

Reaction-diffusion and reaction-subdiffusion equations on arbitrarily evolving domainsE. Abad ^{*}*Departamento de Física Aplicada and Instituto de Computación Científica Avanzada, Centro Universitario de Mérida, Universidad de Extremadura, 06800 Mérida, Spain*C. N. Angstmann,[†] B. I. Henry,[‡] and A. V. McGann[§]*School of Mathematics and Statistics, UNSW, Sydney New South Wales, 2052, Australia*F. Le Vot ^{||} and S. B. Yuste [¶]*Departamento de Física and Instituto de Computación Científica Avanzada, Universidad de Extremadura, 06071 Badajoz, Spain*

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Reaction-diffusion equations are widely used as the governing evolution equations for modeling many physical, chemical, and biological processes. Here we derive reaction-diffusion equations to model transport with reactions on a one-dimensional domain that is evolving. The model equations, which have been derived from generalized continuous time random walks, can incorporate complexities such as subdiffusive transport and inhomogeneous domain stretching and shrinking. Inhomogeneously growing domains are frequently encountered in biological phenomena involving stochastic transport, such as tumor growth and morphogen gradient formation. A method for constructing analytic expressions for short-time moments of the position of the particles is developed and moments calculated from this approach are shown to compare favorably with results from random walk simulations and numerical integration of the reaction transport equation. The results show the important role played by the initial condition. In particular, it strongly affects the time dependence of the moments in the short-time regime by introducing additional drift and diffusion terms. We also discuss how our reaction transport equation could be applied to study the spreading of a population on an evolving interface. From a more general perspective, our findings help to mitigate the scarcity of analytic results for reaction-diffusion problems in geometries displaying nonuniform growth. They are also expected to pave the way for further results, including the treatment of first-passage problems associated with encounter-controlled reactions in such domains.

DOI: [10.1103/PhysRevE.102.032111](https://doi.org/10.1103/PhysRevE.102.032111)**I. INTRODUCTION**

Reaction-diffusion partial differential equations have been widely employed to provide mathematical models across many physical, chemical, and biological processes [1–3], with classic applications including the spread of bushfires, the development of animal coat patterns, and the spread of epidemics. In recent decades the fundamental development of reaction-diffusion equations has focused on extensions to incorporate physical complexities in two key areas: anomalous subdiffusion [4–11] and domain growth [3,12–23]. Anomalous subdiffusion, which has been reported in numerous experimental observations [24–32], refers to diffusion processes in which the mean-square displacement scales as a sublinear power law in time. Domain growth is used generically to refer to stretching and shrinking of the domain over

time. In this work we have developed reaction-diffusion equations to allow for the possibility of including both features, subdiffusion and domain growth, simultaneously.

As a preamble, we comment here briefly on the methodology employed in our derivation of reaction-diffusion equations, including the possibility of subdiffusion, on a growing domain. The first fundamental derivation of the diffusion equation was carried out by Einstein using a random walk formalism [33]. In this approach Einstein considered random walks at fixed intervals of time with steps from a step length probability density with a finite variance. The extension to continuous time random walks (CTRWs) with waiting times between steps, drawn from a power-law probability density, led to the derivation of the fractional diffusion equation for subdiffusion [34–36].

Reaction diffusion equations with standard diffusion were formulated by simply adding reaction kinetics terms to the standard diffusion term [37]. It was not possible to obtain a physically consistent model for subdiffusion with reactions following this simple approach. In particular it was found that negative reaction kinetics terms added to the subdiffusion term could result in negative solutions overall [5]. This led to a reinvestigation of the underlying CTRWs with consideration on how to incorporate particle deaths and births at the level

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of the random walks [5–11]. One can immediately envisage that different system dynamics could ensue depending on whether or not newborn particles inherit the same waiting time as their parent particles before taking a random walk [8]. It is now generally recognized that fractional dynamics, including subdiffusion, cannot be incorporated into model equations involving other complexities such as reactions or space- and time-dependent forces simply by replacing standard macroscopic transport terms with fractional macroscopic transport terms. We have been mindful of this in the present work by deriving the modeling equations from physically consistent CTRWs.

A useful approach, in the CTRW paradigm, for dealing with reaction subdiffusion systems in the case where newborn particles do not inherit the waiting times of parent particles is to construct an ensemble of different species of reacting particles by considering their most elementary representation; that of single particles that are created (birth process) at some point in time and space and then removed (death process) at some later point. In this approach, single particles with death probabilities, undergoing continuous time random walks are considered first, and then collections of such particles arising from the birth processes are considered in an ensemble representation [10,11]. The reaction subdiffusion equation can then be derived by taking the diffusion limit of the master equation for this ensemble of walkers [11]. Standard reaction diffusion equations can also be derived using this methodology, and it is capable of modeling phenomena on a vast array of scales, from single chemical molecules to ecosystems. Examples include a reaction-subdiffusion model for the space and time distribution of degrading chemical morphogens at the cellular level [10] and models for the non-Fickian spread of contaminant plumes with chemical degradation at the macroscopic level [38].

