A + A → ∅ reaction for particles with a dynamic bias to move away from their nearest neighbour in one dimension

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Dynamics of a one dimensional $A + A \rightarrow \emptyset$ system where the particles move towards their nearest neighbour with probability $0.5 + \epsilon$ ($0 \leq \epsilon \leq 0.5$) are well studied. We consider a negative bias ($-0.5 \leq \epsilon < 0$) so that the particles have a preference to move away from their nearest neighbour. Here $\epsilon = -0.5 = \epsilon_c$ implies deterministic motion where the particles always move away from their nearest neighbour. Both the bulk properties and the tagged particle dynamics are studied in this system. We show that the negative bias changes drastically the behaviour of the fraction of surviving particles $\rho(t)$ and persistence probability $P(t)$ with time $t$. $\rho(t)$ decays as $a/(\log t)^b$ where $b$ increases with $\epsilon - \epsilon_c$ and $P(t)$ is found to show a stretched exponential decay. The probability $\Pi(x,t)$ that a tagged particle is at position $x$ from its origin is found to be Gaussian for all $\epsilon < 0$, where the scaling variable is $x/t^\alpha$, $\alpha$ is $\epsilon$ dependent, approaching the known limiting value $1/4$ at $\epsilon \rightarrow \epsilon_c$. Some additional features of the dynamics by tagging the particles are also studied.

I. INTRODUCTION

Reaction diffusion systems have been extensively studied over the last few decades $[1, 2]$. The simplest form of the reaction diffusion system is $A + A \rightarrow \emptyset$, where the particles $A$ diffuse and annihilate on contact. This model in one dimension, with asynchronous updating, also represents the ordering dynamics of the Ising model with Glauber dynamics at zero temperature. One can assume that the particles $A$ occupy the sites of a lattice and at each time step they hop to a nearest neighbour site. The $A + A \rightarrow \emptyset$ system has been studied in the recent past where the particles $A$ move with a bias towards their nearest neighbours $[3, 4]$, in one dimension. The model, in its deterministic limit, maps to a opinion dynamics model studied earlier $[5]$. The reaction diffusion model with parallel updating has also been studied in two dimensions recently $[6]$.

The annihilation process is not affected by the bias but this extension leads to drastic changes in bulk dynamical properties. In a previous work $[5]$, tagged particle dynamics have been reported in the one dimensional $A + A \rightarrow \emptyset$ system where the particle $A$ diffuses towards its nearest neighbour with a probability $0.5 + \epsilon$ ($0 < \epsilon \leq 0.5$) and otherwise in the opposite direction $[5]$. To generalize the problem, in the present paper, the results for a negative bias are reported, i.e., when $\epsilon < 0$. Specifically, $\epsilon = -0.5$ implies purely repulsive motion where the particles always move towards their farther neighbour. These particles with full negative bias can represent the motion of similarly charged particles or in general particles with repulsive interaction which can move both ways. The idea behind the study is to find the universal behaviour in the bulk properties as well as the microscopic features and compare with the positive bias case.

II. THE MODEL, DYNAMICS AND SIMULATION DETAILS

In the $A + A \rightarrow \emptyset$ model, a particle $A$ diffuses to one of its neighbouring sites and undergoes a reaction (annihilation). At each update, a site is randomly chosen and if there is a particle on the selected site, it hops one step towards its nearest neighbour with probability $0.5 + \epsilon$ and otherwise it moves in the opposite direction, here $-0.5 \leq \epsilon < 0$. If the destination site is previously occupied by a particle, both of them will be annihilated simultaneously. We have considered the lattice of size $L$ to be randomly half filled initially. At each step, a site is chosen and the state of the corresponding particle is updated. $L$ such updates constitute one Monte Carlo step. In the rare cases of two equidistant neighbours, the particle moves in either direction with equal probability 0.5. The motion is illustrated in Fig. 1.

![Figure 1](image-url)  
**FIG. 1.** The tagged particle hops to right with probability $0.5 + \epsilon$ as its right neighbour is two lattice separation away and to left with probability $0.5 - \epsilon$ as the left neighbour is four lattice separation away. In the present case as $\epsilon < 0$, the particle has a preference to move in the left direction as its nearest neighbour is in the right. For $\epsilon = -0.5$, the particle definitely moves to the left.

