Finite-size effects of two-particle diffusion-limited reactions

Jae Woo Lee*
Department of Physics, Inha University, Inchon 402-751, Korea

(Received 16 March 2000)

We have studied the finite-size effects of two-particle diffusion-limited reaction $A+B\rightarrow 0$, on a one-dimensional lattice using the Monte Carlo method. The density at a finite lattice follows a power law, $C(t)\sim t^{-x}$ below the crossover time, and shows an exponential decay above the crossover time. The crossover time depends on the lattice size and the bias field. We found second-order correction terms of the density decay as $C(t)\sim t^{-1/4}[1+O(t^{-1/8})]$ for the isotropic diffusion of particles and $C(t)\sim t^{-1/3}[1+O(t^{-1/24})]$ for the maximum drift. We proposed the scaling function of the density given as $C(t)\sim L^{-1/2}f_o(t/L^2)+L^{-3/4}f_1(t/L^2)$ for the isotropic diffusion and $C(t)\sim L^{-1/2}f_o(t/L^{3/2})+L^{-9/16}f_1(t/L^{3/2})$ for the maximum drift where f_o and f_1 are scaling functions.

PACS number(s): 05.40.−a, 05.60.−k, 82.20.−w

Diffusion-limited reactions (DLR's) are interesting for a nonclassical behavior of the density decay [1–7]. DLR have been applied to studies of annihilation and coagulation phenomena such as electron-hole recommbination in semiconductors, exiton-exiton dynamics in tetra-mehtylammonium maganese trichloride, competing species in biology, aerosol dynamics and polymerization [3,8–10]. In one-dimensional systems, the density of single species annihilation, $A+A\rightarrow 0$, and coagulation, $A+A\rightarrow A$, decays much more slowly than a mean-field prediction regardless of a drift field [3–11]. In diffusion-limited reaction of two species, $A+B\rightarrow 0$, the density decays according to a power law $C(t)\sim t^{-x}$ with $x=d/4, d\leqslant d_c=4$ for the isotropic diffusion of particles [12–17]. Sancho *et al.* have studied the chemical reaction $A+B\rightarrow 0$ for different initial distribution of reactants. They observed the long-wavelength components of the initial fluctuations determine the long-time decay of the reactant decay [17]. Lindenberg *et al.* have studied DRL's for the different initial distribution of reactants. They observed the crossover behavior of density decays and predicted the crossover time [18]. When one applies a maximum drift, the density decay exponent increases from $x=1/4$ to $x=1/3$ on a one-dimensional lattice [19–24].

Exact solutions have been reported on single-particle annihilations [25–28] and two-particle annihilations [29,30] for the isotropic diffusion of the particles. Finite-size effects of annihilation models have been studied on the single-particle reactions [30,32]. Simon observed finite-size effects of the single-particle annihilations and crossover from the power law to exponential decay of the density [30]. Cadilhe has studied the finite-size effects of reaction systems for the isotropic diffusion of particles. He estimated the prefactor of the density decay from the simulation [31]. Kreb *et al.* reported the finite-size scaling of reaction-diffusion systems [32]. In the single species coagulation reaction they proposed a scaling relation as $C(z)=L^aF_o(z)+L^bF_1(z)$ with $z=4Dt/L^2$ for the isotropic diffusion of the particles. They obtained the exponents as $a=-1$ and $b=-2$. Noh *et al.* have studied the second-order correction $O(t^{-1/8})$ of the density decay on the two-particle annihilations for the isotropic diffusion [33]. Dimensional crossovers of the reaction system have been studied in tubular geometries where the size of the system in one or two directions is much smaller than in the third direction [34–39]. They observed that the crossover time for the reaction $A+B\rightarrow 0$ is $t_c\sim W^2$ for large W where W is the width of the tube along a narrow direction [35,37]

In the present paper we have studied the finite-size effects and the second-order correction of the density decay on the diffusion-limited reaction of two particles annihilations for the isotropic diffusion of particles and for the maximum drift.

