# Numerical Simulation of the Trapping Reaction with Mobile and Reacting Traps 

Joshua D. Hellerick, ${ }^{1}$ Robert C. Rhoades, ${ }^{2}$ and Benjamin P. Vollmayr-Lee ${ }^{1}$<br>${ }^{1}$ Department of Physics, Bucknell University, Lewisburg PA 17837, USA<br>${ }^{2}$ Center for Communications Research, Princeton, NJ 08534, USA

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#### Abstract

We study a variation of the trapping reaction, $A+B \rightarrow A$, in which both the traps $(A)$ and the particles $(B)$ undergo diffusion, and the traps upon meeting react according to $A+A \rightarrow 0$ or $A$. This two-species reaction-diffusion system is known to exhibit a non-trivial decay exponent for the $B$ particles, and recently renormalization group methods have predicted an anomalous dimension in the $B B$ correlation function. To test these predictions we develop a computer simulation method, motivated by the technique of Mehra and Grassberger, that determines the complete probability distribution of the $B$ particles for a given realization of the $A$ particle dynamics, thus providing a significant increase the quality of statistics. Our numerical results indeed reveal the anomalous dimension predicted by the renormalization group, and compare well quantitatively to precisely known values in cases where the problem can be related to a 4 -walker problem.


## I. INTRODUCTION

Reaction-diffusion processes with irreversible reactions provide an important class of far from equilibrium systems. Interest in these systems stems from the fact that the particles develop nontrivial correlations that cannot be described by equilibrium fluctuations, and these correlations in turn affect the reaction rates and particle densities. Applications for these model systems include chemical reaction kinetics [1], interface growth models [2], aggregation 3], domain coarsening [4], and population dynamics [5].

In the present work, we consider a two-species process consisting of the trapping reaction $A+B \rightarrow A$, in which $A$ particles, or "traps," catalyze the decay of $B$ particles, and where the traps additionally react according to $A+A \rightarrow 0$ (annihilation) or $A+A \rightarrow A$ (coalescence). Both particle types $A$ and $B$ undergo diffusion with corresponding diffusion constants $D_{A}$ and $D_{B}$. This system has been predicted via renormalization group ( RG ) methods to exhibit anomalous dimension in both the $B$ particle density decay [6-8] and separately in the scaling of the $B B$ correlation function [9] for spatial dimension $d<2$. The primary focus of this paper is to test these predictions numerically in one-dimensional systems. For this purpose we develop a hybrid Monte Carlo technique that provides the entire $B$ particle distribution for a given realization of the $A$ particles. This is possible because, as argued below, the $B$ particles remain locally Poissonian.

For the $A+B \rightarrow A$ trapping reaction with mobile but non-reacting traps, the mean-field rate equation predicts the $B$ particle density to decay exponentially with time. However, scaling arguments and rigorous bounds confirm that for dimension $d<2$ nontrivial correlations develop between the traps and the surviving $B$ particles, invalidating the rate equation and causing the $B$ particle density to decay as a stretched exponential $\langle b\rangle \sim \exp \left(-\lambda_{d} t^{d / 2}\right)$ with a universal coefficient $\lambda_{d}$ 1012]. Here and throughout angle brackets are used to indicate averages over the random initial conditions and
over the stochastic processes of reaction and diffusion.
Now consider traps that are additionally reacting according to

$$
A+A \rightarrow \begin{cases}A & (\text { coalescence }) \text { probability } p  \tag{1}\\ 0 & \text { (annihilation) probability } 1-p\end{cases}
$$

