Kinetics of the bosonic $A+B\rightarrow 0$ reaction with on-site attractive interaction

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We investigate kinetics of the uniformly driven bosonic $A+B\rightarrow 0$ reaction with on-site attractive interaction in one dimension. In this model, n_i^λ particles from a site with n_i particles are driven to the right. When particles of opposite species occupy the same site, the reaction takes place instantaneously. Since $n_i^\lambda<n_i$ for $\lambda<1$, λ controls the on-site attractive interaction between like particles. The $\lambda=0$ case corresponds to the hard-core (HC) particle model. With equal initial densities of both species, we numerically confirm that the scaling behaviors of density and lengths are the same as those of the uniformly driven HC particle system. Especially the domain length l satisfies the power law $l\sim t^{2/3}$. The kinetics of the reaction is independent of λ as long as $\lambda<1$. The λ-independent kinetics results from the λ-independent collective motions of single species domains.

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I. INTRODUCTION

The irreversible two species reaction $A+B\rightarrow 0$ has been widely and intensively investigated among diffusion-limited reactions because of its rich kinetics and wide applications to various phenomena such as physics, chemistry, and biology [1–6]. The reaction instantaneously takes place with a rate k when two particles of opposite species encounter on the same site. For homogeneous initial distributions with equal densities of A and B, $\rho_A(0)=\rho_B(0)$, the density $\rho(t)$ algebraically decays in time t. In higher dimensions than the upper critical dimensions ($d\geqslant d_c$), the kinetics follows the mean-field rate equation and ρ decays as $\rho\sim t^{-1}$ in time t. However for $d<d_c$, the kinetics is fluctuation-dominated to depend on both the motion and the mutual statistics of particles [4–18].

For isotropic diffusions, $\rho(t)$ decays as $\rho(t)\sim t^{-d/4}$ with $d_c=4$ [5–9]. However, when the motion of particles is not the simple isotropic diffusion, the kinetics is completely changed. With the global relative drift of one species to the other, $\rho(t)$ scales as $\rho(t)\sim t^{-(d+1)/4}$ for $d\leqslant 3$ [6]. When only boundary particles of domains are relatively driven, the kinetics continuously changes according to the form of the drift velocity [10]. For all cases mentioned above, the hard-core (HC) constraint between identical particles is irrelevant to the asymptotic kinetics. However, when both species are uniformly driven to the same direction, the HC constraint completely changes the kinetics. In one dimension, Janowsky reported that ρ scales as $t^{-1/3}$ for HC particles instead of $t^{-1/4}$ [11]. Since one expects that the motion of particles under the Galilean transformation is isotropic, the $t^{-d/4}$ decay law for the isotropic diffusion is also expected in uniformly driven systems. Furthermore, for the single species reaction $kA\rightarrow 0$, the anisotropy of motion does not affect the kinetics of HC particles [19]. Hence the result of Janowsky is rather surprising. For the uniformly driven $A+B\rightarrow 0$ reaction without the HC constraint, the uniform drift does not change the kinetics, either [20]. Hence the interplay of the uniform drift and the HC constraint is crucial for the anomalous $t^{-1/3}$ decay law.

As an attempt to understand the physical origin of the anomalous decay law $t^{-1/3}$, Ispolatov *et al.* suggested a scaling argument based on the assumption that the motion of particles in a single species domain follows the Burgers equation [12]. From the drift velocity of a single interface between A and B domains, they found that the domain length l satisfies the equation $dl/dt\sim\rho$, where l is defined as the distance between the first particles of adjacent opposite species domains. For the random initial condition of $\rho_A(0)=\rho_B(0)$, ρ scales as $\rho\sim 1/\sqrt{l}$ [6] and thus l scales as $l\sim t^{2/3}$ instead of $t^{1/2}$ for the isotropic case. Hence, the anomalous scaling of the domain length l may result in the anomalous density decay. In d dimensions, l scales as $l\sim t^{(5-d)/6}$. So ρ decays as $\rho\sim t^{-(d+1)/6}$ for $d\leqslant 2$, $t^{-d/4}$ for $2<d\leqslant d_c(=4)$ [12]. For $d>2$ the drift is irrelevant. In addition to the domain length l, the interparticle distance (l_{AA}) and the distance between two adjacent particles of opposite species (l_{AB}) also characterize the spatial organization of particles [7]. Janowsky numerically showed that l_{AA} and l_{AB} scale as $l_{AA}\sim t^{1/3}$ and $l_{AB}\sim t^{3/8}$, respectively [13]. Intriguingly, the scaling of l_{AB} is not changed by the drift. Using the scaling of l_{AB}, it was suggested that the domain length l scales as $t^{7/12}$ [13]. The further extensive simulation results [14] supported the result of Janowsky, but it conflicts with the prediction of Ref. [12].