Monte Carlo simulations were performed for the cases of isotropic diffusion and maximum drift of hopping particles on a one-dimensional lattice. In the isotropic case, a randomly selected particle attempts to hop to the left or right nearest-neighbor site with equal probabilities. In the drift case, the particle attempts to hop the right with probability $(1+p)/2$ or to the left with probability $(1-p)/2$. In the present paper we took the maximum bias $p=1$, i.e., the chosen particle only attempts to hop to the right direction. We used lattices up to 10^6 sites with periodic boundary conditions. One Monte Carlo step corresponds to the number of hopping attempts equal to the number of remaining particles. Initial densities were 20% of the full occupancy. Data of the density were averaged over 1000 configurations for $L=10^3$, 200 configurations for $L=10^4$, 20 configurations for $L=10^5$, and $L=10^6$.

In Fig. 1 we show the log-log plot of the density versus time with $C_A(0)=C_B(0)=0.1$ for the isotropic diffusion as shown in Fig. 1(a), and for the maximum drift case as shown in Fig. 1(b). Density decays according to a power law $C(t)\sim t^{-x}$ with $x=0.256\pm 0.005$ for the isotropic diffusion and $x=0.31\pm 0.02$ for the maximum drift at long times and large lattice $L=10^6$. At a small lattice, we observed the finite-size effects as shown in Fig. 1(a) and Fig. 1(b). At long times the density decays exponentially at the small lattice. As shown in Fig. 1(c) the finite-size effects are also observed at the size of lattice $L=10^5$. The crossover time of density decays from the power law to the exponential decay is given by $t_c\sim L^2$ for the isotropic diffusion and $t_c\sim L^{3/2}$ for the maximum