Since the traps are unaffected by the $B$ particles, their dynamics reduces to the well-studied single-species reaction, where mean-field rate equations (see below), exact solutions in one spatial dimension [13-15], and field-theoretic RG methods [16 18] for general dimension demonstrate that the $A$ particle density decays as power law (with a multiplicative logarithmic correction in $d=2$ ). This decaying trap density then enhances the survival probability of the $B$ particles, resulting in a power law decay with time, $\langle b\rangle \sim t^{-\theta}$. For example, the rate equations, valid for $d>2$ where diffusion manages to keep the reactants well mixed, are

$$
\begin{equation*}
\partial_{t}\langle a\rangle=-\Gamma\langle a\rangle^{2}, \quad \partial_{t}\langle b\rangle=-\Gamma^{\prime}\langle a\rangle\langle b\rangle \tag{2}
\end{equation*}
$$

with solutions $\langle a\rangle \sim 1 /(\Gamma t)$ and $\langle b\rangle$ decay exponent determined by the nonuniversal rate constants, $\theta=\Gamma^{\prime} / \Gamma$.

For $d<2$ the depletion caused by reactions competes with diffusion, developing correlations that modify the reaction rate. This results in the trap density decay $\langle a\rangle \sim A_{d}\left(D_{A} t\right)^{-d / 2}$ with a universal coefficient $A_{d}$. The $B$ particle density in this fluctuation-dominated case has been studied with Smoluchowski theory [19], which is an improved rate equation that incorporates the depletion with a time-dependent rate constant, and with RG techniques [6-9]. In both cases the $B$ particle density was found to decay as a power law with a universal exponent $\theta$ depending only on the diffusion constant ratio $\delta=D_{B} / D_{A}$ and the trap reaction parameter $p$ defined in Eq. (1). Smoluchowski theory gives

$$
\begin{equation*}
\theta_{S}=\frac{d}{2-p}\left(\frac{1+\delta}{2}\right)^{d / 2} \tag{3}
\end{equation*}
$$

while the RG analysis predicts

$$
\begin{equation*}
\theta=\theta_{S}+\frac{1}{2} \gamma_{b}^{*} \tag{4}
\end{equation*}
$$

where $\gamma_{b}^{*}$ is an anomalous dimension of order $\epsilon=2-d$ which stems from a field renormalization of the density [7, 9].

Recently it was shown by RG methods that an additional anomalous dimension occurs due to the field renormalization of the $b^{2}$ density operator [9], with the consequence that the $B$ particle correlation function scales as

$$
\begin{equation*}
C_{B B}(r, t) \equiv \frac{\langle b(r, t) b(0, t)\rangle-\langle b(t)\rangle^{2}}{\langle b(t)\rangle^{2}} \sim t^{\phi} f(r / \sqrt{t}) \tag{5}
\end{equation*}
$$

where $\phi$ is a universal exponent of order $\epsilon$. In contrast, the scaled correlation functions $C_{A A}$ and $C_{A B}$ are simply functions of $r / \sqrt{t}$ with no time-dependent prefactor. We note that $\chi_{B B}(t) \equiv C_{B B}(0, t)$ is a measure of the local fluctuations, and Eq. (5) predicts that $\chi_{B B}$ grows as a universal power of time. In Ref. [9] the exponent $\phi$ was computed to first order in $\epsilon$. Additionally, an exact value of $\phi$ was obtained for the case of $p=\delta=1$ in one spatial dimension by mapping to a four walker problem [9] and solving an eigenvalue problem numerically [20].

Here we aim to use numerical simulations to test the predicted scaling form Eq. (5) and to measure the exponents $\theta$ and $\phi$. These simulations are challenging since the window of scaling behavior is limited by transients at early times and finite size effects and vanishing particle numbers at late times. In the present work we circumvent the small number statistics of the $B$ particles by determining the entire $B$ particle probability distribution conditioned on a particular realization of the $A$ particle dynamics. Our technique was inspired by and is a converse to the method of Mehra and Grassberger [21], who studied the trapping reaction by monitoring a single particle and updating the distribution of traps. With greatly improved statistical accuracy, we were able to demonstrate the scaling collapse of the $A A, A B$, and $B B$ correlation functions and measure the dynamical exponents $\theta$ and $\phi$ to high accuracy.