Recently there have been some attempts to describe systems of HC particles in field-theoretic formalisms [16,21,22]. Park *et al.* [16] systematically derived the $\rho\sim t^{-1/3}$ decay law. Even though the decay law of ρ is well understood from such analytic formalisms, the scaling behaviors of various lengths are not still convincingly conclusive. Since the asymptotic scaling regime is extremely slowly approached due to strong corrections [12,14], it is difficult to observe the true scaling behaviors directly via simulations. Hence it is desirable to devise and study another model which exhibits the same scaling behavior, but reaches the true scaling regime within moderate simulation time. On the other hand, HC interaction can be generalized by allowing multiple occupation with a certain attractive interaction between particles on the same site. The on-site attractive interaction would give more general understanding about the scaling behavior HC particles exhibit.

For this aim we introduce a two species bosonic model with on-site attractive interaction. In this model, the HC constraint is replaced by the attractive interaction between like

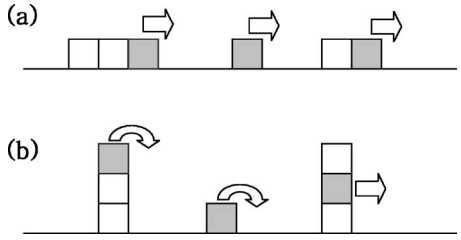

FIG. 1. Motions of particles driven to the right. (a) Motions of HC particles. Only boundary particles (gray boxes) can hop to the right. (b) Motions of bosonic particles with $\lambda=0$. A randomly selected particle (gray box) hops to the right.

particles on the same site. For simplicity, we only consider the particles driven to the right. To implement the on-site attraction, n^λ particles from a site with n particles are made to move simultaneously to the right nearest neighbor site. When two particles of opposite species meet on the same site, they annihilate instantaneously. For $\lambda=1$, the whole particles at a site moves to the right so the $\lambda=1$ case corresponds to a noninteracting bosonic model. Since the number of hopping particles (n^λ) is less than n for $\lambda<1$, the attractive interaction between like particles on the same site exists. Our model generalizes the HC interaction and enables us to investigate how the kinetics of the reaction depends on the interaction strength λ.

Especially, for $\lambda=0$, only one particle hops to the right with the unit rate. Since only the right boundary particle of a HC cluster hops with the unit rate, the $\lambda=0$ case corresponds to HC interaction (Fig. 1). In some bosonic lattice gas model only the top particle on the pile of particles at each site hops to the bottom of the pile at the nearest neighbor site. In this model, the order of particles is conserved, so that we call this model the ordered bosonic lattice gas (BLG) model. It was shown for the drift case that the motion of BLG particles follows the Burgers equation as in HC particle systems [23]. Since particles on a site are identical, the ordered BLG describes the motion of particles inside single species domains of the $\lambda=0$ case in our model. Hence the kinetics for $\lambda=0$ is expected to be the same as that for HC particles. For $0<\lambda<1$, n^λ is larger than one, but n^λ is still smaller than n. Hence the interaction is weaker than HC constraint. However, the interaction for $\lambda<0$ is stronger than HC interaction because of $n^\lambda<1$.

We study the kinetics of the reaction $A+B\to 0$ with the hopping rate of a site $D(n)=n^\lambda$ for random initial distributions with $\rho_A(0)=\rho_B(0)$. For the uniform drift of both species to the right, we find for several values of λ that the scaling of ρ, l_{AA}, and l_{AB} coincide with the results of Refs. [13,14]. However the domain length l scales as $l\sim t^{2/3}$ [12] rather than $t^{7/12}$ [13]. Interestingly, the observed scaling behaviors of density and lengths seem to be independent of λ as long as $\lambda<1$. In the next section, we introduce our model in detail and present simulation results of several values of λ. In Sec. III, we discuss the collective motion of single species domain to understand the λ-independent kinetics for the reaction. Finally, we conclude with a summary in Sec. IV.