The study of subdiffusion on growing domains is still in its infancy, and the inclusion of reactions within this framework is an outstanding problem. Reaction diffusion models with standard diffusion on a growing domain have been studied in a series of papers [12–18,39]. Specific examples include a model with diffusion and degradation for the formation of morphogen gradients on a growing domain [20], and a model with diffusion, a constant per capita birth rate, and a population size dependent death rate, for insect dispersal on a growing domain [16]. In the case of morphogen gradients, say, degradation may occur at timescales over which both diffusive transport arising from concentration differences and advection mediated by tissue growth are non-negligible. This justifies the inclusion of death terms in the relevant PDEs [40,41].

We now proceed to give a brief overview of recent progress on subdiffusion on growing domains and how it relates to the goals of this paper. In Refs. [42,43], Ali *et al.* put forward a procedure to map the behavior of stochastic trajectories from time-dependent domains (especially, expanding radial domains) onto fixed domains for the case of fractional Brownian motion (as well as for normal Brownian motion and Lévy flights). Le Vot, Abad, and Yuste [44] used a CTRW approach to obtain evolution equations for unbiased diffusion, including anomalous diffusion, in uniformly expanding or contracting media. Later these results were extended to account for the effect of a biasing force field [45] or a velocity field [46].

Another significant advance was made by Angstmann, Henry, and MacGann [47], which employed a generalized CTRW formalism [36,48] to deal with the general case of random walkers that move diffusively or subdiffusively in domains with inhomogeneous growth and contraction rates. In particular, this means that some regions of the domain may expand, while others may simultaneously shrink. The next step was the inclusion of chemical reactions in models with normal diffusion. This was done in Refs. [22,49,50], where evolution equations for encounter-controlled reactions between reactants performing normal diffusive walks in uniformly evolving domains were derived and solved for the special cases of particle coalescence and annihilation. Here we take the formalism developed in Ref. [47] as a starting point by including chemical reactions in the transport equations that hold for arbitrarily evolving domains. Such reactions are not restricted to death processes as in Refs. [22,49,50] but may also involve particle birth.

Because of the notorious difficulties to deal with inhomogeneous domain growth, the problem is often studied numerically (see, e.g., Refs. [39,51]), even in the case of normal diffusion without ongoing reactions. We are actually not aware of previous works where extensive analytical results are presented, as we do here both for normal and for anomalous subdiffusion in the early-time regime. We see this as a first step to develop approximations beyond this regime and to obtain acceptable approximations for the positional PDF on the basis of the behavior of the associated moments.

In turn, an improved knowledge of reaction-diffusion in arbitrarily evolving domains will help to refine some of the existing models for biological systems and phenomena such as tumor growth. In Ref. [52] the spreading of a specific mutant population on the growing surface of tumoral spheroids was studied. The portion of the surface occupied by such mutants (“mutant sector” in the language of Ref. [52]) may increase or decrease deterministically due a selective advantage or disadvantage. However, genetic drift introduces stochasticity at the boundary of the mutant sector. In two dimensions the two boundary points of the corresponding arc of circumference move randomly and can be thought of as coalescing random walks. The extinction of the mutant surface population subject to genetic drift is thus tantamount to vanishing separation distance of the boundary points. A sufficiently fast surface growth is able to avoid such an extinction, since it keeps the separation positive except in a vanishingly small number of statistical realizations. The underlying first-passage problem can be described in terms of a diffusion equation for the separation distance of both boundary points on the growing circular boundary. The type of surface growth considered in Ref. [52] was a homogeneous one, but a more realistic description would clearly involve nonuniform growth.

Inhomogeneous surface growth also plays a critical role in the formation of stromatolites, i.e., laminated, sedimentary rocks originally formed by layer-upon-layer deposition of dead microbes such as cyanobacteria (single-celled photosynthesizing microbes), whereby only the most superficial layer contains living microbes. Recently, a KPZ-like deterministic equation has been used to model its surface growth [53,54]. In Sec. VI we will discuss in detail how the motion on such surfaces of microbicides subject to birth and

death processes could in principle be modeled with our equations.

We begin in Sec. II by setting up a formalism and coordinate system to describe nonuniform domain growth. In Sec. III we first consider a single-particle CTRW on a growing domain, with a death probability between steps. The CTRW on the growing domain is mapped to an auxiliary CTRW in terms of comoving coordinates, i.e., spatial coordinates referring to the initial fixed domain. Then the master equation is obtained for this auxiliary process. We subsequently consider an ensemble of particles undergoing CTRWs with death probabilities and creation probabilities between steps and the master equation for the auxiliary CTRW on the fixed domain with reactions is obtained. In Sec. IV we derive the diffusion limits of the auxiliary CTRW master equation with a jump length density corresponding to unbiased jumps of fixed length on the evolving domain, and with two distinct waiting time densities, exponential and Mittag-Leffler. These densities are known to limit to standard diffusion, and subdiffusion respectively on fixed domains. The fixed length jump on the growing domain maps to a space- and time-varying jump length for the auxiliary CTRW on the fixed domain. An iterative method for evaluating moments to higher orders in time is introduced and moments are evaluated for special cases. These moments are first evaluated for the auxiliary process and then mapped to moments on the evolving domain. The moment calculations are shown to compare favorably with numerical simulations, both on the auxiliary domain and on the evolving domain. In Sec. V we map the diffusion limit equations for the auxiliary CTRW on the fixed domain back to the evolving domain. This yields reaction-diffusion equations for systems undergoing standard diffusion, or subdiffusion, including reactions, on arbitrarily evolving domains. In Sec. VI we deal with the aforementioned problem of stromatolite growth. We conclude with a brief summary and outlook in Sec. VII.