The layout of this paper is as follows. In Sec. II we present our hybrid simulation method, which also serves to define the model we are considering. In Sec. III we report our measurements of the density decay exponent $\theta$ for a variety of $\delta$ and $p$ values, and compare these to known exact solutions, RG calculations, and the Smoluchowski approximation. Then in Sec. IV we present our data for the anomalous dimension $\phi$, and compare to the RG prediction and the exact solution from the 4 -walker problem, while in Sec. V we test the pair correlation functions for scaling collapse. Finally, in Sec. VI we summarize our results and suggest future work.

## II. HYBRID MONTE CARLO AND MASTER EQUATION METHOD

Reaction-diffusion systems are typically simulated via Monte Carlo methods: a lattice is populated randomly by particles, and then updated according to the particular rules for reaction and stochastic diffusion. Quantities of interest are then averaged over multiple realizations of the stochastic processes. Monte Carlo is employed rather than direct computation of the probabilities in a master equation because of the impossibility in dealing with such a large number of configurations.

However, for the trapping reaction the $B$ particles are non-interacting, and this allows for a much simpler description of the $B$ particle probabilities. We use this to construct a hybrid approach in which we use Monte Carlo for the $A$ particles, but for each realization of the $A$ particle dynamics we calculate the entire $B$ particle probability distribution. This is possible because the $B$ particle distribution remains Poissonian at each lattice site.

We now define our model for concreteness. We consider a $d$-dimensional hypercubic lattice and use a parallel update. The $A$ and $B$ particles are initially randomly distributed on sites whose lattice indices sum to an even number. In a diffusion step each particle will simultaneously hop in one of the $\pm \hat{x}_{i}$ directions along the principle axes of the lattice, so that after an even (odd) number of steps, the particles reside in the even (odd) sector of the bi-partite lattice. Reactions are then performed subsequent to the diffusion hops. In the simplest scenario, for any site containing both $A$ and $B$ particles, the $B$ particles are removed. A variant of this rule would be for each $B$ particle to be removed with probability $p^{\prime}$. Any site containing two $A$ particles reacts according to Eq. (1), governed by the parameter $p$.

When the $A$ and $B$ diffusion constants are equal, both particle types step simultaneously, resulting in the diffusion constant $D=\Delta x^{2} /(2 d \Delta t)$ for a lattice constant $\Delta x$ and a hop time $\Delta t$. For unequal diffusion constants we can take an odd number of multiple steps for one of the species. For example, if $\delta=D_{B} / D_{A}=3$ we take two steps with the $B$ particles, check the $A+B \rightarrow B$ reaction, take one more step with both particle types, and then check the reactions again. For $\delta=2$ we first do the process just described and then take one more step with both particle types. In this way any rational value of the diffusion constant ratio $\delta$ can be realized.

Our hybrid technique relies on the following two wellknown properties of Poisson distributions:
P1. The sum of two independent Poisson distributed random variables with mean values $\mu$ and $\nu$ is a Poisson random variate with mean $\mu+\nu$.

P2. The compound of a Poisson distribution with mean $\mu$ and a binomial distribution with probability $q$ is a Poisson distribution with mean $q \mu$.
The second property says that if a number of elements is a Poissonian random variate and then a random subset


FIG. 1: A characteristic segment of our simulation. The blue lines are $A$ particles (traps), which undergo both coalescence and annihilation reactions. The $B$ particle probability distribution is shaded in red, with the intensity representing the local Poissonian mean.
of elements are selected with independent probabilities, the selected number of elements is a Poissonian random variate.