II. MODEL AND SIMULATION RESULTS

Our model is defined on the finite one-dimensional lattice width of the size L. We always impose the periodic condition. Particles in our model are always uniformly driven to the right. First, randomly select a site. If the selected site i is occupied by n_i particles, $n_i^\lambda(\equiv m)$ particles simultaneously hop to the right with the unit probability. When n_{i+1} particles of opposite species occupy the site $i+1$, the reaction $n_{i+1}\to n_{i+1}-m$ occurs instantaneously. If $m>n_{i+1}$, the $m-n_{i+1}$ particles remain on the site $i+1$. Then, the color of the remaining particles becomes of the same type as the moved m particles. When the same species occupies the site $i+1$, the reaction $n_{i+1}\to n_{i+1}+m$ takes place.

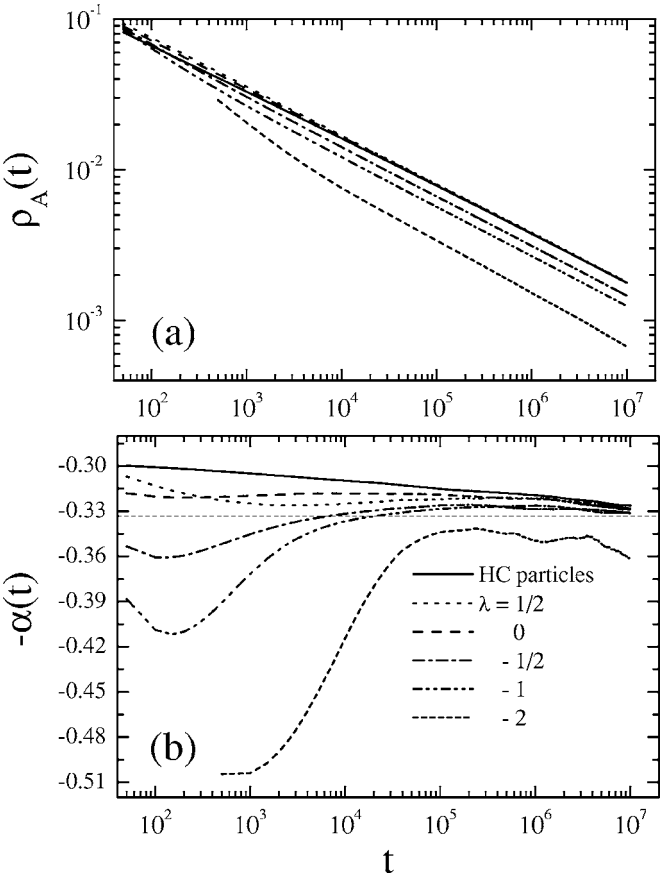

FIG. 2. (a) Plot of ρ_A against time t. (b) Plot of effective exponent $\alpha(t)$ against t. The dotted horizontal straight line denotes "$\alpha=1/3$." The line style of each line is the same in both panels.

We use the following algorithm for determining the number of hopping particles from a site i (m). For $\lambda>0$, the number $m(=n_i^\lambda)$ is not an integer. In that case, integer $[n_i^\lambda]$ particles hop and then one particle hops with the probability $n_i^\lambda-[n_i^\lambda]$. The symbol $[x]$ denotes an integer not greater than the real number x. For $\lambda\leqslant 0$, only one particle among n_i particles attempts to hop with the probability n_i^λ. With random initial distributions of $\rho_A(0)=\rho_B(0)=1/2$, we perform Monte Carlo simulations on a chain of the size $L=1\times 10^7$ for $\lambda=-1$ and $L=3\times 10^6$ for other values of λ up to $t=10^7$. We average densities and various lengths over from 50 to 150 independent runs.

