Continuously varying exponents in $A + B \rightarrow 0$ reaction with long-ranged attractive interaction

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(Dated: December 29, 2018)

We investigate the kinetics of the $A + B \rightarrow 0$ reaction with long-range attractive interaction $V(r) \sim -r^{-2\sigma}$ between $A$ and $B$ or with the drift velocity $v \sim r^{-\sigma}$ in one dimension, where $r$ is the closest distance between $A$ and $B$. It is analytically show that the dynamical exponents for density of particles ($\rho$) and the size of domains ($\ell$) continuously vary with $\sigma$ when $\sigma < \sigma_c = 1/2$, while that for the distance between adjacent opposite species ($\ell_{AB}$) varies when $\sigma < \sigma_{c}^{AB} = 7/6$. Beyond $\sigma_{c}^{AB}$, diffusive motions dominate the kinetics, so that the dynamical behavior for diffusive systems is completely recovered. These anomalous behaviors with the two crossover values of $\sigma$ are supported by numerical simulations and the argument of effective repulsion between the opposite species domains.

PACS numbers: 05.70.Ln, 05.40.-a

The irreversible two-species reaction $A + B \rightarrow 0$ has been intensively and widely investigated as a basic model for various phenomena in physics [1, 2], chemistry [3], and biology [4]. When an $A$ and a $B$ particle meet on the same site, they instantly and irreversibly combine to form an inert species. Until now the studies for the reaction have been focused on understanding the effect of the fluctuations of the initial particle density or the global bias of particle motions on the kinetics without careful consideration of the interactions between $A$ and $B$ even for charged particles [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]. However, in situations where the kinetics of reaction is affected by certain attractive interactions between $A$ and $B$ such as the Coulomb interaction, the interactions should be much more important than the simple diffusive motions or global biases to understand the kinetics. Such situations may include matter-antimatter annihilation in the universe, soliton-antisoliton recombination, charge recombination in clouds [12] and electron-hole recombination in irradiated semiconductor structures [4].

It has recently been shown through a simple model that the underlying attractive interaction between opposite species leads to completely different scaling behaviors from those studied so far [13]. In the model, the fluctuation-dominated kinetics leads to the segregation of alternating $A$–rich and $B$–rich domains as usual [4]. In addition, domain-boundary particles feel the attractive interaction and are assumed to move to the adjacent opposite species domain with a constant drift velocity. Since the bias is a constant regardless of the distance between $A$ and $B$, the interaction strength in the model [13] is infinite. In contrast the particles inside the domain are screened by the same neighboring particles and the motion of bulk particles is naturally assumed to be isotropic diffusion. As a result, the interaction causes the alternatively changing bias at domain boundaries which is neither the relative nor the uniform bias of Refs. [6] and [11] (Fig. 1(a)). In non-interacting systems, the density decay has been known to depend on the motion and the mutual statistics of particles. For isotropic diffusions, the particle density $\rho(t)$ scales as $\rho(t) \sim t^{-\sigma}$ in $d$ dimensions $(d \leq 4)$ [6, 7, 8, 9, 10]. With the global relative drift, $\rho(t)$ scales as $\rho(t) \sim t^{-(d+1)/4}$ for $d \leq 3$ [6]. With the uniform drift of both species, the hard-core (HC) constraint between identical particles leads to the scaling of $\rho(t) \sim t^{-1/3}$ in one dimension [11]. With the infinite interaction, $\rho(t)$ scales as $t^{-\sigma}$ regardless of the HC constraint [13]. In one dimension, the uniform bias of HC particles and the infinite interaction lead to the same scaling law, but the scaling behaviors of basic lengths are different. Hence the infinite interaction results in new dynamical scaling behaviors [13].