Now consider a Poisson distribution of $B$ particles on site $i$ with mean value $b_{i}$. In the diffusion step the probability of a particle making the hop to a particular nearest neighbor $j$ is $1 /(2 d)$. Thus from property P 2 these particles will contribute a Poissonian distributed number of particles with mean $b_{i} /(2 d)$ to each of their neighboring sites. The new distribution at a particular site $j$ is a sum of Poisson random variates, thus by property P1 it is Poissonian with mean given by

$$
\begin{equation*}
b_{j, t+\Delta t}=\frac{1}{2 d} \sum_{k} b_{k, t} \tag{6}
\end{equation*}
$$

where $k$ are the nearest neighbors of $j$.
To incorporate the trapping reaction, we take

$$
\begin{equation*}
b_{i, t} \rightarrow\left(1-p^{\prime}\right) b_{i, t} \tag{7}
\end{equation*}
$$

at any site $i$ containing an $A$ particle at time $t$, which derives from property P 2 , recalling that each $B$ particle independently reacts with probability $p^{\prime}$, or survives with probability $1-p^{\prime}$.

With this method, an explicit realization of the $A$ particles is evolved, and simultaneously the local means of the Poissonian $B$ particles are updated by use of Eqs. (6) and (7). The computational cost of this method in comparison to a Monte Carlo simulation of the $B$ particles is the introduction of a floating point variable that has to be updated at each lattice site at each time step. The gain is vastly improved statistics, particularly for parameter values where $\theta$ is large, for which the $B$ particle density decays rapidly and Monte Carlo simulations would yield vanishing particle numbers.


FIG. 2: Log-log plot of the average $B$ particle density versus time, demonstrating multiple decades of scaling for the case $p=1$ (traps undergoing $A+A \rightarrow A$ ) for various diffusion constant ratios $\delta=D_{B} / D_{A}$. The error bars are significantly smaller than the points plotted.

## III. $B$ PARTICLE DENSITY

We measured the $B$ particle density for onedimensional systems with lattice size ranging from $10^{6}$ up to $3 \times 10^{7}$ sites. We set $\Delta x=\Delta t=1$ and used an initial condition of $\langle a(0)\rangle=0.5$ for the trap density and without loss of generality we set $\langle b(0)\rangle$ to unity.

Simulations were performed for diffusion constant ra$\operatorname{tios} \delta=D_{B} / D_{A}=1 / 4,1 / 2,1,2$, and 4 for both the $A+A \rightarrow 0(p=0)$ and the $A+A \rightarrow A(p=1)$ trap reactions. Additionally, for equal diffusion constants $\delta=1$ we simulated mixed trap reactions with $p=1 / 4,1 / 2$, and $3 / 4$, with $p$ defined in Eq. (11). We also varied the trapping probability parameter $p^{\prime}$ in Eq. (7) to confirm the universality of our results. The data presented here and below correspond to $p^{\prime}=1$. In each case we performed between 100 and 400 independent runs. In order for the statistical uncertainties at different times to be uncorrelated, we used an independent set of runs for each time value where we collected data. The onset time for finite size effects depended strongly on the parameters $\delta$ and $p$, decreasing with respect to both parameters. As such, we chose the system size and simulation run time accordingly for each parameter set to optimize the scaling regime.

Representative data for the $B$ particle density with $p=1$ and varying $\delta$ values are presented in Fig. 2] along with the best fit power law. Not all data points shown are used in the fits.

We fit our data with independent errors at each time value to a power law, choosing our minimum and maximum times according to goodness of fit. We estimated the uncertainty of the exponent by varying the minimum and maximum times. We can evaluate the effectiveness of this procedure by comparing to two exact solutions:

- For $p=1$, the $B$ particle density decays like the

| $\delta$ | $p$ | $\theta_{\text {measured }}$ | $\theta_{\text {exact }}$ |
| :---: | :---: | :--- | :--- |
| $1 / 4$ | 0 | $0.4129(7)$ |  |
| $1 / 2$ | 0 | $0.4434(4)$ |  |
| 1 | 0 | $0.5004(3)$ | 0.5 |
| 2 | 0 | $0.5899(7)$ |  |
| 4 | 0 | $0.7285(9)$ |  |
| $1 / 4$ | 1 | $1.1468(7)$ | 1.14704 |
| $1 / 2$ | 1 | $1.2768(9)$ | 1.27607 |
| 1 | 1 | $1.4992(9)$ | 1.5 |
| 2 | 1 | $1.8650(11)$ | 1.86762 |
| 4 | 1 | $2.438(2)$ | 2.44102 |
| 1 | $1 / 4$ | $0.5923(3)$ |  |
| 1 | $1 / 2$ | $0.7299(10)$ |  |
| 1 | $3 / 4$ | $0.9581(16)$ |  |