In Fig. 2, we plot the density of A species $[\rho_A(t)]$ and its effective exponent defined as $-\alpha(t)=\ln[\rho_A(t)/\rho_A(t/b)]/\ln b$ with $b=5$ for $\lambda=1/2$, 0, $-1/2$, -1, -2, respectively. For the comparison with the HC particle model, we also plot the

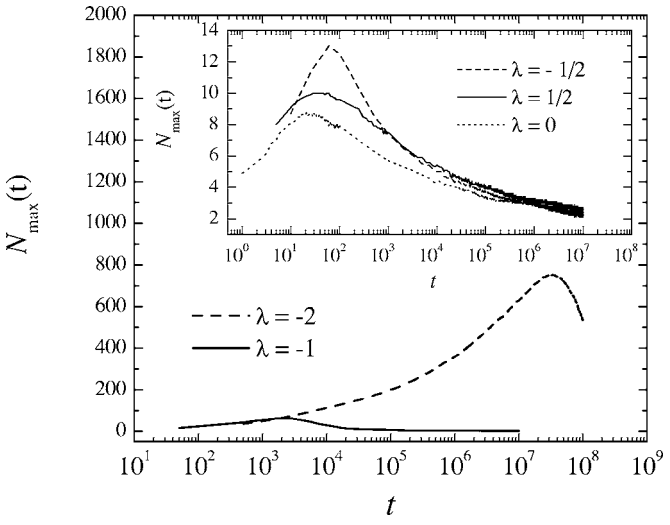

FIG. 3. Plot of $N_{\max}$ against t. The main plot shows $N_{\max}$ for $\lambda=-1$, -2. In the inset, $N_{\max}$ for $\lambda=1/2$, 0, $-1/2$ are plotted.

results for HC particles. The density $\rho_A(t)$ decays as $\rho_A \sim t^{-\alpha}$, and decays faster than that for HC particles in all stages of time for $\lambda<1$. Especially in the early stage, the density decay becomes faster as λ decreases for $\lambda<0$, which is reflected by bumps in $\alpha(t)$. After the early stage, $\rho_A(t)$ slowly gets into the asymptotic scaling regime of $\alpha=1/3$. From the scaling plot of $t^{\alpha}\rho(t)$ against t, we estimate $\alpha=0.329(2)$, 0.331(3), 0.333(2), and 0.331(2) for $\lambda=1/2$, 0, $-1/2$, and -1, respectively which agree well with previous studies [11–14]. For HC particles, we estimate $\alpha=0.327(3)$. Hence our model approaches to the scaling regime faster than the HC particle model does. For $\lambda=-2$, we estimate $\alpha=0.37(1)$. It indicates that the asymptotic scaling region is not reached yet. The physical argument for the slow approach to the asymptotic scaling for the $\lambda=-2$ case is discussed in the following paragraph.

To understand the slow approach to the asymptotic scaling for the $\lambda=-2$ case, we measure the maximum number of particles occupying a single site at time t, $N_{\max}(t)$. By definition, the inequality $n_i(t)\leqslant N_{\max}(t)$ always holds. Figure 3 shows the plot of $N_{\max}(t)$ against t for several λ values. In early time, like particles pile up on several sites due to multiple occupation. Hence $N_{\max}$ increases to a certain maximum value, and after then decreases monotonously. The maximum of $N_{\max}$ and the time it takes to reach the maximum tend to diverge as $\lambda\rightarrow-\infty$. Hence the time it takes to reach the asymptotic scaling regime of $N_{\max}\sim O(1)$ also diverges as $\lambda\rightarrow-\infty$. For example, the maximum of $N_{\max}$ for $\lambda=-2$ is reached at $t\sim 3\times 10^7$. It means that the asymptotic scaling regime of $N_{\max}\sim O(1)$ is very slowly approached after $t \gg 3\times 10^7$. Hence the system already feels the finite size before $t=10^7$, which results in the larger estimate of α. For this reason, we perform simulations only for $\lambda>-2$.