*Email address: jaewlee@inha.ac.kr

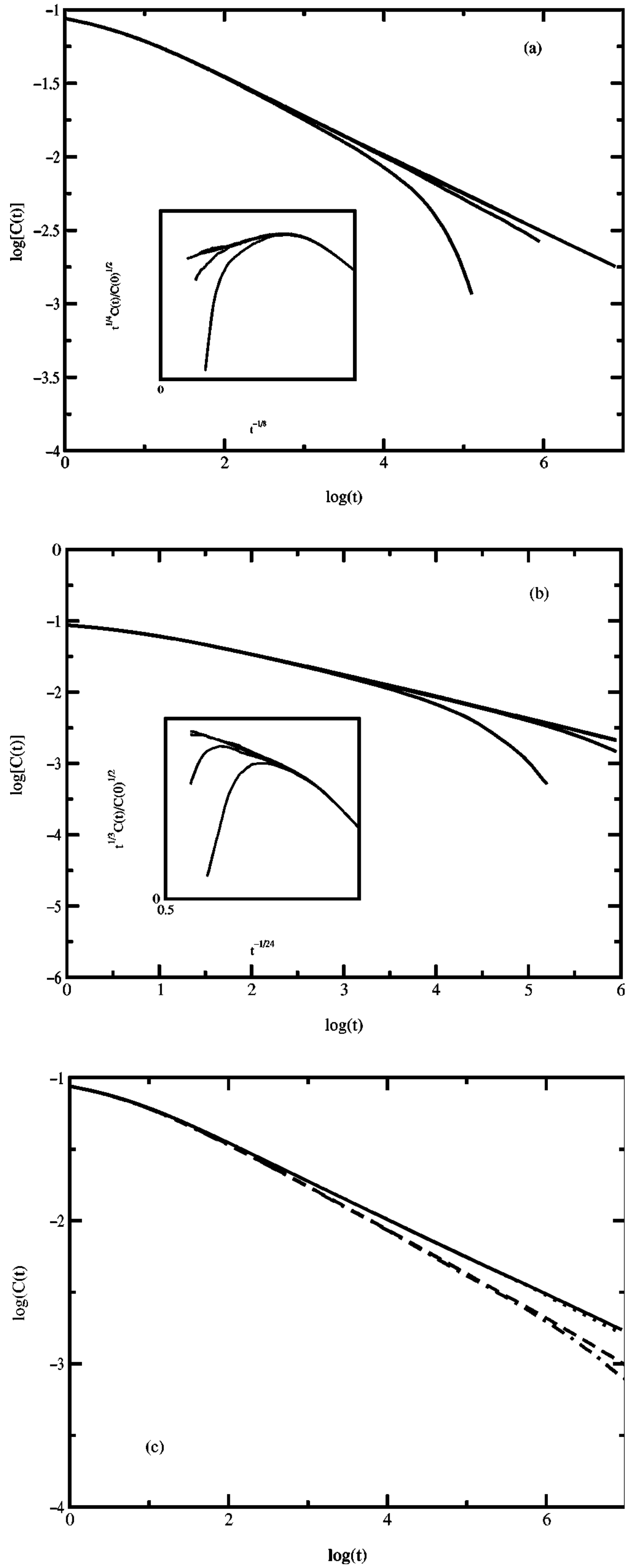

FIG. 1. The log-log plot of density versus time (a) for the isotropic diffusion of particles, (b) for the maximum drift for $L=10^3$, 10^4, 10^5, and 10^6 from bottom to top, and (c) for the isotropic diffusion (upper curves) and for the maximum drift (lower curves) for $L=10^5$ and $L=10^6$. Inset is the log-log plot of (a) $t^{1/4}C(0)^{-1/2}C(t)$ versus $t^{-1/8}$ and (b) $t^{1/3}C(0)^{-1/2}C(t)$ versus $t^{-1/24}$.

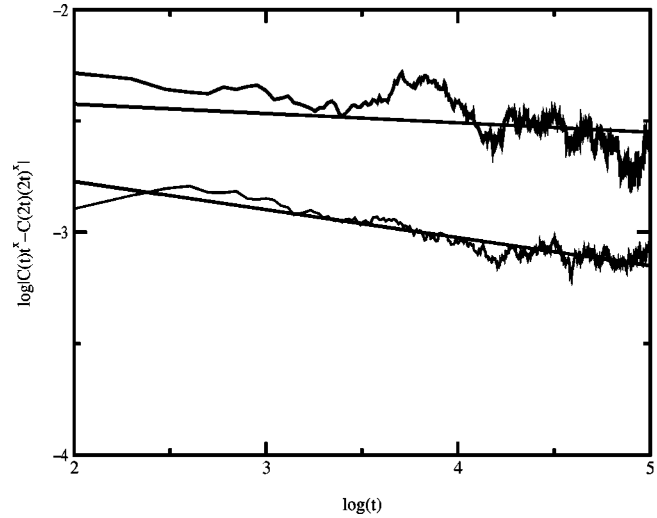

FIG. 2. The log-log plot of $|C(t)t^x - C(2t)(2t)^x|$ versus time for the isotropic case (lower curves) with $x=1/4$ and for the maximum drift (upper curves) with $x=1/3$. The straight lines are with the slope $-1/8$ (lower line) and $-1/24$ (upper line).

drift. In the inset of Fig. 1(a) we plot $t^{1/4}C(t)/\sqrt{C(0)}$ versus $t^{-1/8}$. At long times we observed, the straight line regime from which we concluded the second-order correction of the density decays $C(t)\sim t^{-x}[1+O(t^{-y})]$ with $x=1/4$ and $y=1/8$.

Let us consider some physical quantities that characterize the structure of the domain of the particles. These include the density $C(t)\sim t^{-x}$, the average distance between the nearest particles of the same species $l_{AA}(t)\sim t^{\beta}$, the average distance between nearest particles of different species $l_{AB}(t)\sim t^{\gamma}$, the average number of pairs of same-species particles per a site $N_{AA}(t)\sim t^{-\mu}$, and the average number of pairs of different-species particles per site $N_{AB}(t)\sim t^{-\nu}$. The density of particles is a sum of the number of pairs of the particle [33]

$$C(t)\sim N_{AA}(t)+N_{BB}(t)+N_{AB}(t)=2N_{AA}(t)+N_{AB}(t). \tag{1}$$

The sum of the all interparticle distances adds up to the size of the system

$$[N_{AA}(t)+N_{BB}(t)]l_{AA}(t)+N_{AB}(t)l_{AB}(t)\sim 1. \tag{2}$$

For the isotropic diffusion, the asymptotic behavior of the domain is given as $l_{AA}(t)\sim t^{1/4}, l_{AB}(t)\sim t^{3/8}, N_{AA}(t)\sim t^{-1/4}$, and $N_{AB}(t)\sim t^{-1/2}$ [19,20,22]. From Eq. (1) and Eq. (2) we obtain $C(t)\sim 2N_{AA}+(1-2N_{AA}l_{AA})/l_{AB}=AN_{AA}+Bl_{AB}^{-1}$, where A and B are constants. Therefore, the density decays according to $C(t)=At^{-1/4}+Bt^{-3/8}=t^{-1/4}[A+Bt^{-1/8}]$. In Fig. 2 we show the log-log plot of $|C(t)t^x - C(2t)(2t)^x|$ versus time with $x=1/4$. We find the slope $-1/8$ that supports the second-order correction $O(t^{-1/8})$ in the isotropic diffusion. In Fig. 1(b) we present the density decay for the maximum drift. The inset shows a log-log plot of $t^{1/3}C(t)/\sqrt{C(0)}$ versus $t^{-1/24}$. We observed the second-order correction $O(t^{-1/24})$ from the linear dependence in the inset.