TABLE I: Measured values of $\theta$ for various diffusion constant ratios $\delta=D_{B} / D_{A}$ and trap reaction parameter $p$, defined in Eq. (11). The exact values from the vicious walker problem are included for comparison.
survival probability in a three-walker problem [22], giving

$$
\begin{equation*}
\theta=\frac{\pi}{2 \arccos [\delta /(1+\delta)]} \tag{8}
\end{equation*}
$$

- For $p=0$ and $\delta=1$, the $B$ particles behave exactly like $A$ particles, $\langle b\rangle \sim\langle a\rangle$, giving $\theta=1 / 2$.

Our measured values along with their uncertainties are reported in Table. IT The uncertainty estimates appear to be reasonable.

Theoretical results for $\theta$ include the exact solutions described above, as well as Smoluchowski theory, which provides the value $\theta_{S}$ given in Eq. (3), and the RG $\epsilon=$ $2-d$ expansion. Smoluchowski theory has proved to be surprisingly effective, e.g., it correctly predicts the $A$ particle decay exponent for all dimensions 19], but is an uncontrolled approximation. By contrast, the RG $\epsilon$ expansion is systematic, but has only been computed to first order in $\epsilon[\underline{6}, \underline{8}, \underline{9}]$. For completeness we provide the result here:

$$
\begin{equation*}
\theta=\theta_{S}+\frac{1}{4}\left[\frac{1+\delta}{2-p}+\left(\frac{1+\delta}{2-p}\right)^{2} f(\delta)\right] \epsilon+O\left(\epsilon^{2}\right) \tag{9}
\end{equation*}
$$

where
$f(\delta)=1+2 \delta\left[\ln \left(\frac{2}{1+\delta}\right)-1\right]+\left(1-\delta^{2}\right)\left[\operatorname{Li}_{2}\left(\frac{\delta-1}{\delta+1}\right)-\frac{\pi^{2}}{6}\right]$
and $\operatorname{Li}_{2}(v)=-\int_{0}^{v} d u \ln (1-u) / u$ is the dilogarithm function [23].

For coalescing traps, $A+A \rightarrow A$, Smoluchowski theory in $d=1$ and the truncated $R G$ expansion with $\epsilon=1$ can be compared directly to the vicious walker result, as was done in Ref. [8]. We reproduce the comparison


FIG. 3: Measured values of the $B$-particle decay exponent $\theta$ plotted versus the diffusion constant ratio, along with the Smoluchowski prediction, Eq. (3), the RG expansion truncated at first order in $\epsilon=2-d$, and exact solutions. The upper (lower) curves and points correspond to the $A+A \rightarrow A$ $(A+A \rightarrow 0)$ trap reaction. The error bars on the data are much smaller than the points plotted.
here as the upper curves in Fig. 3, and add to the plot our measured values. Primarily, this demonstrates that our simulations and data analysis technique are accurate. Also, as noted in Ref. [8], the truncated RG does a remarkable job of matching the exact solution, while the Smoluchoswki result is considerably low.

The lower set of curves and points in Fig. 3are the corresponding $\theta$ values for annihilating traps, $A+A \rightarrow 0$, where the vicious walker solution is not available. Our measured values for $\theta$ indicate that the Smoluchowski approximation, while faring poorly for $p=1$, is reasonably accurate for $p=0$. The non-monotonicity of $\theta$ with respect to $\delta$ in the truncated RG is likely an artifact of the truncation at $O(\epsilon)$.