As shown in Fig. 2, our model approaches to the scaling regime faster than the HC particle model does. Furthermore the density decays faster as λ becomes smaller. The λ-dependent decay continues until the system reaches the asymptotic scaling region. Since a site may contain more than one particle, the difference of the particle number between adjacent sites causes the difference of the particle velocity between the sites. The velocity difference enhances the reaction, which results in the fast decay of the density. To explain the fast decay, we define the relative velocity between two adjacent sites. When the number of particles of two adjacent sites i and j $(j<i)$ occupied by opposite species are n_i and n_j, respectively, the relative velocity of a particle at site i to j is $v_{ij}=n_i^{\lambda}-n_j^{\lambda}=[1-(n_i/n_j)^{-\lambda}]/n_i^{-\lambda}$. For $\lambda<0$ and $n_i>n_j$, v_{ij} is negative so the reaction is accelerated. On the other hand, for $\lambda<0$ and $n_i<n_j$, a particle on the site j is difficult to react with a particle on the site i due to $v_{ij}>0$. For $n_i=n_j$, $v_{ij}=0$ and thus diffusive motions lead to the reaction as in the HC particle model. As a result, the reactions are much more enhanced between domain boundaries with $v_{ij}<0$. The enhancement becomes more and more prominent as $\lambda\rightarrow-\infty$ in early stage. Although $N_{\max}$ decreases as the scaling regime is approached, the enhanced reactions from the difference of the number of particles should be still dominant due to $N_{\max}>1$. The similar enhancement of reactions also occurs for $0<\lambda<1$. For this reason, the densities of $\lambda<1$ decay faster than that for the HC particle model in the whole stage.

Next, we present simulation results of various lengths characterizing the spatial organization of particles. The average length of a single species domains (l) is defined as the distance between the first occupied site of two adjacent opposite species domains. The length l_{AA} and l_{AB} are defined as the interparticle distance between two adjacent particles of the same species and of opposite species, respectively [7]. The lengths algebraically increase in time t for $\rho_A(0)=\rho_B(0)$ as

$$l_{AA}\sim t^{1/z_{AA}},\quad l_{AB}\sim t^{1/z_{AB}},\quad l\sim t^{1/z}. \tag{1}$$

Figure 4 shows the scaling plots of $l_{AA}t^{-1/z_{AA}}$ for $\lambda=3/4$, 0, -1. We obtain the best scaling plots with $1/z_{AA}=1/3$ for $\lambda=3/4$ and 0.332 for $\lambda=0$, -1 respectively. For HC particle system, the best scaling plot is obtained with $1/z_{AA}=1/3$ as expected. For the length l_{AB} (Fig. 5), we obtain the best scaling plot of $l_{AB}t^{-1/z_{AB}}$ with $1/z_{AB}=3/8$ for $\lambda=3/4$, 0, and 0.37 for $\lambda=-1$, respectively. For HC particles, $1/z_{AB}=3/8$ gives a nice scaling plot as expected. The simulation results of l_{AA} and l_{AB} agree very well with the prediction $1/z_{AA}=1/3$ and $1/z_{AB}=3/8$ of previous studies [13,14].

For the domain length l, $1/z=2/3$ is predicted by Ref. [12], while $1/z=7/12$ is predicted and are numerically supported by Refs. [13,14]. Our simulation results support $1/z=2/3$ rather than 7/12. Figure 6 shows the scaling plots of $lt^{-1/z}$ for $\lambda=3/4$, 0, -1 and HC particles. We obtain the best scaling plots with $1/z=0.65$ for $\lambda=3/4$, -1, HC particles and 0.64 for $\lambda=0$, respectively. These values are close to the prediction $1/z=2/3$ [12]. The inset shows the effective exponent $1/z(t)$ defined as $\ln[l(bt)/l(t)]/\ln b$ with $b=5$. The effective exponent shows that our model reaches asymptotic region faster than the HC particle model does. On the other hand, $1/z=7/12$ indicates the violation of the relation $\rho\sim 1/\sqrt{l}$ in the drift case, while $1/z=2/3$ satisfies the relation. We check the relation of $\rho\sim 1/\sqrt{l}$ by investigating the scal-