II. SPATIAL AND TEMPORAL DOMAIN EVOLUTION FUNCTION

To obtain the governing evolution equations for diffusing particles on an evolving domain it is useful to establish a mapping between points on the evolving domain at time t and points on the initial fixed domain at time $t = 0$ [47].

For simplicity, in the following, we will assume a finite domain of initial size $L(t = 0) \equiv L_0$. At a given time t we associate each point on the evolving domain $y(t) \in [0, L(t)]$, with a point on the initial domain $x \in [0, L_0]$ through a one-to-one mapping $y(t) = \bar{g}(x, t)$. It should be noted that, although in the present discussion we assume that the domain remains finite at all times, there is no problem in considering it as large as necessary, or even infinite (see Sec. IV). Here, and subsequently, we use a bar to denote any function of the space variable x on the original domain. Especially in cosmology, this x coordinate is also termed “comoving distance” [19,49]. The mapping must satisfy the initial condition $\bar{g}(x, 0) = x$, the boundary conditions $\bar{g}(0, t) = 0$ and $\bar{g}(L, t) = L(t)$, and the non-negativity condition $\bar{g}(x, t) \geq 0$.

Assuming that the domain is a differentiable manifold, the mapping $\bar{g}(x, t)$ can be represented uniquely in terms of

a local growth rate function $\bar{\mu}(x, t)$, which has dimensions of $[T]^{-1}$. We partition the initial domain into n intervals of equal length, $\delta x = L_0/n$. On the evolving domain, the length of each partitioned interval may change in time. We let $\delta y_i(t)$ denote the length of the i th partition at time t . We can now define a local growth function $\bar{\mu}(x_i, t)$ through the evolution equation [47]

$$\frac{d\delta y_i}{dt} = \bar{\mu}(x_i, t)\delta y_i. \quad (1)$$

Integrating Eq. (1), and using the initial condition $\delta y_i(0) = \delta x$ results in the expression

$$\delta y_i(t) = \left[\exp \int_0^t \bar{\mu}(x_i, s) ds \right] \delta x = \bar{v}(x_i, t) \delta x, \quad (2)$$

where, in the rightmost equation, the dimensionless quantity

$$\bar{v}(x, t) \equiv e^{\int_0^t \bar{\mu}(x, s) ds} \quad (3)$$

has been introduced. In the language of cosmology, this quantity is referred to as “the scale factor.” Summing all the δy_i intervals and taking the limit as $n \rightarrow \infty$ produces the mapping between the domains, which can be expressed as a function of the local growth rate. Explicitly,

$$y = \lim_{n \rightarrow \infty} \sum_{i=0}^n \delta y_i = \int_0^x \bar{v}(z, t) dz = \bar{g}(x, t). \quad (4)$$

The local growth rate function might be positive or negative, at different locations, allowing for local expansion and contraction, respectively. This may result in a significant distortion of the original morphology of the domain, as illustrated schematically in Fig. 1 for the particular case of periodic boundary conditions. The evolution equations that we derive are unaffected by the complexity of the distortions, with the only restriction being that the domain remains a differentiable manifold.

Our derivation of the governing evolution equations for reaction and diffusion on an evolving domain utilizes the mapping between the growing domain and the fixed domain. Note that if $f(y, t)$ represents a function of the space variable on the evolving domain y , and $\bar{f}(x, t)$ represents the corresponding function on the fixed domain x , then these functions are related through the mapping $\bar{g}(x, t)$ via

$$f(y, t) = \bar{f}(\bar{g}^{-1}(y, t), t) = \bar{f}(x, t). \quad (5)$$

The advantage in using the representation on the fixed domain is that this enables us to employ standard time derivatives and then map them to the evolving domain.

It should be noted that our results are also valid for d -dimensional evolving domains when the diffusion processes along each Cartesian direction are independent, that is, when

$$\frac{d\delta y_i^{(j)}}{dt} = \bar{\mu}^{(j)}(x_i, t)\delta y_i^{(j)}, \quad (6)$$

where the superscript j denotes the j th Cartesian direction. An important special case is obtained when $\bar{\mu}^{(j)}(x_i, t) = \bar{\mu}(t)$, which corresponds to an isotropic d -dimensional exponential domain evolution.

The use of auxiliary fixed domain formulations to investigate growing domain problems in the analysis of systems