The constant drift or the infinite attractive interaction is unnatural [13] and cannot explain more general or real situations where the attractive interaction depends on the distance $r$ between $A$ and $B$. Some of physically realistic attractive interactions should be those described by a conserved attractive potential $V(r) \sim -r^{-2\sigma}$. The drift velocity $v$ is then given as $v(r) \sim \sqrt{|V|} \sim r^{-\sigma}$. In this paper, we investigate the kinetics of $A + B \rightarrow 0$ with the attractive potential $V(r) \sim -r^{-2\sigma}$ or with the drift velocity to opposite species $v(r) = r^{-\sigma}$. In reality the motions of boundary particles cannot be determined only by the interaction, because there should exist various noises, which are normally believed to make the background diffusive motions. In this reason, a boundary particle is assumed to stochastically move to its opposite species domain with the rate $p = (1 + v(r))/2$, and to its own domain with $1 - p$ for a unit time. Hence this model naturally includes the competition between the attractive interaction and the diffusive motion. The drifted motions at boundaries and the competition are expected to lead rich and interesting scaling behavior as $\sigma$ varies. Fig. 1(b) shows the space-time trajectories for $\sigma = 0.3$. Using the trajectories schematically depicted in Fig. 1(c), we analytically derive asymptotic scaling
behavior. Intriguingly, we find that all dynamical exponents for various densities and lengths continuously vary when $\sigma < \sigma_c$. Furthermore the scaling behaviors for the present model manifest unique anomalous behaviors, which have not seen in dynamical critical models with the continuous varying exponents [14]. In addition, the anomalous behavior is that there exist two different crossover values of $\sigma_c$, $\sigma_c$ for the density of particles ($\rho$) and the size of domains ($\ell$) is $\sigma_c = 1/2$, while that for the distance between adjacent opposite species ($\ell_{AB}$) is $\sigma_{cAB}^AB = 7/6$. Hence the interaction completely changes the scaling behavior of kinetics when $\sigma < \sigma_{cAB}^B$. However, when $\sigma \geq \sigma_{cAB}^B$, the kinetics for diffusive motions is completely recovered [8]. As in the $\sigma = 0$ case, the HC constraint is irrelevant due to the isotropic diffusions inside domains. We also numerically confirm our analytical results.

With the equal initial density $\rho_A(0) = \rho_B(0)$, particles are randomly distributed on a one-dimensional lattice of size $L$. When the selected particle has two opposite species neighbors such as $(A \cdots A \cdots B)$, the central particle $(A)$ hops to the opposite species $(B)$ with rate $p = (1 + v(r))/2$ and to the same species $(A)$ with rate $1 - p$, where $v(r) = r^{-\sigma}$ with $\sigma \geq 0$ and $r$ is the distance between $A$ and $B$. Otherwise, particles diffuse isotropically. In the region of a length $\ell$, the number of $A$ species is initially $N_A = \rho_A(0)\ell \pm \sqrt{\rho_A(0)\ell}$ and the same for $N_B$. After a time $t \sim \ell^2$, particles travel throughout the whole of the region, and annihilate by pairs. The residual particle number is the number fluctuation in the region, so we have the relation $N_A \sim \sqrt{\ell}$ or $\rho_A \sim 1/\sqrt{\ell}$ for a given length $\ell$ [3, 6]. As the processes evolve, the system becomes a collection of alternating $A$-rich and $B$-rich domains. To characterize the structure of segregated domains, we introduce three length scales as in Ref. [3].

The length of the domain ($\ell$) is defined as the distance between the first particles of adjacent opposite species domains [2]. The length $\ell_{AB}$ is defined as the distance between two adjacent particles of opposite species, while $\ell_{AA}(\ell_{BB})$ is the distance between adjacent $A(B)$ particles in a $A(B)$ domain. These lengths scale asymptotically as

$$\ell \sim t^{1/z}, \quad \ell_{AA} \sim t^{1/z_{AA}}, \quad \ell_{AB} \sim t^{1/z_{AB}}. \quad (1)$$

A bulk particle inside single species domains diffuses isotropically and the mean position of the bulk particle is not substantially changed until it becomes a boundary particle. Once it becomes boundary, it drifts to its neighboring opposite species with velocity $v(r)$ until it annihilates in the midway between two opposite species domains. From this situation in mind we now analytically calculate the scaling behaviors of the kinetics when the drift velocity is $v(r) \sim r^{-\sigma}$. For an $AB$ pair with the distance $\ell_{AB}$, the time interval for annihilation of the $AB$ pair is $\tau_{AB} \sim \ell_{AB}/v(\ell_{AB}) \sim \ell_{AB}^{\sigma+1}$. For $\sigma \geq 0$, the space-time trajectory of a particle is arch-shaped. In the $\sigma = 0$ case the trajectory is very close to a pentagon [12]. These arch-shaped trajectories should be self-similar (self-affine) fractal structures, because they should have the scaling symmetry due to the power-law scaling behavior (1). A typical base unit of the self-similar arch-shaped trajectories of adjacent opposite domains are schematically depicted in Fig. 1(c). This base unit allows us to calculate a time $\tau_n$ needed to remove the unit of size $\ell$ surrounded by one scale larger ones. Then the size of the larger unit increases by $\ell$ during $\tau_n$ and we have