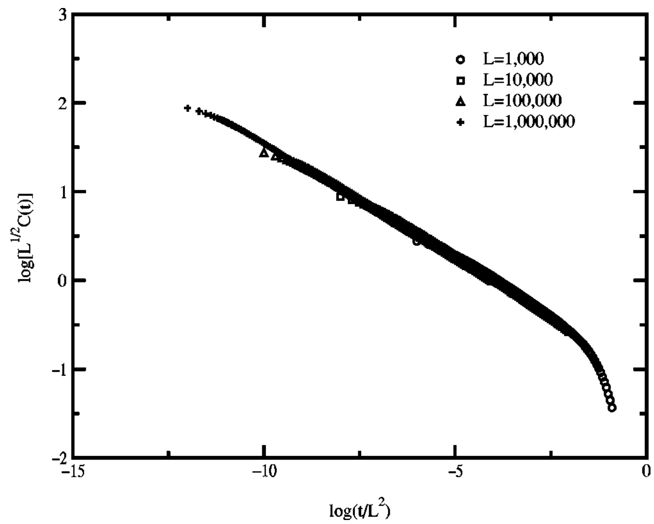

FIG. 3. The log-log plot of $L^{1/2}C(t)$ versus t/L^2 for the isotropic diffusion for $L=10^3(\bigcirc),10^4(\square),10^5(\triangle)$, and $L=10^6(+)$.

The crossover time of the density is $t_c \sim L^{3/2}$ for the maximum drift. In Fig. 2 we show the log-log plot of $|C(t)t^x - C(2t)(2t)^x|$ versus time with $x=1/3$ for the maximum drift. The estimated slope is $-1/24$. In the maximum drift case, the asymptotic behavior of the domain is given as $N_{AA} \sim t^{-1/3}, N_{AB} \sim t^{-7/12}, l_{AA} \sim t^{1/3}$, and $l_{AB} \sim t^{3/8}$ [19,22–24]. From Eq. (1) and Eq. (2), we obtain $C(t)=Ct^{-1/3}+Dt^{-3/8} = t^{-1/3}[C+Dt^{-1/24}]$ for the maximum drift where C and D are constant. Our results of simulation support this prediction for the second-order correction.

We showed the finite-size scaling of density decay for the isotropic diffusion of the particle as shown in Fig. 3 and for the maximum drift as shown in Fig. 4 for various lattice sizes. We consider the scaling function as

$$C(z)=L^a F_o(z)+L^b F_1(z),$$

where F_o and F_1 are scaling functions and $z=t/L^2$ for the isotropic diffusion and $z=t/L^{3/2}$ for the maximum drift. At long-time limits $L\to\infty$ and $t\to\infty$, kept constant z, the density is independent on the lattice size. Thus, we obtain the exponents as $a=-2x$, $b=-2(x+y)$ for the isotropic case and $a=-3x/2$, $b=-3(x+y)/2$ for the maximum drift case where y is the exponent of the second-order correction of the density. From the scaling function we obtained the leading-order scaling function such as $L^{1/2}C(z)=F_o(z=t/L^2)$ for the isotropic diffusion. Data with different lattice sizes are all collapsed on a single line as shown in Fig. 3. Similar collapses of data observed for the maximum drift case by $L^{3x/2}C(z)=F_o(z=t/L^{3/2})$ are shown in Fig. 4. In the maximum drift the typical length of particles is given by the super diffusive behavior $L \sim t^{2/3}$. So the scaling variable is $z = t/L^{3/2}$ for the maximum drift. We presented the data collapses with three different values of x as shown in Fig. 4. For the maximum drift the exponent x was predicted to 1/3 by the scaling argument [19,20]. However, the exponent x always observed lower value $x=0.31$ in Monte Carlo simulation [19,22–24]. In our simulation we observed the exponent $x=0.31(2)$ for the maximum drift. However, the data collapses of the scaling function were better for $x=1/3$ than for $x=0.31$. But it is inconclusive to fix the exponent x through our data because we only consider the leading term in data collapses of the scaling function. The exponent of second-order scaling function are predicted by $b=-3/4$ for the isotropic diffusion and $b=-9/16$ for the maximum drift.