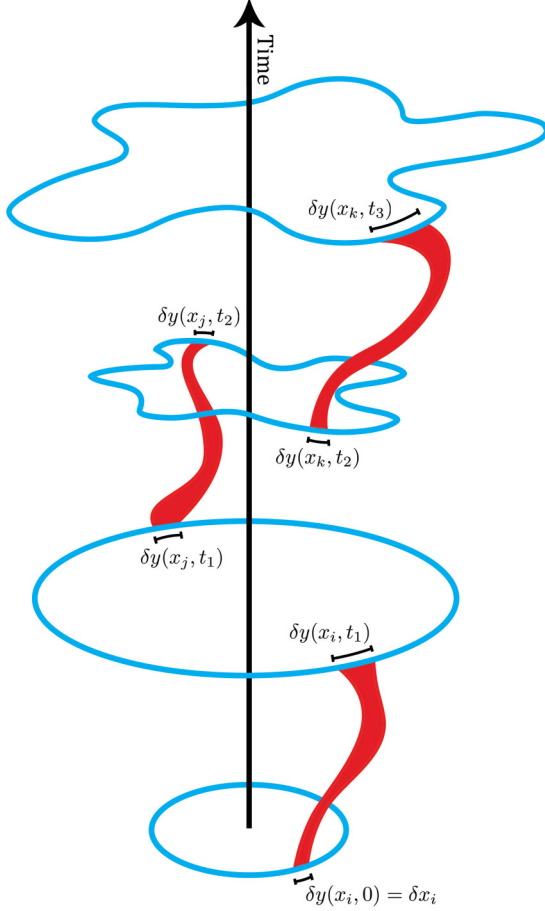


FIG. 1. Schematic illustration of an evolving domain. Here the domain initially expands uniformly as an ellipse before local expansions and contractions lead to a more irregular profile. The red shading is used to illustrate how particular intervals evolve in time with different local space- and time-dependent growth rates. Note that, although we have depicted the one-dimensional domain as a ring, in general, the medium would be a line with two independent ends.

involving reaction and diffusion on a growing domain is not new. For example, Mackenzie and Madzvamuse [39] used a Lagrangian reduction of the arbitrary Lagrange-Eulerian (ALE) mapping [55] to investigate numerical approximations to a reaction-diffusion problem on a growing domain. The ALE scheme had been widely used in numerical methods for fluid flow switching between Lagrangian and Eulerian descriptions. While such approaches involve deterministic PDEs, it is also possible to develop equivalent descriptions in terms of Langevin equations, as done in Refs. [42,43]. In the case of normal diffusion, the main advantage of the Langevin description is that it provides a good starting point for numerical simulations. However, in the case of subdiffusive walks, Langevin equations become much less intuitive and thus harder to deal with.

Here we will follow a different path, and we will consider mappings from growing domain coordinates to fixed domain coordinates at the level of the random walks. As discussed above, this level of description is required for obtaining fundamental results in subdiffusive systems with reactions or forces,

and it also covers the case of standard diffusion with reactions and forces (see also Ref. [47] for the case without reactions).

III. MASTER EQUATIONS IN FIXED DOMAIN COORDINATES FOR CTRWs ON A GROWING DOMAIN

As discussed above, a CTRW on a growing domain can be mapped to a unique CTRW on a fixed domain—the domain at time zero. In this section we derive the master equation for this auxiliary CTRW on the fixed domain. We begin by constructing the probability density function for a single particle undergoing a CTRW on a growing domain with possible particle death. This function is then mapped to the fixed domain and the evolution equation for the mapped function is obtained by differentiating with respect to time. In the next step a collection of such particles, created at different points in space and time, is considered, and we find the master equation in the coordinates of the fixed domain for this ensemble.

A. Single particles with death probabilities

We begin by deriving the governing equation for single-particle diffusion on a growing domain with an associated death probability.

Subsequently we consider an ensemble of such particles, and we also include birth events. We let $q_n(y, t|y_0, 0)$ denote the probability per unit time for a particle that started at y_0 at time $t = 0$ to arrive at y at time t after n jumps, and we suppose that initially

$$q_0(y, t|y_0, 0) = \delta(y - y_0)\delta(t - 0^+). \quad (7)$$

After $n + 1$ steps, the arrival probability rate can be expressed with a recursion relation as

$$q_{n+1}(y, t|y_0, 0) = \int_0^{L(t)} \int_0^t \Psi(y, y'', t, t')\theta(y', t, t') \times q_n(y', t'|y_0, 0) dt' dy'. \quad (8)$$

The interpretation of this is that the probability rate for a particle to arrive at y at time t after $n + 1$ steps is the probability rate for a particle that arrived at y' at an earlier time t' , then waited for a time $t - t'$, and survived death, before jumping to y at time t . The position y'' represents the location on the growing domain of a point at time t that was at a point y' at the earlier time t' . The term $\theta(y', t, t')$ is the probability of surviving death at a point on the domain, referenced as y' at time t' , and $\Psi(y, y'', t, t')$ is the probability density for waiting a time $t - t'$ and transitioning from y'' to y at time t .

The probability per unit time for a particle to arrive at y at time t after any number of steps is obtained by summing over all n in Eq. (8). This results in

$$q(y, t|y_0, 0) = q_0(y, t|y_0, 0) + \int_0^{L(t)} \int_0^t \Psi(y, y'', t, t') \times \theta(y', t, t')q(y', t'|y_0, 0) dt' dy', \quad (9)$$

where

$$q(y, t|y_0, 0) = \sum_{n=0}^{\infty} q_n(y, t|y_0, 0). \quad (10)$$

In Eq. (9) the quantity

$$\theta(y', t, t') = e^{-\int_{t'}^t \omega(y', s) ds} \quad (11)$$

stands for the survival probability of a particle arriving at location y' at time t' , where $\omega(y, s)\delta s$ is the (infinitesimal) probability of a particle dying between times s and $s + \delta s$, and the quantity $\omega(y, s)$ has dimensions of $[T]^{-1}$. At this stage, it is worth noting that, while the above mortality law may not be the most general one, it does not preclude a dependence of the form $\omega = \omega(\rho(y, t))$, i.e., an explicit dependence of the survival probability θ on the probability density (or ‘‘concentration’’) $\rho(y, t)$ of finding a particle at position y at time t .

