D_A \Delta \rho_A + \epsilon \rho_A (\rho_0 - \rho_A)$$  \tag{1}

Here, $\rho_A(x,t)$ is the local density of $A$ particle at position $x$ and time $t$, $D_A$ is its diffusion coefficient and $\epsilon$ is the reaction rate of the particle. In the second line we have used $\rho_A + \rho_B = \rho_0$ which is constant. Equation (1) arises in the macroscopic description of diverse physical processes and serves as a generic model for front propagation in a system in which a stable state invades an unstable state [2]. Equation (1) allows a family of travelling wave solutions with speed $V \geq 2\sqrt{\epsilon \rho_0 D_A}$ invading the unstable state $\rho_A = 0$ from the stable state $\rho_A = \rho_0$. However, for steep enough initial conditions, the selected asymptotic speed is the minimum speed $V_0 = 2\sqrt{\epsilon \rho_0 D_A}$ [2]. In the microscopic lattice model in low dimensions, the discreteness effects alter the dynamical properties of the propagating front and the results obtained are different from that using deterministic mean field equation [3] [4]. Here, in this paper we will present the Monte Carlo simulation results and approximate analytic prediction for the front velocity in a one dimensional lattice model for $A + B \rightarrow 2A$ defined in the next section (II).

II. MODEL AND FRONT VELOCITY

In our simulation, we start with a 1D lattice $[0, \infty)$ initially randomly filled with $B$ particles with overall concentration $\rho_0$. We have taken hard core exclusion into account: any site can be occupied by maximum one particle. At the left end of the lattice we place an $A$ particle. We allow both the particles $A$ and $B$ to diffuse to the nearest neighbour empty sites with rates $D_A$ and $D_B$ respectively. When a 'sick' particle $A$ encounters the 'healthy' one $B$ sitting on a neighbouring site, then $B$ gets infected with rate $\epsilon$ and is converted to an $A$ particle.

In this way the front (rightmost $A$) propagates and we wish to find the velocity of this front.

In Ref. [2], authors studied a similar problem using Smoluchowski approach [6] and obtained the steady state density for $B$ and $A$ particles at a distance $x$ from the moving front particle $(x = 0)$ as: $\rho_B(x > 0) = \rho_0 (1 - e^{-\epsilon x/(D_A + D_B)})$ and $\rho_A(x < 0) = \rho_A$ respectively. By invoking the equality of particle fluxes to the left and right, they found $\rho_A = \rho_0$, but it does not fix the front propagation velocity $V$. In the present paper, we try to find the expression for the front velocity by visualising the front as random walker moving with forward and backward rates as $P_+$ and $P_-$ respectively, and thus speed of the front $V = P_+ - P_-$. In order to compute $P_+$, we notice that there are two ways in which the front will move to the right: (1) when the front diffuses to the right neighbouring site, provided it is empty with rate $D_B(1 - \rho_B^*)$, here $\rho_B^*$ is the probability that site just ahead of the front is occupied, (2) when the site just ahead of front is occupied by $B$ particle, then due to reaction it changes the neighbouring $B$ into $A$ and thus the front moves forward with rate $\epsilon \rho_B^*$ and hence $P_+ = \epsilon \rho_B^* + D_A(1 - \rho_B^*)$. Similarly, the front moves backward due to its diffuse move to the left empty neighbouring site and hence $P_- = D_A(1 - \rho_B^*)$, $\rho_B^*$ is the probability that site just behind the front is occupied. Using these values for $P_+$ and $P_-$, we have for the asymptotic velocity,

$$V = \epsilon \rho_B^* + D_A(\rho_B^- - \rho_B^*),$$  \tag{2}

which is exact, given $\rho_B^*$ and $\rho_B^-$. The multi-particle nature of the problem is embodied in finding $\rho_B^*$ and $\rho_B^-$. The fact that equation (2) is exact can be seen from the excellent agreement between simulation result of $V$ and its estimate using values of $\rho_B^*$ and $\rho_B^-$ obtained directly from simulation, Fig. (I). Here, we also observe a
FIG. 1: Front velocity $V$ as a function of $D_A$ for $D_B = 0.05, \epsilon = 0.2, \rho_0 = 0.5$. The broken line represents the front velocity obtained by simulation while the filled circles correspond to the velocity obtained by using Eq. (2) and substituting the values of $\rho^+_1$ and $\rho^-_1$ from simulation. Inset: The difference $|\rho^-_1 - \rho_0|$ as a function of $D_A$, $\rho^-_1$ taken directly from simulation.