$$\frac{dt}{dt} \sim \ell/\tau_n,$$

which gives the dynamic exponent $z$. In following calculations, we consider only the mean positions of bulk particles, and assume $\ell_{AA}(t)$ to be a constant during the annihilation of the base unit. After a smaller unit is completely annihilated, the remainder of particles redistribute over the larger unit increased by the size of the annihilated unit. Hence we approximate $\ell_{AA}(t) = \cdots = \ell_{AA}(t + \tau_n) = \cdots = \ell_{AA}(t + \tau_2)$ during the annihilation of a smaller unit.

As only boundary particles of each domain have two opposite species neighbors, the annihilation of boundary particles comes from the attractive interaction. It takes a time $\tau_1 = \ell_{AB}^{\sigma+1}$ for the first boundary pair, $A_1$ and $B_1$ in Fig. 1(c), to annihilate. The second pair ($A_2$ and $B_2$) from the boundary isotropically diffuse during time $\tau_1$ until $A_1$ and $B_1$ annihilate. After the time $\tau_1$, the second pair becomes a new boundary pair, and the $t_2 \sim (\ell_{AB} + \ell_{AA})^{\sigma+1}$ is needed for the annihilation. So it takes time $\tau_2 = \tau_1 + t_2$ in total for the second pair to annihilate. Similarly, the $n$th pair from the initial boundary will annihilate after $\tau_n \sim \tau_{n-1} + t_n$, where $t_n = (\ell_{AB} + (n-1)\ell_{AA})^{\sigma+1}$ for $n \geq 2$. From the recurrence

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{image.png}
\caption{(Color online) Snapshot of trajectories of $A + B \rightarrow 0$ with the attractive interaction between $A$ and $B$ of (a) $\sigma = 0$ and (b) $\sigma = 0.3$. (c) The magnified schematic trajectories of adjacent opposite species domains. Subscripts $\{1, 2, \ldots, n\}$ indicate the order of the positions of particles from a given domain boundary.
\end{figure}
relation of $\tau_n$, we find

$$\tau_n \sim \ell^{\sigma+1}_{AB} + \sum_{k=1}^{n-1} (\ell_{AB} + k\ell_{AA})^{\sigma+1},$$

$$\sim \ell^{\sigma+1}_{AB} + [(\ell_{AB} + n\ell_{AA})^{\sigma+2} - \ell^{\sigma+2}_{AB}] / \ell_{AA}. \tag{3}$$

The second line is obtained by integrating out the summation over $k$. As the number of particles $N_\ell$ and the length $\ell_{AA}$ in a domain of size $\ell$ scale as $N_\ell \sim \ell^2$ and $\ell_{AA} \sim 1/\rho \sim \ell^2$, the time $\tau_\ell$ needed to annihilate the domain of size $\ell$ in the unit box is given by

$$\tau_\ell \sim \ell^{\sigma+3/2} \tag{4}$$

Because of $\ell > \ell_{AB}$ by definition, we finally find the leading scaling of $\tau_\ell$ as

$$\tau_\ell \sim \ell^{\sigma+3/2}, \tag{5}$$

and $z$ is given as $z = \sigma + 3/2$ from Eq. [2]. Intriguingly, $z$ increases continuously and linearly with $\sigma$. However, $z$ cannot increase beyond the upper bound $z_c = 2$, because domains cannot spread more slowly than those of random diffusion. Hence for $\sigma \geq \sigma_c = 1/2$, we have $z = 2$ regardless of $\sigma$. The scaling of $\ell_{AA}$ is easily obtained from the relation $\ell_{AA} \sim \sqrt{\ell} \sim t^{1/\alpha_{AA}}$. One finds $z_{AA} = 2z = 2\sigma + 3$. Since $\ell_{AB}$ with the diffusion only scales as $\ell_{AB} \sim \ell^{1/\alpha_{AB}}$, the critical value of $\sigma$ is also $\sigma_{c\AA} = 1/2$. For $\ell_{AB}$, we consider the change of density during time $\tau_{AB} \tag{6}$. During $\tau_{AB}$, one pair of $AB$ particle annihilate only between boundaries, the change of particle density is given as $d\rho/dt \sim -\rho_{AB}/\tau_{AB}$, where $\rho_{AB}$ is the density of $AB$ pairs. Using relations, $\rho \sim 1/\sqrt{\ell}$, $\rho_{AB} = 1/\ell$, and $\tau_{AB} \sim \ell^\sigma_{AB}$, one finds $\ell_{AB} \sim \ell^{1/\sigma_{AB}}$ with $z_{AB} = z = \sigma + 3/2$. Interestingly, $\ell_{AB}$ scales with the scaling of $\ell$. However, $\ell_{AB}$ with the diffusion only scales as $\ell_{AB} \sim \ell^{3/8}$ and thus $\sigma_{c\AB} = 7/6$. The scaling exponents of three lengths and their critical values of $\sigma$, beyond which the diffusive scaling behaviors recover, are summarized as follows.