We assume that the transition probability density is composed of two independent probability densities: the jump density, $\lambda(y, y'') = \lambda(y - y'')$, for a jump of length $y - y''$, and the waiting time density, $\psi(t, t') = \psi(t - t')$, for a particle to wait for $t - t'$ time before jumping. Hence we write

$$\Psi(y, y'', t, t') = \lambda(y - y'')\psi(t - t'). \quad (12)$$

The probability of finding a particle, undergoing a CTRW on a growing domain, in the infinitesimal volume interval $[y'', y'' + dy'']$ at time t can be written as

$$\begin{aligned} &\rho(y'', t|y_0, 0) dy'' \\ &= \int_0^t \Phi(t - t')\theta(y', t, t')q(y', t'|y_0, 0) dy' dt', \end{aligned} \quad (13)$$

where

$$\Phi(t - t') = 1 - \int_0^{t-t'} \psi(s) ds \quad (14)$$

is the jump probability survival function, and $\rho(y'', t|y_0, 0)$ is the probability density for being at y'' at time t . In order to formulate a master equation for the evolution of $\rho(y, t|y_0, 0)$, we find it convenient to consider an auxiliary CTRW process on the initial fixed domain [47]. One advantage of this is that standard time derivatives can be carried out on the fixed domain, and the corresponding functions can then be mapped back to the growing domain. A second advantage is that the equations for the auxiliary process on the fixed domain can be solved in this coordinate system, and the solutions can then be mapped on to the evolving domain. First we relate the densities on the evolving domain to associated densities on a fixed domain using the transformation of Eq. (4). Explicitly, the probability of finding a particle at time t within the interval $[y, y + dy]$ is given by

$$\begin{aligned} \rho(y, t|x_0, 0) dy &= \rho(y, t|x_0, 0) \frac{dy}{dx} dx \\ &= \rho(g(x, t), t|x_0, 0)\bar{v}(x, t) dx \\ &= \bar{\rho}(x, t|x_0, 0)\bar{v}(x, t) dx \\ &= \rho(x, t|x_0, 0) dx. \end{aligned} \quad (15)$$

The quantity $\rho(x, t|x_0, 0)dx$ defined in the last line has a clear physical interpretation: it is the probability of finding a particle at time t within the interval $[x, x + dx]$ on the fixed domain, $[x, x + dx]$ being the x interval corresponding to $[y, y + dy]$ at time t . Because of probability conservation,

one has the relation $\rho(y, t|x_0, 0) = (dy/dx)\rho(x, t|x_0, 0)$. Similarly, one has

$$q(y, t|x_0, 0) dy = q(x, t|x_0, 0) dx = \bar{q}(x, t|x_0, 0)\bar{v}(x, t) dx. \quad (16)$$

Along the same lines, the jump length density on the fixed domain is obtained from probability conservation:

$$\lambda(x, x', t) dx' = \lambda(y, y') dy', \quad (17)$$

implying

$$\lambda(x, x', t) = \bar{v}(x', t)\bar{\lambda}(x, x', t). \quad (18)$$

On the fixed domain we now have the arrival rate probability density, for arriving at x at time t ,

$$\begin{aligned} \bar{q}(x, t|x_0, 0) &= \bar{q}_0(x, t|x_0, 0) + \int_0^{L_0} \lambda(x, x', t) \\ &\times \int_0^t \psi(t - t')\bar{\sigma}(x', t, t')\bar{q}(x', t'|x_0, 0) dt' dx' \end{aligned} \quad (19)$$

and

$$\bar{\rho}(x, t|x_0, 0) = \int_0^t \Phi(t - t')\bar{\sigma}(x, t, t')\bar{q}(x, t'|x_0, 0) dt', \quad (20)$$

where we have defined

$$\bar{\sigma}(x, t, t') = e^{-\int_{t'}^t \bar{\mu}(x, s) ds} \bar{\theta}(x, t, t') = \frac{\bar{v}(x, t')}{\bar{v}(x, t)} \bar{\theta}(x, t, t') \quad (21)$$

with $\bar{\theta}(x, t, t') = \theta(y, t, t')$.

To derive the evolution equation for $\bar{\rho}$, we differentiate Eq. (20) with respect to time. This results in (see Appendix A)

$$\begin{aligned} \frac{\partial \bar{\rho}(x, t|x_0, 0)}{\partial t} &= \int_0^{L_0} \lambda(x, x', t) \int_0^t K(t - t')\bar{\sigma}(x', t, t') \\ &\times \bar{\rho}(x', t'|x_0, 0) dt' dx' \\ &- \int_0^t K(t - t')\bar{\sigma}(x, t, t')\bar{\rho}(x, t'|x_0, 0) dt' \\ &- [\bar{\mu}(x, t) + \bar{\omega}(x, t)]\bar{\rho}(x, t|x_0, 0), \end{aligned} \quad (22)$$

where

$$K(t) = \mathcal{L}^{-1} \left[\frac{\mathcal{L}[\psi(t)]}{\mathcal{L}[\Phi(t)]} \right] \quad (23)$$

is a memory kernel and $\mathcal{L}[Y(t)]$ denotes a Laplace transform of $Y(t)$ with respect to time.