FIG. 2: Log-log plot for the front velocity as a function of $D_A$ for $D_B = 0.05, \epsilon = 0.2, \rho_0 = 0.5$. Here $V \propto D_A^{\alpha}$ and we notice a crossover from $\alpha \approx 1.0$ to $\alpha \approx 0.5$. Crossover from linear dependence of $V$ on $D_A$ for small $D_A$ to $V \propto \sqrt{D_A}$ for large $D_A$ as shown in Fig. 2, although we have verified that $V \neq V_0$ (mean field value).

From Fig. 2, the density profile of $A$ particles behind the front is constant and equal to $\rho_0$. Thus we can make approximation $\rho^-_1 = \rho_0$. But we note that this approximation fails to work when $D_A = 0$ where we get $\rho_A = 1$ at all the sites behind the front irrespective of $\rho_0$. Thus the approximation $\rho^+_1 = \rho_0$ works better for larger values of $D_A$ while for smaller $D_A$ it appears to be a poor approximation as shown in the Fig. 1 inset. Now using the approximation $\rho^+_1 = \rho_0$ we try to find analytic expression for $\rho^+_1$. In the following we find an approximate analytic expression for $\rho^+_1$ using the technique developed in [11].

The technique involves writing a truncated master equation in a frame moving with the front (i.e. the rightmost $A$ particle). For example, the simplest one is the set of two states $\{A\phi, AB\}$. In this truncated representation each state contains the occupancy at two sites ($l = 2$), the leftmost $A$ represents the front particle while $\phi$ and $B$ stand for empty and a site occupied by $B$ just ahead of the front respectively. These two states make transitions between each other due to reaction or diffusion of particles, see Fig. 3. For example, in the transition shown in Fig. (3a), the configuration $AB$ changes to $A\phi$ if $A$ particle diffuses to its left empty site and it takes place with rate $D_A(1 - \rho^-_1)$. In Fig. (3b), diffusion of $B$ particle in the configuration $AB$ to its right neighbouring empty site changes $AB$ to $A\phi$. If the probability of occupancy of $B$ particle at a second site ahead of the front is denoted by $\rho^+_2$, then $AB \rightarrow A\phi$ with rate $D_B(1 - \rho^+_2)$. In the Fig. (3c), when $A$ infects $B$ in the configuration $AB$ then $AB \rightarrow A\phi$ if the second site ahead of the front is empty and this occurs with rate $\epsilon(1 - \rho^+_2)$. Similarly, in Fig (3d), $A\phi$ changes to $AB$ with rate $D_B\rho^+_2$. Thus considering all the transitions between the two states $A\phi$ and $AB$ and approximating $\rho^-_1 = \rho_0$, the following master equation may be written [11]:

$$\frac{dp_A}{dt} = \{D_B(1 - \rho^+_2) + D_A(1 - \rho_0) + \epsilon(1 - \rho^+_2)\}p_{AB} - \{D_A + D_B\rho^+_2\}p_{A\phi},$$

$$\frac{dp_{AB}}{dt} = \{D_A + D_B\rho^+_2\}p_{A\phi} - \{D_B(1 - \rho^+_2) + D_A(1 - \rho_0) + \epsilon(1 - \rho^+_2)\}p_{AB}.$$  \hspace{1cm} (3)

In the steady state, by definition, $\rho^+_1 = p_{AB}$ and thus from Eq. 2 with the normalization $p_{A\phi} + p_{AB} = 1$ we obtain

$$\rho^+_1 = \frac{(D_A + D_B)\rho^+_2}{\{D_B + D_A\rho^+_2 + D_A(1 - \rho_0) + \epsilon(1 - \rho^+_2)\}}.$$  \hspace{1cm} (4)