$$z = \sigma + 3/2, \quad z_{AA} = 2z, \quad z_{AB} = z, \quad \sigma_c = 1/2, \quad \sigma_{c\AA} = 1/2, \quad \sigma_{c\AB} = 7/6. \tag{6}$$

From the scaling of lengths, asymptotic decays of various densities can be extracted. The density of total particles ($\rho = 2\rho_A$), adjacent pairs of same species ($\rho_{AA} = \rho_{BB}$) and adjacent pairs of opposite species ($\rho_{AB}$) scale as

$$\rho \sim t^{-\alpha}, \rho_{AA} \sim t^{-\alpha_{AA}}, \rho_{AB} \sim t^{-\alpha_{AB}}. \tag{7}$$

As $\rho \sim 1/\sqrt{\ell}$, we have $\rho \sim t^{-1/2z}$ with $\alpha = 1/2z = 1/(2\sigma + 3)$. $\rho_{AA}$ follows the same scaling of $\rho$ due to $\rho_{AA} \sim 1/\ell_{AA} \sim 1/\sqrt{\ell}$ so $\rho_{AA} \sim t^{-\alpha}$ with $\alpha_{AA} = \alpha$. Finally $\rho_{AB}$ scales as $\rho_{AB} \sim 1/\ell$, which leads to $\rho_{AB} \sim t^{-1/2}$ with $\alpha_{AB} = 1/z = 1/(\sigma + 3/2)$. As densities with the diffusion only scale as $\rho \sim \rho_{AA} \sim t^{-1/4}$ and $\rho_{AB} \sim t^{-1/2}$, the upper bound of $\sigma$ is $\sigma_c = 1/2$ for all densities. All decay exponents of various densities are simply given as

$$\alpha = 1/2z, \quad \alpha_{AA} = \alpha, \quad \alpha_{AB} = 1/z, \quad \sigma_{c\AA} = 1/2, \quad \sigma_{c\AB} = 7/6. \tag{8}$$

and the critical value of $\sigma$ is $\sigma_c = 1/2$ for all densities. For $\sigma = 0$, the all scaling behaviors of the constant drift are fully recovered [8]. As shown in Eqs. (6) and (7), there exists two different crossover values of $\sigma$, $\sigma_c(= \sigma_{c\AA} = 1/2$ and $\sigma_{c\AB} = 7/6$), where $\sigma_c < \sigma_{c\AB}$. It is very peculiar that there exists two crossover values. However the inequality $\sigma_c < \sigma_{c\AB}$ directly comes from the anomalous scaling of $\ell_{AB}$ with diffusion only. With diffusion only, adjacent opposite domains are effectively repulsive by preferential annihilations of nearby $AB$ pairs. Hence, opposite species pairs are further apart than the typical interparticle distance $\ell_{AA}$ and, as a result, $\ell_{AB}$ increases anomalously as $t^{3/8}$. This anomalous scaling of $\ell_{AB}$ leads to another crossover in addition to the crossover by diffusion.

As the strength of the interaction becomes weak, the effect of the random fluctuation by diffusion becomes weak. The competition between the fluctuation by diffusion and the drift by the interaction leads to the continuously decaying exponents and the critical values of $\sigma$ above which diffusive motions dominate the kinetics. On the other hand, since the interaction maintains the Galilean invariance of the domain structure, the predictions [8] and [5] are expected to be independent of the HC constraint.