As asynchronous dynamics have been used, the net displacement of a particle can be zero or more than one after a MC step $[4]$. The studies were performed on lattices of maximum size $L = 24000$ and the maximum number of configurations taken is 2000. Periodic boundary condition has been used in all the simulations.
III. SIMULATION RESULTS

We took snapshots of the system to check the motion of individual particles. The world lines of the motion of the particles are shown for $\epsilon = -0.1$ and $-0.5$ in Fig. 2 and they are strikingly different from each other. It is obvious that the number of annihilations is larger for $\epsilon = -0.1$. To probe the dynamics of the particles, we have studied the following quantities: (i) fraction of surviving particles at time $t$, (ii) persistence probability of the lattice sites $P(t)$, (iii) the probability distribution $\Pi(x, t)$ of finding a particle A at distance $x$ from its origin at time $t$, (iv) the probability $S(t)$ of the change in the direction in the motion of a particle at time $t$ and (v) the distribution $D(\tau)$ of the time interval $\tau$ between two successive changes in the direction of the motion of a particle. The results for each of these quantities are presented in the following subsections.

A. Bulk properties

1. Fraction of surviving particles $\rho(t)$

For the purely diffusive system ($\epsilon = 0$), it is well known that the fraction of surviving particles shows a power law behaviour in time; $\rho(t) \sim t^{-\alpha}$ with $\alpha = 0.5$. If a positive bias in introduced in the system, $\alpha \approx 1$ for all $\epsilon > 0$ [3, 4]. The exponent increases as the attractive dynamics result in an increased number of annihilations. As $\epsilon$ is made negative, number of annihilations decreases as reaction becomes less probable because of the repulsion. So, $\rho(t)$ shows a slow decay in time and can be fitted to the following form

$$\rho(t) = a/(\log t)^b,$$

where $a$ and $b$ are constants, depending on $\epsilon$. Fig. 3 shows the data for $\rho(t)$ against $t$ for different $\epsilon$. Here it may be mentioned that for the extreme point $\epsilon = -0.5$, the particles ideally attain an equidistant configuration. However, the dynamical rule is such that the particles have to make a move and hence they perform a nearly oscillatory motion. Annihilations take place extremely rarely at large times such that $b$ decreases as the magnitude of $\epsilon$ increases (see inset of Fig. 3).

![FIG. 3. Variation of fraction of surviving particles $\rho(t)$ in time $t$. Inset shows the variation of $b$ with $\epsilon - \epsilon_c$, where $\epsilon_c = -0.5$. The best fit lines (shifted vertically for better view) are shown along with for different $\epsilon$ in the same order.](image)

2. Persistence probability $P(t)$

Persistence probability $P(t)$ in this model is defined as the probability that a site is unvisited till time $t$. For $\epsilon = 0$, $P(t)$ decays as $P(t) \sim t^{-\theta}$ with $\theta \approx 0.375$ [8]. For $\epsilon > 0$, $\theta \approx 0.235$, however small be the bias [3]. As $\epsilon$ becomes negative, $P(t)$ falls off rapidly (see Fig. 4). $P(t)$ shows a stretched exponential decay in time:

$$P(t) = q_0 \exp(-qt^\gamma).$$

Both $q$ and $\gamma$ increase as $\epsilon \to \epsilon_c$.

![FIG. 4. Variation of persistence probability $P(t)$ with $t$ for different $\epsilon$. The best fit lines are shown along with for different $\epsilon$ in the same order.](image)
B. Tagged particle features

1. Probability distribution $\Pi(x,t)$

For pure random walk ($\epsilon = 0$), the probability distribution $\Pi(x,t)$ is known to be Gaussian and $\Pi(x,t)t^{1/2}$ shows a data collapse for different times when plotted against $x/t^{1/2}$. This is also true for the unbiased annihilating random walkers because they perform purely diffusive motion until they are annihilated. For $\epsilon < 0$, the distributions are still Gaussian (see Fig. 5). However the scaling variable is in general $x/t^\alpha$ with $\alpha < 0.5$. To obtain data collapse for different times we have plotted $\Pi(x,t)t^\alpha$ against $x/t^\alpha$.

![Figure 5](image)

FIG. 5. Data collapse of $\Pi(x,t)t^\alpha$ against $x/t^\alpha$ for $\epsilon = -0.1$ (a) and $\epsilon = -0.5$ (b).

The scaling variable $\alpha$ shows a dependence on $\epsilon$, shown in Fig. 6. As $\epsilon$ decreases from zero, at first $\alpha$ decays rapidly from the value 0.5 at $\epsilon = 0$ until $\epsilon \simeq -0.1$ where it attains a value close to 0.3. Below $\epsilon = -0.1$, $\alpha$ shows a slow decrease and at $\epsilon = -0.5$, it equals 0.25, the value expected for repulsive random walkers [11]. At large time as the walkers do not annihilate, effectively they perform repulsive random walk in the lattice.

![Figure 6](image)

FIG. 6. Variation of scaling variable $\alpha$ with $\epsilon$ for several system sizes.

2. Probability of direction change $S(t)$

The probability of direction change of a particle is measured by estimating the number of particles that changes direction of motion at time $t$ divided by the number of surviving particles at that time. Fig. 7 shows the data for $S(t)$ for different $\epsilon$. For purely diffusive system ($\epsilon = 0$), $S(t)$ is independent of time, $S(t) = p_0$. $p_0$ turns out to be $\sim 0.27$ numerically with the updating rule used here.