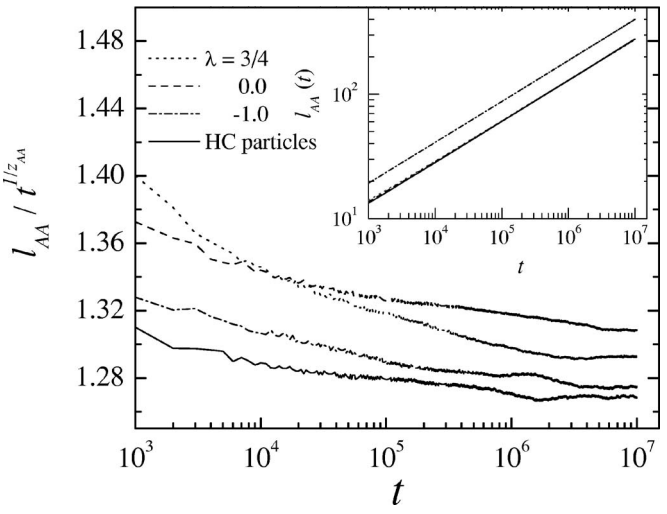

FIG. 4. The scaling plot of l_{AA} against t. The main plot shows the scaling plot of $l_{AA}t^{-1/z_{AA}}$. We use $1/z_{AA}=1/3$ for $\lambda=3/4$, HC particles and 0.332 for $\lambda=0$, -1. We add -0.62 to the scaled value of $\lambda=-1$ and -0.02 to that of HC particles for the better presentation. The inset shows the double logarithmic plot of l_{AA} against t.

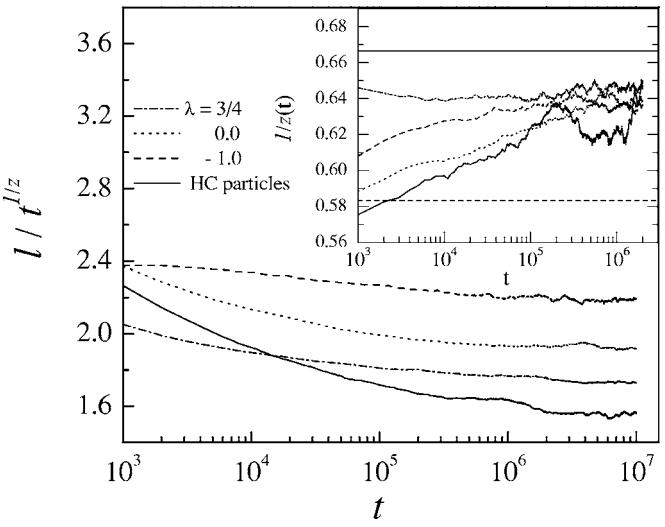

FIG. 6. The scaling plot of l against t. The main plot shows the scaling plot of $lt^{-1/z}$. We use $1/z=0.65$ for $\lambda=3/4$, -1, HC particles and 0.64 for $\lambda=0$. The inset shows the effective exponent $1/z(t)$. The solid and dotted horizontal lines in the inset correspond to $1/z=2/3$ and $7/12$, respectively.

ing plot of ρl^x. We obtain the best scaling plot with $x=0.51(2)$ for several λ and the HC particle model (not shown), which numerically confirm the relation $\rho \sim 1/\sqrt{l}$ in this uniformly driven case. With $\alpha=1/3$, we also expect $1/z=2/3$ from the relation $\rho \sim 1/\sqrt{l}$. Therefore our numerical results agree well with the prediction of $1/z=2/3$ [12].

Our simulation results indicate that the kinetics of the bosonic reaction with the on-site attractive interaction does not depend on the exponent $\lambda(<1)$. $m(=n_i^\lambda)$ particles simultaneously hop to the right in our model, while only the boundary particle can hop in the HC particle model. The m hopping particles can be selected in various ways such as random selection or the ordered selection from the top of the pile. Hence no direct mapping between our model and the HC particle model is available. In the ordered BLG model [23], it was shown that the dynamics of the density is described by Burgers equation and the dispersion of the center of mass (c.m.) scales as $t^{4/3}$, which is the characteristic of asymmetric exclusion process (ASEP) [24]. For the same kinetics of our model as that of the HC particle model, collective motions of single species domain should share the important physical features of ASEP. However, to the best of our knowledge, there are no such studies on bosonic model with the present kind of the on-site attractive interaction. In the next section, we discuss the collective motion of a driven single species domain with the on-site attractive interaction.