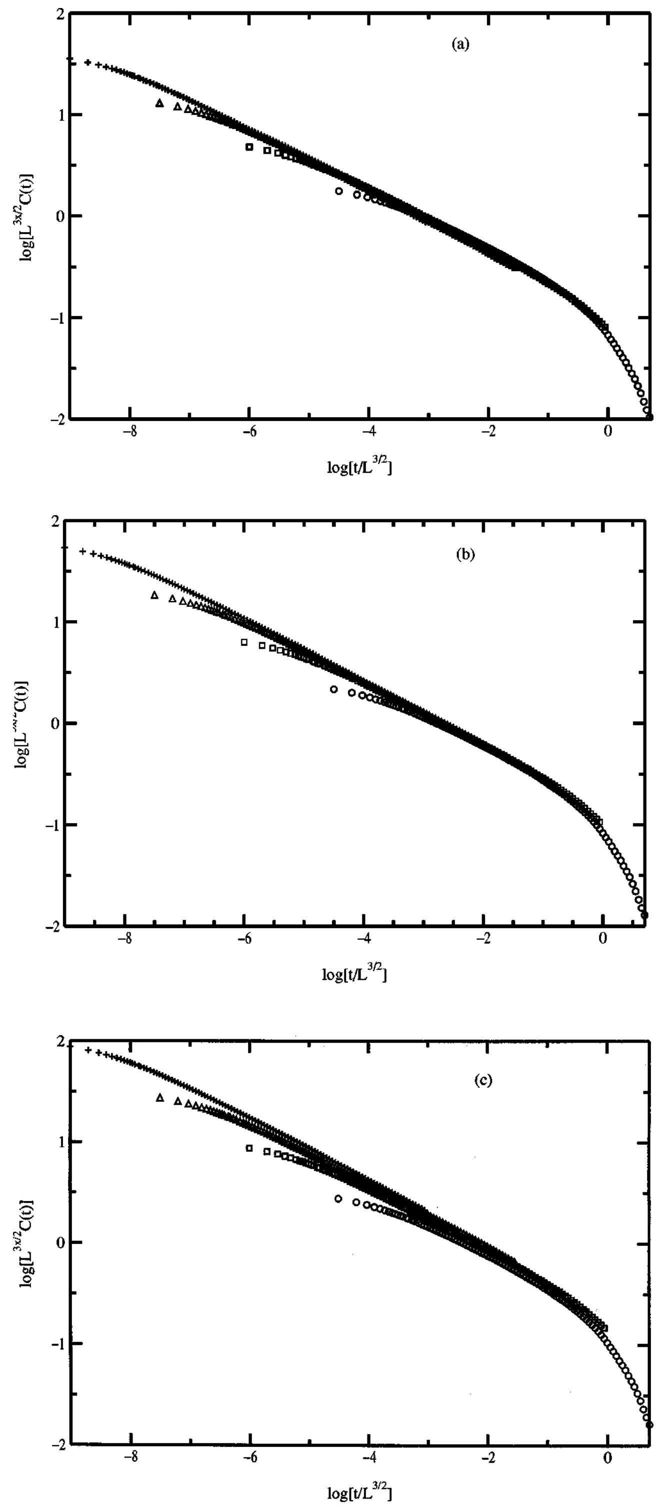

FIG. 4. The log-log plot of $L^{3x/2}C(t)$ versus $t/L^{3/2}$ for the maximum drift with (a) $x=0.32$, (b) $x=1/3$, and (c) $x=0.33$ for $L=10^3(\bigcirc),10^4(\square),10^5(\triangle)$, and $L=10^6(+)$.

In summary we have observed the finite-size effects of two species diffusion-limited annihilations. The second correction of the density is give by $O(t^{-1/8})$ for the isotropic diffusion and $O(t^{-1/24})$ for the maximum drift. We proposed a scaling function of the density decay. We obtained the scaling exponent as $a=-1/2$, $b=-1/4$ for the isotropic diffusion and as $a=-1/2$, $b=-1/12$ the maximum drift.

This work was supported by Brain Korea 21, BSRI 1998-015-D00125, and Korea Research Foundation for the 21st Century.

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