For $\epsilon < 0$, at first $S(t)$ increases with time, then it reaches a constant value $S_{sat}$. Repulsion between the neighbouring particle is mainly responsible for the change in direction of motion. When $\epsilon$ decreases from zero the repulsive factor becomes stronger, particles change their direction more rapidly, $S(t)$ increases. At the extreme limit $\epsilon = -0.5$, the change in direction is maximum as the particles perform nearly oscillatory motion. A systematic decrease of the saturation value is obtained when $S_{sat}$ with $\epsilon - \epsilon_c$ (see inset of Fig. 7).

![Figure 7](image)

FIG. 7. Probability of direction change $S(t)$ of a tagged particle at time $t$ for different $\epsilon$. Inset shows variation of $S_{sat}$ with $\epsilon - \epsilon_c$.

3. Distribution of time interval spent without change in direction of motion $D(\tau)$

Another quantity calculated is $D(\tau)$, the interval of time $\tau$ spent without change in direction of motion. For random walkers with $\epsilon = 0$, the probability that in the time interval $\tau$, there is no direction change is given by

$$D(\tau) = p_0^2(1-p_0)^\tau,$$

which reduces to an exponential form: $D(\tau) \propto \exp[-\tau \text{ln}(1/(1-p_0))]$. As for $\epsilon < 0$ at large time $S(t)$ is a constant, $D(\tau)$ is expected to show an exponential decay [5]. Therefore, the tail of the distribution $D(\tau)$ is fitted according to

$$D(\tau) = c \exp(-d\tau).$$

Fig. 8 shows the data for $D(\tau)$ against $\tau$ for different $\epsilon$. $1/d$ is an effective ‘time scale’ which increases with


\[\epsilon - \epsilon_c\], shown in the inset of Fig. 8. It shows that for \(\epsilon_c\), the tendency to oscillate is maximum.

IV. CONCLUDING REMARKS

In this paper, we have studied the behaviour of the \(A+ A \rightarrow 0\) model in one dimension, where the particles tend to avoid their nearest neighbour. The probability to move towards the nearest neighbour is taken parametrically as \(0.5 + \epsilon\) where \(\epsilon < 0\). The case with \(\epsilon > 0\) has been studied earlier [3–5]. The bulk properties of the system show abrupt changes for any \(\epsilon \neq 0\). In particular, a significant result in the present paper is that the fraction of surviving walker shows an inverse logarithmic decay for \(\epsilon < 0\). Usually we find a power law decay in one dimension with possibly a logarithmic corrections, e.g., in [6] and purely logarithmic in rare cases, an example in higher than two dimensions can be found in [10].

For \(\epsilon > 0\) the bulk properties (e.g., persistence probability, fraction of surviving particles) show universality in the sense there is a unique scaling behaviour of the dynamical quantities independent of \(\epsilon\). As a negative bias is incorporated in the system, both the fraction of surviving particles and persistence probability show a \(\epsilon\) dependent behaviour. The persistence probability also does not show a power law dependence on time. The behaviour of the bulk properties can be qualitatively understood; the nature of the bias makes the particles more long lived and as a consequence, the probability of a site remaining unvisited decays faster than a power law.

At the microscopic level the system also shows completely different behaviour for positive and negative bias. First, the distributions have a different nature (Gaussian, single peaked) and also show a \(\epsilon\) dependent scaling behaviour for the negative bias. Secondly, there is no crossover behaviour as found for the positive bias case. The negative bias case is entirely dominated by the repulsion from an early stage which causes rapid change of direction such that \(S(t)\) increases as \(\epsilon\) becomes more negative.

For the fully biased case, \(\epsilon = -0.5\), the motion is effectively the same as the repulsive motion between random walkers [11] where the scaling behaviour is known to be \(x \sim t^{4/5}\), which is also obtained from the simulations. Here we find in general \(x \sim t^\alpha\). An interesting question is the dependence of \(\alpha\) on \(\epsilon\). The present results suggest that \(\alpha\) has a weak dependence on \(\epsilon\) for \(\epsilon < -0.1\); it continuously decreases from \(\sim 0.3\) to \(0.25\) for \(-0.1 \geq \epsilon \geq -0.5\). On the other hand there is a sharp decay in the value of \(\alpha\) from 0.5 to \(0.3\) as \(\epsilon\) deviates from zero. The results being numerical, the possibilities that (a) \(\alpha\) becomes 1/4 for any \(\epsilon < 0\) or (b) \(\alpha\) has two distinct values \(\sim 0.3\) and 0.25 for \(\epsilon < -0.1\) are not excluded and we would like to keep this question open and subject to further investigations.

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