Thus, in order to find $\rho^+_1$ we need to know $\rho^+_2$ and as
a first approximation assuming $\rho_1^+ = \rho_0$, we find

$$\rho_1^+ = \frac{(D_A + D_B)\rho_0}{D_A + D_B + \epsilon/(1 - \rho_0)} \quad (5)$$

Using this approximation for $\rho_1^+$ in Eq. (2) we obtain the following expression for the velocity,

$$V = \frac{\epsilon \rho_0 (2D_A + D_B - D_A \rho_0)}{D_A + D_B + \epsilon/(1 - \rho_0)} \quad (6)$$

We have shown the estimate for the velocity as obtained from Eq. (3) in Fig. 4. Here we note that when $D_A = \epsilon$ the expression for $V$ is independent of $\rho_1^+$ and hence we obtain nice agreement between the theory and simulation results. But the dependence of $V$ on $\rho_1^+$ increases gradually with the increasing magnitude of $\epsilon - D_A$ and hence we observe poor agreement between analytic and simulation results as we move away from the point $D_A = \epsilon$. In order to get better prediction for the velocity, especially for larger values of $\epsilon - D_A$, we need to study the states having larger number of particles. For example, we studied the following set of states ($l = 3$): $\{A\phi\phi, AB\phi, A\phi B, ABB\}$. If we denote the probability of occupancy at third site ahead of the front as $\rho_3^+$, the evolution of these states is described by the following master equation.

$$\begin{align*}
\frac{dp_{A\phi\phi}}{dt} &= \{DB(1 - \rho_3^+) + DA(1 - \rho_0)\}p_{A\phi\phi} + \epsilon(1 - \rho_3^+)p_{AB\phi} - (DA + DB)\rho_3^+ p_{A\phi\phi}, \\
\frac{dp_{A\phi B}}{dt} &= (DA + DB)\rho_3^+ p_{A\phi\phi} + \{(DA + DB)\rho_3^+ + DB + DA(1 - \rho_0)\}p_{A\phi B} + \epsilon\rho_3^+ p_{AB\phi} + DA(1 - \rho_0)p_{ABB} - 2DA + 2DB - DA\rho_0 - DB\rho_3^+ p_{A\phi\phi}, \\
\frac{dp_{AB\phi}}{dt} &= \{(DB + DA(1 - \rho_3^+)\}p_{AB\phi} + DB(1 - \rho_3^+) + \epsilon(1 - \rho_3^+)\}p_{ABB} - \{DA + DB + \epsilon - DA\rho_0 - DB\rho_3^+\}p_{AB\phi}, \\
\frac{dp_{ABB}}{dt} &= DArho_0 + DB\rho_3^+ p_{ABB} - \{DA + DB + \epsilon - DA\rho_0\}p_{AB\phi}.
\end{align*} \quad (7)$$

In order to solve the Eqs. (7) we need to know $\rho_3^+$. To find the steady state solution of Eq. (7), and thus $\rho_3^+ = p_{AB\phi} + p_{ABB}$, one could approximate $\rho_3^+ = \rho_0$, as was done for $l = 2$ case. However, a better estimate for $\rho_3^+$ can be obtained by writing a mean field equation for the densities $\rho_2^+$ and $\rho_3^+$ at second and third site ahead of the front,

$$\begin{align*}
\frac{d\rho_2^+}{dt} &= (\rho_1^+ + \rho_2^+)(1 - \rho_2^+)DB - DB\rho_2^+ (2 - \rho_1^+ - \rho_3^+), \\
\frac{d\rho_3^+}{dt} &= (\rho_2^+ + \rho_3^+)(1 - \rho_3^+)DB - DB\rho_3^+ (2 - \rho_1^+ - \rho_3^+).
\end{align*} \quad (8)$$