B. Ensemble of particles with birth and death probabilities

We now consider an ensemble of particles composed of individual particles that are created at particular locations, undergo random walks, and are annihilated at other locations. We hereafter assume that newborn particles are created with zero age, i.e., their ‘‘internal clock’’ used as a reference for the waiting time distribution is set to zero. Let us denote by $\chi(y, t) dt dy$ the probability of a particle being created in the region $[y, y + dy]$ during the interval $[t, t + dt]$. Here $\chi(y, t)$ has dimensions of $[L]^{-1}[T]^{-1}$. The ensemble density

of particles at location y at time t , found by summing over all possible starting points y_0 and birth times t_0 , is then given by

$$u(y, t) = \int_0^{L(t)} \int_0^t \rho(y, t|y_0, t_0) \chi(y_0, t_0) dt_0 dy_0. \quad (24)$$

The case of a single particle initially located at y_i which gives rise to no offspring is recovered by setting $\chi(y_0, t_0) = \delta(y_i - y_0) \delta(t_0 - 0^+)$.

Again we find it convenient to consider the auxiliary system on the fixed domain using the mapping given by Eq. (15) and the auxiliary function definitions

$$\bar{u}(x, t) = u(y, t) \quad \text{and} \quad \bar{\chi}(x, t) = \chi(y, t). \quad (25)$$

The ensemble density of particles for the auxiliary system on the fixed initial domain is then

$$\bar{u}(x, t) = \int_0^t \int_0^{L_0} \bar{v}(x_0, t) \bar{\rho}(x, t|x_0, t_0) \bar{\chi}(x_0, t_0) dx_0 dt_0. \quad (26)$$

The master equation for the ensemble is found by differentiating with respect to time. In this way we find

$$\begin{aligned} \frac{\partial \bar{u}(x, t)}{\partial t} &= \int_0^t \int_0^{L_0} \bar{v}(x_0, t) \frac{\partial \bar{\rho}(x, t|x_0, t_0)}{\partial t} \bar{\chi}(x_0, t_0) dx_0 dt_0 \\ &+ \int_0^{L_0} \bar{v}(x_0, t) \bar{\rho}(x, t|x_0, t) \bar{\chi}(x_0, t) dx_0. \end{aligned} \quad (27)$$

This can be simplified by noting that

$$\chi(y, t) = \int_0^{L(t)} \rho(y, t|y_0, t) \chi(y_0, t) dy_0, \quad (28)$$

and thus

$$\bar{\chi}(x, t) = \int_0^{L_0} \bar{v}(x_0, t) \bar{\rho}(x, t|x_0, t) \bar{\chi}(x_0, t) dx_0. \quad (29)$$

We further replace the derivative in Eq. (27) using the single-particle master equation (22), together with Eq. (26), so that

$$\begin{aligned} \frac{\partial \bar{u}(x, t)}{\partial t} &= \int_0^{L_0} \lambda(x, x', t) \int_0^t K(t-t') \bar{u}(x', t') \\ &\times \bar{\sigma}(x', t, t') dt' dx' \\ &- \int_0^t K(t-t') \bar{u}(x, t') \bar{\sigma}(x, t, t') dt' \\ &- [\bar{\mu}(x, t) + \bar{\omega}(x, t)] \bar{u}(x, t) + \bar{\chi}(x, t). \end{aligned} \quad (30)$$

Equation (30) is the master equation for an ensemble of CTRWs, including reaction kinetics, on a fixed domain. The ensemble density at position x and time t maps to the ensemble density for CTRWs, including reaction kinetics, on a growing domain at position y and time t .

It is worth noting that in the limit of a nongrowing domain $\bar{\mu}(x, t) \equiv 0$, one recovers results previously known from the literature. For example, taking $\bar{\theta}(x, t, t') \equiv \exp\{-\int_{t'}^t r_-[\bar{u}(x, s)] ds\}$ and $\bar{\chi}(x, t) \equiv r_+[\bar{u}(x, t)] \bar{u}(x, t)$ leads to Eq. (26) in Ref. [8] upon performing the appropriate changes in notation.

IV. REACTION DIFFUSION EQUATIONS AND REACTION SUBDIFFUSION EQUATIONS IN FIXED DOMAIN COORDINATES FOR GROWING DOMAIN PROBLEMS

In this section we consider the governing equations in the diffusion limit of the master equations for CTRWs in the fixed domain coordinates corresponding to CTRWs on an evolving domain. This yields the partial differential equations and fractional partial differential equations that can be used to model the evolution of an ensemble of CTRWs on a growing domain with reactions. These governing equations are used as a basis for moment calculations on growing domains with standard diffusion, and with subdiffusion. When deriving the equations or discussing the behavior of their solutions, we will assume that boundary and finite size effects are absent and thus deal with the case of free normal or anomalous diffusion. This implies that the particle concentration in the vicinity of the interval end points must remain negligible at any finite time. This is formally attained by considering the case of an infinite system (in our formalism, this could be achieved, for example, by rewriting the interval $[0, L_0]$ as $[-L_0/2, L_0/2]$ and then letting $L_0 \rightarrow \infty$) and an initial condition for the diffusing particle(s) with a sufficiently strong localization, which will be our implicit assumptions in what follows.

First we consider the diffusion limit. The latter requires a simultaneous limit where length scales and timescales approach zero without introducing singularities. The details of this depend on the details of the jump length and waiting time densities. For CTRWs on fixed domains a jump length density for unbiased jumps of fixed length, can result in standard diffusion if the waiting time density is an exponential, or subdiffusion if the waiting time density decays as a power law in time. We now consider these possibilities on the growing domain.