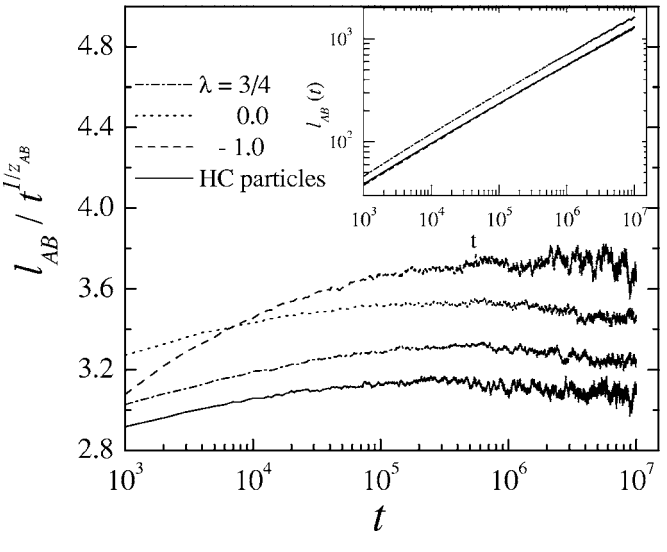

FIG. 5. The scaling plot of l_{AB} against t. The main plot shows the scaling plot of $l_{AB}t^{-1/z_{AB}}$. We use $1/z_{AB}=3/8$ for $\lambda=3/4$, 0, HC particles and 0.37 for $\lambda=-1$. We add 0.2, 0.4, and 0.5 to the scaled value of $\lambda=3/4$, 0, and -1, respectively, to avoid overlap. The inset shows the double logarithmic plot of l_{AB} against t.

III. THE COLLECTIVE MOTION OF A SINGLE DOMAIN

For simplicity, we only consider particles driven to the right. Particles of the same kind are randomly distributed on a ring of size L, while matching the initial density ρ. When a randomly selected site i is occupied by n_i particles, $m=n_i^\lambda$ particles randomly selected and moves simultaneously to the right. When the site $i+1$ has n_{i+1} particles, the coagulation $n_{i+1} \rightarrow n_{i+1}+m$ takes place instantaneously.

We measure the dispersion of the center of mass $(\sigma^2_{\text{c.m.}})$ defined as $\sigma^2_{\text{c.m.}}=\bar{X}^2_{\text{c.m.}}-\bar{X}^2_{\text{c.m.}}$. $X_{\text{c.m.}}$ is the displacement of the center of mass defined as $X_{\text{c.m.}}=\sum_i^N x_i/N$, where N is the total number of particles and x_i is the displacement of the ith particle from its initial position. The dispersion $\sigma^2_{\text{c.m.}}$ is 0 for driven bosonic particles and scales as $t^{4/3}$ for driven HC particles [24]. We perform Monte Carlo simulations for various values of λ from $1/2$ to -1 on chains of the size $L=10^4$ with the periodic boundary condition. We average $\sigma^2_{\text{c.m.}}$ over 3×10^4 independent runs up to $t=10^4$ time steps. In simula-

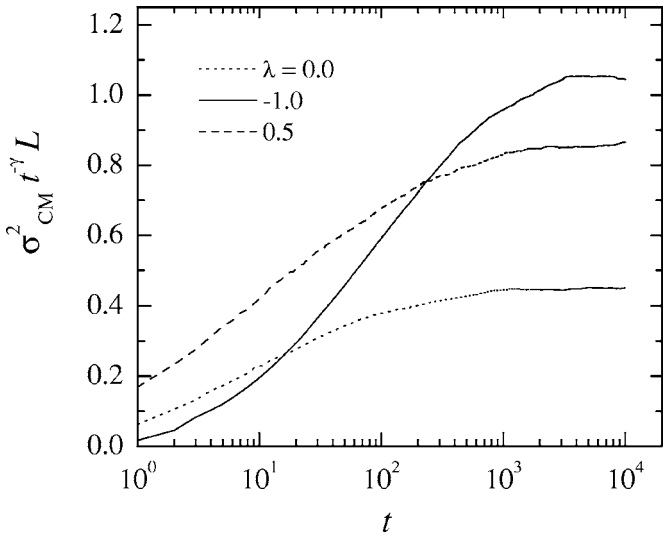

FIG. 7. The scaling plot of $\sigma^2_{\text{c.m.}} t^{-\gamma} L$ against t for $L=10^4$. We use $\gamma=1.38$ for $\lambda=0.5$, and 1.37 for both $\lambda=-1$ and 0. We multiply the data of $\lambda=-1$ by 0.04 for the better presentation.

tions, we exactly set $\rho=0.2$ for $\lambda=1/2$, $\rho=0.5$ for $\lambda=0$, and $\rho=0.01$ for $\lambda=-1$.