In steady state Eqs. (8) gives, $\rho_3^+ = (\rho_1^+ + 2\rho_2^+)/3$. Now using the value of $\rho_1^+$ from Eq. (4) and approximating $\rho_4^+ = \rho_0$, we obtain the following approximate expression for $\rho_3^+$.

$$\rho_3^+ = \frac{3DA\rho_0 + 3DB\rho_0 + 2\epsilon\rho_0(1 - \rho_0)}{3\{DA + DB + \epsilon(1 - \rho_0)\}} \quad (9)$$

Using this value of $\rho_3^+$ in Eqs. (7), we obtain the steady state solution satisfying the normalisation $p_{A\phi\phi} + p_{A\phi B} + p_{AB\phi} + p_{ABB} = 1$. Once we know these probabilities the density at site just ahead of the front is obtained as: $\rho_1^+ = p_{ABB} + p_{ABB}$. Substituting this value of $\rho_1^+$ in Eq. (4), we obtained an improved analytic estimates for the velocity as shown in the Fig. 4. Here we notice that as $l$ increases the data corresponding to the analytic estimate comes closer to the simulation result. In this approach one can systematically improve upon the estimates for $\rho_1^+$ and thus $V$ by including states having successively larger number of particles. We have also observed that when $D_A = 0$, the front position $x$ grows with time $t$ as $t^{1/2}$ as was reported in [3]. Hence, when $D_A = 0$, the asymptotic velocity $V$ approaches to zero. Using Eq. (4) for $D_A = 0$, velocity is given as $V = \epsilon \rho_1^+$. The condition for zero velocity simply implies that $\rho_1^+ \to 0$. In the Fig. 4, we have shown the simulation results for the density profile ahead of the front for different values of $D_A$ and notice that as $D_A \to 0$, $\rho_1^+ \to 0$, which gives $V \to 0$. We also note that when $D_A = 0$, all particles form a compact cluster while $B$ particles keep on moving diffusively. The number of $A$ particles created during time interval $dt$, $dN_A = V dtdt$ should be equal to the number of consumed $B$ particles, $dN_B = V\rho_0 dt$. However, the equality $dN_A = dN_B$ holds for non zero $V$ only if $\rho_0 = 1$ while for $\rho_0 \neq 1$, it gives $V = 0$. We also notice that when $D_A = 0$, the front dynamics is like a DLA in 1d, where, $A$ particles are static and growth occurs when $B$ particle diffuses and sticks with the neighbouring $A$ particle.

### III. CONCLUSION

In this paper we have analyzed the reaction $A + B \to 2A$ using an approximate analytic method and Monte Carlo simulation. Considering the front as the position of rightmost $A$ particle we have been able to obtain analytic estimate for its velocity by writing master equation in the frame moving with the front. One can improve upon the results systematically by including states with successively larger number of sites in front of the leading
A particle. The mean field equation (1) gives $V \propto \sqrt{D_A}$, but we observe linear dependence, $V \propto D_A$ for small $D_A$ reflecting the important role of discrete fluctuations which is neglected in the deterministic mean field equation (1).

FIG. 4: Velocity $V$ as a function of $D_A$ for $D_B = 0.05$, $\epsilon = 0.20$, $\rho_0 = 0.5$. Filled circle (●) represents analytic estimate for $l = 2$, that is, for states $\{A\phi, AB\}$. Filled square corresponds to the results obtained for $l = 3$, that is, for the states: $\{A\phi\phi, A\phi B, AB\phi, ABB\}$ while the open circle (○) is the simulation results for the front velocity. Here, we note that as $l$ increases the analytic prediction curve comes closer to the simulation results.

FIG. 5: Density profile ahead of the front particle as a function of $D_A$ while keeping $D_B = 0.05$, $\epsilon = 0.20$, and $\rho_0 = 0.5$ fixed. The simulation data from top to bottom corresponds to $D_A = 0.025, 0.015, 0.005, 0.004, 0.002, 0.0005, 0.0$. Here we note that as $D_A \to 0$, $\rho_1 \to 0$.

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