The jump length density for unbiased jumps of fixed length on the growing domain can be written as

$$\lambda(y, y') = \frac{1}{2} [\delta(y - \Delta y - y') + \delta(y + \Delta y - y')], \quad (31)$$

where Δy is a fixed length interval on the growing domain. The master equations that we derived above describe the evolution of an auxiliary CTRW on the fixed domain; thus we need to map the jump density on the growing domain, Eq. (31), to a jump density on the fixed domain. The end positions $y - \Delta y$ and $y + \Delta y$ after a jump are related to their corresponding positions $x - \epsilon^-$ and $x + \epsilon^+$ in the fixed domain by Eq. (4), i.e., $y - \Delta y = \bar{g}(x - \epsilon^-, t)$ and $y + \Delta y = \bar{g}(x + \epsilon^+, t)$. Therefore, the jump density in the fixed domain is just

$$\lambda(x, x', t) = \frac{1}{2} [\delta(x - \epsilon^- - x') + \delta(x + \epsilon^+ - x')]. \quad (32)$$

After replacing the jump density in Eq. (30) with Eq. (32) we obtain

$$\begin{aligned} \frac{\partial \bar{u}(x, t)}{\partial t} &= \frac{1}{2} \int_0^t K(t-t') \bar{u}(x-\epsilon^-, t') \bar{\sigma}(x-\epsilon^-, t, t') dt' \\ &+ \frac{1}{2} \int_0^t K(t-t') \bar{u}(x+\epsilon^+, t') \bar{\sigma}(x+\epsilon^+, t, t') dt' \\ &- \int_0^t K(t-t') \bar{u}(x, t') \bar{\sigma}(x, t, t') dt' \\ &- [\bar{\mu}(x, t) + \bar{\omega}(x, t)] \bar{u}(x, t) + \bar{\chi}(x, t). \end{aligned} \quad (33)$$

In order to advance further, one now needs explicit expressions for ϵ^\pm in terms of Δy . While we have not been able to write an explicit expression for the step sizes ϵ^+ and ϵ^- , it is straightforward to obtain the approximations (see Appendix B)

$$\epsilon^\pm = \frac{\Delta y}{\bar{v}(x, t)} \mp \frac{1}{2\bar{v}(x, t)^2} \left[\int_0^t \frac{\partial \bar{\mu}(x, s)}{\partial x} ds \right] \Delta y^2 + O(\Delta y^3). \quad (34)$$

Using the relations (34), we can perform a Taylor expansion of the functions in Eq. (33) around the point x , retaining terms up to order Δy^2 . This results in

$$\begin{aligned} \frac{\partial \bar{u}(x, t)}{\partial t} &= \frac{\Delta y^2}{2\bar{v}(x, t)^2} \left\{ \frac{\partial^2}{\partial x^2} \int_0^t K(t-t') \bar{u}(x, t') \bar{\sigma}(x, t, t') dt' \right. \\ &- \left[\int_0^t \frac{\partial \bar{\mu}(x, s)}{\partial x} ds \right] \\ &\times \frac{\partial}{\partial x} \int_0^t K(t-t') \bar{u}(x, t') \bar{\sigma}(x, t, t') dt' \left. \right\} \\ &- [\bar{\mu}(x, t) + \bar{\omega}(x, t)] \bar{u}(x, t) + \bar{\chi}(x, t) + O(\Delta y^3). \end{aligned} \quad (35)$$

A. Standard diffusion

In the theory of CTRWs it is well known that the standard diffusion equation can be derived from the diffusion limit of the master equation for a CTRW with nearest-neighbor steps and an exponential waiting time density [36],

$$\psi(t) = \frac{1}{\tau} e^{-t/\tau}. \quad (36)$$

The memory kernel given by Eq. (23) can readily be evaluated in this case yielding

$$K(t) = \frac{1}{\tau} \delta(t). \quad (37)$$

Substituting this memory kernel into the master equation for the auxiliary CTRW, Eq. (33), we obtain the result

$$\begin{aligned} \frac{\partial \bar{u}(x, t)}{\partial t} &= \frac{\Delta y^2}{2\tau \bar{v}(x, t)^2} \left\{ \frac{\partial^2}{\partial x^2} \bar{u}(x, t) \bar{\sigma}(x, t, t) \right. \\ &- \left[\int_0^t \frac{\partial \bar{\mu}(x, s)}{\partial x} ds \right] \frac{\partial}{\partial x} \bar{u}(x, t) \bar{\sigma}(x, t, t) \left. \right\} \\ &- [\bar{\mu}(x, t) + \bar{\omega}(x, t)] \bar{u}(x, t) + \bar{\chi}(x, t) + O(\Delta y^3). \end{aligned} \quad (38)$$