Figure 7 shows the plot of $\sigma^2_{\text{c.m.}} t^{-\gamma} L$ against t. $\sigma^2_{\text{c.m.}}$ reaches t^{γ} scaling regime after the moderated transient time. We obtain the best scaling plot with $\gamma=1.38(1)$ for $\lambda=1/2$, and 1.37(1) for $\lambda=-1$ and 0, respectively, which is slightly larger than $\gamma=4/3$ for HC particles. In the ordered BLG model [23], the velocity of c.m. is given as $v_{\text{c.m.}}=1/(1+\rho)$ when the particles drift to the right. For $\lambda=0$ with $\rho=0.5$, we estimate $v_{\text{c.m.}}=0.669(1)$ which agree well with the prediction $v_{\text{c.m.}}=1/(1+\rho)$ [23]. For $\lambda=0$ with other densities, we also confirm the prediction $v_{\text{c.m.}}=1/(1+\rho)$. Hence we are convinced that the $\lambda=0$ case is kinetically the same as the ordered BLG model in spite of somewhat larger numerical values of γ. On the other hand, for $\lambda\neq 0$, there are no theoretical predictions for $v_{\text{c.m.}}$ and $\sigma^2_{\text{c.m.}}$. However the exponent γ indicates that the collective motions for $\lambda<1$ are very close to that for HC particles rather than that for bosonic particles.

We conclude that the collective driven motions of particles with the on-site attractive interaction is kinetically the same as HC particles as long as $\lambda<1$. It results in λ-independent kinetics of $A+B\rightarrow 0$ reaction with on-site attractive interaction.

IV. SUMMARY

In summary, we investigate the kinetics of uniformly driven bosonic $A+B\rightarrow 0$ reaction with on-site attractive interaction. In this model, the number of selected particles (m) from a site with n_i particles is given as $m=n_i^{\lambda}$, and these particles are driven to the right. When particles of opposite species occupy the same site, the reaction takes place instantaneously. Since $m<n_i$ for $\lambda<1$, the exponent λ controls the strength of the on-site attractive interaction between like particles occupying the same site. The $\lambda=0$ case corresponds to the uniformly driven HC particle model, because only one particle from a selected site hops to the right. Compared to the $\lambda=0$ case, the attractive interaction for $\lambda>0$ is weaker than HC interaction, while the interaction for $\lambda<0$ is stronger. Our model generalizes the HC interaction and enables to investigate how the kinetics of the reaction depends on the interaction strength. Our model gets into the asymptotic scaling regime faster than the HC particle model does, since the HC constraint is somewhat relaxed in our model by allowing any particle on a site to move.

We perform Monte Carlo simulations in one dimension for several values of λ to measure the exponents of density and various lengths, which exhibit power-law scaling for $\rho_A(0)=\rho_B(0)$. The scaling behaviors of density and lengths except the domain length l are the same as those of the HC particle model [11,13,14]. The scaling behavior of l are close to $t^{2/3}$ [12] rather than $t^{7/12}$ [13]. Interestingly, the kinetics of the reaction is independent of λ as long as $\lambda<1$. To understand the λ-independent behavior, we investigate the collective driven motions of single domains. The dispersion of the center of mass ($\sigma^2_{\text{c.m.}}$) scales as t^{γ} with $\gamma=4/3$ for driven HC particles [24] and $\sigma^2_{\text{c.m.}}$ is zero for bosonic particles. For various λ values, we find that γ is slightly larger than, but close to, 4/3. The collective motion of single domains is thus kinetically very close to that for the HC particle system. Furthermore the motion is independent of λ, which results in the λ-independent kinetics of the reaction. However for the quantitative understanding of the collective motion, another analytical study is needed.

ACKNOWLEDGMENTS

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