Finally, in Fig. 4 we present a similar comparison for the case of equal diffusion constants but varying $p . \mathrm{Cu}-$ riously, the truncated RG expansion matches the exact solutions available at $p=0$ and $p=1$, while faring reasonably in between.

## IV. ANOMALOUS DIMENSION $\phi$

From the field theoretic RG calculation it was determined that $b^{2}$, the square of the field associated with the $B$ density, must be renormalized independently of the $b$ itself. A consequence of this renormalization is that the local fluctuations grow as a power law in time, as measured by

$$
\begin{equation*}
\chi_{B B}(t)=\frac{\left\langle b^{2}\right\rangle-\langle b\rangle^{2}}{\langle b\rangle^{2}} \sim t^{\phi}, \tag{11}
\end{equation*}
$$



FIG. 4: A similar comparison as in Fig. 3 for the equal diffusion constant case $\delta=1$ and varying $p$ as defined in Eq. (1).


FIG. 5: Log-log plot of the local fluctuations $\chi_{B B}$ plotted versus time, for the case $p=1$ and varying $\delta$. The straight lines are power law fits. Finite-size effects are visible at later times, and these data are not included in the fits.
in contrast to the analogous measures

$$
\begin{equation*}
\chi_{A A}=\frac{\left\langle a^{2}\right\rangle-\langle a\rangle^{2}}{\langle a\rangle^{2}}=-1 \tag{12}
\end{equation*}
$$

and

$$
\begin{equation*}
\chi_{A B}=\frac{\langle a b\rangle-\langle a\rangle\langle b\rangle}{\langle a\rangle\langle b\rangle}=-1 \tag{13}
\end{equation*}
$$

which maintain constant values [9]. Our measured values for $\chi_{B B}$ versus time are plotted in Fig. 55, for the case of coalescing traps ( $p=1$ ). We observe power law behavior until the onset of finite-size effects. Curiously, finite-size effects appear much earlier in $\chi_{B B}$ than they do in the density, by a factor of $10^{2}$ or $10^{3}$ (compare Fig. (2).

We were unable to demonstrate power law behavior in $\chi_{B B}$ when the traps are annihilating $(p=0)$ or for any of the mixed reactions we simulated $(p=0.25,0.5$,


FIG. 6: Log-log plot of the local fluctuations $\chi_{B B}$ plotted versus time, for the case equal diffusion constants $\delta=1$ and varying the trap reaction parameter $p$. For $p<1$ we do not reach the scaling regime.

| $\delta$ | $\phi_{\text {measured }}$ | $\phi_{\text {exact }}$ |
| :---: | :--- | :--- |
| $1 / 4$ | $0.452(2)$ |  |
| $1 / 2$ | $0.505(3)$ |  |
| 1 | $0.628(3)$ | 0.6262475 |
| 2 | $0.820(5)$ |  |
| 4 | $1.08(4)$ |  |

TABLE II: Measured values of $\phi$ for various diffusion constant ratios $\delta=D_{B} / D_{A}$ and trap reaction parameter $p=1$, defined in Eq. (11). The exact value from the four-walker problem is included (to 7 digits) for comparison.
and 0.75 ), as shown in Fig. 6. The data are consistent with an asymptotic approach to a power law with a small exponent $\phi$.

Our measured values of $\phi$ for $p=1$ are reported in Table III Our uncertainties were estimated by varying the fitting range within the scaling regime. For the case $\delta=1$, an exact value of $\phi$ can be obtained by considering a four-walker problem, where the walkers on a line are in the order $A-B-B-A$. The bracketing $A$ walkers are unaffected by any subsequent coalescence events with exterior $A$ particles, so they may be regarded as simple random walkers. The $B$ particle density squared will decay as the probability for the two interior walkers to survive until and meet at time $t$ 9]. This exponent can be reduced to an eigenvalue problem [20] and the corresponding value is reported in Table II.