To confirm our analytic results numerically, we now present the simulation results. With $\rho_A(0) = \rho_B(0)$, $A$ and $B$ particles distribute randomly on a chain of size $L$. In the simulations we consider both HC particles and the particles without the HC constraint, which we call bosonic particles. In the model with HC particles there can be at most one particle of a given species on a site. In the bosonic model there can be many identical particles on a site. All the simulations are done on the chain of size $L = 3 \times 10^6$ and with $\rho_A(0) = \rho_B(0) = 0.1$. We average densities and lengths over 100 independent runs. Fig. 2(a) shows densities (inset) and their effective exponents defined as $-\alpha(t) = \log[\rho(2t)/\rho(t)]/\log 2$ for $\sigma = 0.1$ case of HC particles. We estimate $\alpha = 0.317(5)$, $\alpha_{AA} = 0.3125(25)$, and $\alpha_{AB} = 0.625(25)$ respectively. All results agree well with the prediction [5]: $\alpha = \alpha_{AA} = 0.3125$ and $\alpha_{AB} = 0.625$ for $\sigma = 0.1$. Fig. 2(b) shows the various lengths and their effective exponents $\alpha_{AA} = 3.20(5)$ and $\alpha_{AB} = 3.60(5)$ which also agree very well with the prediction [8]: $\alpha = 3.6, \alpha_{AA} = 3.2$ and $\alpha_{AB} = 1.6$ for $\sigma = 0.1$. For bosonic particles, we also obtain nearly the same results.

To check the crossover from the continuously varying dynamic scaling to the completely diffusive one, we perform Monte Carlo simulations under the same initial con-
In each panel, horizontal lines from top to bottom show the predictions \( \alpha = 0.313 \) and \( \alpha_{AB} = 0.63 \) (b) \( 1/z = 0.625 \) and \( 1/z_{AA} = 0.313 \).

In conclusion, we investigate the kinetics of irreversible reaction \( A + B \to 0 \) with the attractive interaction \( V(r) \sim -r^{-2\sigma} \) between \( A \) and \( B \) or with the drift velocity \( v(r) \sim r^{-\sigma} \) to opposite species at segregated domain boundaries. The drift leads to arch-shaped space-time trajectories of particles with which we analytically derive asymptotic scaling behaviors, and numerically confirm them. Intriguingly, the drift results in continuously varying scaling behavior by certain critical values, \( \sigma_c \) or \( \sigma_c^{AB} \). above which diffusive motions dominate the kinetics. In our derivations, we only consider the mean positions of particles and neglect the expansion of domains by the random fluctuations during the annihilations of domains. Hence when the interaction dominate the kinetics, the fluctuation does not affect the asymptotic scaling behavior.

This work is supported by Grant No. R01-2004-000-10148-0 from the Basic Research Program of KOSEF.

[1] A. A. Ovchinnikov and Ya. B. Zeldovich, Chem. Phys. 28, 215 (1978).
[2] P. G. de Gennes, J. Chem. Phys. 76, 3316 (1982).
[3] N. G. van Kampen, Stochastic processes in Physics and Chemistry (North-Holland, Amsterdam, 1981).
[4] A. M. Turing, Philos. Trans.R. Soc. London Ser B 237, 37 (1952).
[5] D. Toussaint and F. Wilczek, J. Chem. Phys. 78, 2642 (1983).
[6] K. Kang and S. Redner, Phys. Rev. Lett. 52, 955 (1984); K. Kang and S. Redner, Phys. Rev. A 32, 435 (1985).
[7] G. Zumofen, A. Blumen, and J. Klafter, J. Chem. Phys. 82, 3198 (1985).
[8] S. Cornell, M. droz, and B. Chopard, Physica A 188, 322 (1992).
[9] F. Leyvraz and S. Redner, Phys. Rev. A 46, 3132 (1992).
[10] B. P. Lee and J. Cardy, J. Stat. Phys. 80, 971 (1995).
[11] S. A. Janowsky, Phys. Rev. E 51, 1858 (1995); I. Ipsolatov, P. L. Krapivsky, and S. Redner, Phys. Rev. E 52, 2540 (1995).
[12] K. Lindenberg, B. J. West, and R. Kopelman, Phys. Rev. Lett. 60, 1777 (1988).
[13] S. Kwon, S. Y. Yoon, and Y. Kim, Phys. Rev. E 73, 025102(R) (2006).
[14] H. Hinrichsen, Adv. Phys. 49, 815 (2000); D. ben-Abraham, V. Privman and D. Zhong, Phys. Rev. E 52, 6889 (1995).