The RG calculation of $\phi$ in Ref. 9] gives

$$
\begin{equation*}
\phi=\frac{13}{24-18 p} \epsilon+O\left(\epsilon^{2}\right) \tag{14}
\end{equation*}
$$

where $\epsilon=2-d$. The truncated expansion does not compare well quantitatively with our data, most notably in the absence of $\delta$ dependence. Plugging in $\epsilon=1$ gives $\phi=13 / 6 \simeq 2.17$, which is significantly higher than the


FIG. 7: Scaling collapse of the measured correlation functions for times ranging over three decades. The cross correlation function $C_{A B}(x, t)$ parameters are (a) $p=1, \delta=1 / 4$, (b) $p=1, \delta=1$, and (c) $p=0, \delta=1$. The inset shows the measured $C_{A A}(x, t)$ for $p=0,1 / 2$, and 1 , as well as the exact solution, Eq. (16), with striking agreement.
values we measured. A qualitative feature that the RG calculation does capture is that $\phi$ is a strongly decreasing function of $p$. Presumably, the RG $\epsilon$ expansion is poorly convergent, as was found with the simple annihilation reaction 17.

## V. CORRELATION FUNCTIONS

Associated with power law behavior with universal exponents is the phenomenon of dynamical scaling. These share a common origin in the underlying RG fixed point that controls the asymptotic dynamics and structure. We test for this dynamical scaling by measuring the trap and particle two-particle correlation functions, as well as their cross-correlation function.

We first consider the traps, which undergo the singlespecies $A+A \rightarrow 0, A$ reactions. An exact solution for the correlation function in $d=1$ was obtained by Masser and ben-Avraham, with the result 24]

$$
\begin{equation*}
C_{A A}(x, t)=\frac{\langle a(x, t) a(0, t)\rangle-\langle a(t)\rangle^{2}}{\langle a(t)\rangle^{2}} \sim f_{A A}\left(x / \sqrt{D_{A} t}\right) \tag{15}
\end{equation*}
$$

where

$$
\begin{equation*}
f_{A A}(z)=-e^{-z^{2} / 4}+\sqrt{\frac{\pi}{8}} z e^{-z^{2} / 8} \operatorname{erfc}(z / \sqrt{8}) \tag{16}
\end{equation*}
$$

Interestingly, this result applies to both annihilating and coalescing particles, as well as mixed reactions. We measured these correlation functions via the Monte Carlo realization of our trap dynamics and found convincing scaling collapse and perfect agreement with the exact solution, as shown in the inset of Fig. 7

We next turn to the cross correlation function

$$
\begin{equation*}
C_{A B}(x, t)=\frac{\langle a(x, t) b(0, t)\rangle-\langle a(t)\rangle\langle b(t)\rangle}{\langle a(t)\rangle\langle b(t)\rangle} \tag{17}
\end{equation*}
$$

which is plotted in Fig. 7 With our hybrid simulation method we measure the correlation between the realized $A$ particles and the associated $B$ probability distribution. The data again exhibit convincing scaling collapse, with a scaling function that depends on the parameters $\delta$ and $p$. Both $C_{A A}$ and $C_{A B}$ exhibit anti-correlations at short distances, a direct consequence of the $A+A \rightarrow(0, A)$ and $A+B \rightarrow A$ reactions. However, depending on the parameter values, the cross-correlation function $C_{A B}$ can be non-monotonic with positive correlations at larger separation. We depict three choices of parameters in Fig. 7, but we found similar scaling collapse for all investigated cases.

Finally, we turn to the $B$ particle correlation function defined in Eq. (5) and measured by the sampled set of $B$ particle distributions. Since the $B$ particles do not react with each other, we do not expect them to be anticorrelated at short distances. Instead, a surviving $B$ particle is likely to be found in a region with few $A$ traps nearby, which results in an enhanced probability of other $B$ particles nearby, i.e., positive correlations.

Our measured values for correlation function confirm this, as shown in Fig. 8. The inset shows that when $C_{B B}(x, t)$ is plotted versus the scaled distance $x / \sqrt{D_{A} t}$, as was done in Fig. 7] we do not find collapse, but rather the correlations are growing in magnitude with time. However, when we also scale the vertical axis by the expected $\chi_{B B} \sim A t^{\phi}$, with $A$ and $\phi$ taken from our fitted values, we indeed see scaling collapse, as shown in the main part of Fig. 8. Thus we have confirmed the RG prediction of the scaling form in Eq. (5).

The scaled correlations for $p=1$ show a significant dependence on the diffusion constant ratio. The similarity of the scaling functions suggest that a rescaling of the horizontal axis to the form $x / \sqrt{D_{A}^{1-k} D_{B}^{k} t}$ might collapse all measured functions to a single curve. Indeed, the value $k=0.60$ comes close though slight differences are observable. Evidently the power-law dependence captures a dominant feature of the $\delta$-dependence on the scaling function, but is not an exact result and there is currently no theoretical basis to expect such behavior.

When $p<1$ we cannot make a scaling plot similar to Fig. 8 since we are unable to simulate late enough to get into the regime where $\chi_{B B}$ is a power law. If we instead rescale the vertical scale by $C_{B B}(0, t)$ we find reasonable scaling collapse, suggesting the shape of the correlation function converges more quickly than $\chi_{B B}$ itself.

## VI. SUMMARY

We have developed a hybrid simulation method for the coupled two-species reactions $A+B \rightarrow A$ and $A+A \rightarrow$


FIG. 8: Scaling collapse of the measured correlation functions $C_{B B}(x, t)$ for times ranging over two decades, which requires rescaling the vertical axis by $\chi_{B B} \sim A t^{\phi}$. All plots are for coalescing traps ( $p=1$ ). The inset shows $C_{B B}$ for $\delta=1$ without the vertical rescaling; the intercept is increasing with time.
$(0, A)$ that involves a Monte Carlo simulation of the traps combined with the full probability distribution for the particles. This method provides significant improvement for statistics and avoids the problem of vanishing $B$ particle numbers.

With this technique, we explored the behavior of this reaction-diffusion system for a variety of diffusion constant ratios and trap reaction types. In all cases we were able to obtain convincing power law decay of the $B$ particle density and measure the decay exponent to $0.1 \%$ accuracy, as shown in Table with results that are consistent
with known exact values. Our data were compared with theoretical results from the $\mathrm{RG} \epsilon=2-d$ expansion and from Smoluchowski theory.

We further tested the recently calculated anamolous dimension in the $B$ particle correlation function, or equivalently in the local fluctuations of the $B$ particles: $\chi_{B B}=$ $C_{B B}(0, t) \sim t^{\phi}$. For the case of coalescing traps we were able to obtain multiple decades of power law scaling and measure the exponent $\phi$ to $0.5 \%$ accuracy (see Table II). Our measured values do not match the truncated RG calculation, but are consistent with one exact value.

We have also tested for universality by varying the trapping reaction probability $p^{\prime}$, defined in Eq. (7). We confirmed that the exponents $\theta$ and $\phi$ and the correlation functions are not dependent on this parameter, consistent with them being universal functions of $\delta$ and $p$. In contrast, the amplitude of the density decay $\langle b\rangle \sim A t^{-\theta}$ does dependent on $p^{\prime}$ and is nonuniversal.

It is noteworthy that the power law behavior in the correlation function $C_{B B}(x, t)$ and fluctuations $\chi_{B B}$ encountered finite-size effects much earlier than the density $\langle b\rangle$. From Fig. 5w see finite size effects entering around $t=3 \times 10^{4}$ for the equal diffusion constant case, at which time the diffusion length is $\sqrt{D t} \sim 100$ in a system of size $3 \times 10^{7}$. The origin of this extreme sensitivity merits further investigation, both analytically and numerically.

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