Finally we consider the diffusion limit, $\Delta y \rightarrow 0$ and $\tau \rightarrow 0$ with

$$D = \lim_{\Delta y, \tau \rightarrow 0} \frac{\Delta y^2}{2\tau} \quad (39)$$

and note that $\sigma(x, t, t) = 1$, to obtain

$$\begin{aligned} \frac{\partial \bar{u}(x, t)}{\partial t} &= \frac{D}{\bar{v}(x, t)^2} \left\{ \frac{\partial^2}{\partial x^2} \bar{u}(x, t) - \left[\int_0^t \frac{\partial \bar{\mu}(x, s)}{\partial x} ds \right] \frac{\partial}{\partial x} \bar{u}(x, t) \right\} \\ &- [\bar{\mu}(x, t) + \bar{\omega}(x, t)] \bar{u}(x, t) + \bar{\chi}(x, t). \end{aligned} \quad (40)$$

As it turns out, the equation for the ensemble density of particles $u(x, t)$ on the fixed domain is significantly simpler. Indeed, from Eq. (15) one finds

$$u(x, t) = \bar{v}(x, t) \bar{u}(x, t), \quad (41)$$

and then

$$\begin{aligned} \frac{\partial u(x, t)}{\partial t} &= D \frac{\partial}{\partial x} \frac{1}{\bar{v}(x, t)} \frac{\partial}{\partial x} \frac{1}{\bar{v}(x, t)} u(x, t) \\ &- \bar{\omega}(x, t) u(x, t) + \bar{\chi}(x, t) \bar{v}(x, t). \end{aligned} \quad (42)$$

Equations (40) and (42) are the main results of the first part of this paper. They are the reaction diffusion equations, in fixed domain coordinates, for particles undergoing standard diffusion with reactions, on a growing domain. Solutions to these equations at position x and time t can be mapped to provide the concentrations of diffusing particles with reactions on a growing domain at position y and time t . The mapping requires the identification $u(y, t) = \bar{u}(x, t)$ with $y = \bar{g}(x, t)$, $\bar{\mu}(x, t) = \frac{\partial}{\partial t} \log \left(\frac{\partial y}{\partial x} \right)$ and $\bar{v}(x, t) = \exp \left[\int_0^t \bar{\mu}(x, s) ds \right]$.

The first term on the right-hand side (rhs) can be interpreted as a net probability flux, whose divergence accounts for the time change of the particle concentration inside the interval $[x, x+dx]$ in the absence of chemical reactions. In this latter case, one has the following continuity equation:

$$\frac{\partial u(x, t)}{\partial t} = D \frac{\partial}{\partial x} \frac{1}{\bar{v}(x, t)} \frac{\partial}{\partial x} \frac{1}{\bar{v}(x, t)} u(x, t). \quad (43)$$

The same equation holds if $u(x, t)$ is replaced with a density $\rho(x, t|x_0, 0)$ referring to a deterministic initial condition. Note that in the case of a uniformly evolving domain $\bar{v} \equiv v(t)$, one obtains the diffusion equation

$$\frac{\partial u(x, t)}{\partial t} = \frac{D}{v(t)^2} \frac{\partial^2 u(x, t)}{\partial x^2}, \quad (44)$$

a result already known from previous works [it follows, e.g., by taking $v = 0$ in Eq. (36) of Ref. [19]]. For $\bar{\mu} > 0$, say, the shortening of the jump lengths on the fixed domain due to the growth process is described by a time-dependent effective diffusion coefficient which decreases as the inverse of the squared scale factor. The time dependence of the diffusion coefficient can be eliminated by introducing a new Brownian conformal time $\tau(t) \equiv \int_0^t v(s)^{-2} ds$ [19]. In general, writing $D(t) = \frac{D}{v(t)^2}$, we can relate Eq. (44) to the class of diffusion problems referred to as rescaled Brownian motion, where [56–58] $D(t) = \alpha \kappa_\alpha t^{\alpha-1}$. In this rescaled Brownian motion, if $0 < \alpha < 1$, the long-time growth of the mean-square displacement of a freely diffusing particle is described by a sublinear

power law, and it is interesting to note in this context that subdiffusion can also be observed on a uniformly evolving domain, if the growth scale factor $\nu(t) \propto t^\beta$ with $0 < \beta < \frac{1}{2}$.

1. Moments of $u(x, t)$ for short times

The analytical solution of Eq. (42) is not easy to obtain in general. An exception is the case of homogeneous expansion where $\bar{\nu} \equiv \nu(t)$. Fortunately, in more general cases, some useful information can still be extracted directly from Eq. (42). In what follows, we will show how to obtain the short-time behavior of the moments of $u(x, t)$ in a systematic way. We will illustrate the procedure for the case where $\bar{\mu}(x, t) = \mu_0 x^2$, i.e., for $\bar{\nu}(x, t) = \exp[\mu_0 x^2 t]$, but the procedure can readily be carried out for other forms of the local growth function. For further simplicity, we will assume that there are no reactions, i.e., $\omega(x, t) = \bar{\chi} = 0$.

We start by inserting the short-time power expansion of $\bar{\nu}(x, t)$ into Eq. (43), which yields

$$\frac{\partial u}{\partial t} = D \frac{\partial u^2}{\partial x^2} + D \sum_{m=1}^{\infty} \sum_{r=0}^2 (-1)^m c_{m,r} \mu_0^m t^m x^{2m+r-2} \frac{\partial^r u}{\partial x^r} \quad (45)$$

with $c_{1,0} = 2$, $c_{1,1} = 6$, $c_{1,2} = 2$, $c_{2,0} = 12$, etc. Multiplying this equation by x^n , integrating the resulting equation over the whole interval, and assuming that $x^m u$ and $x^m \partial_x u$ are negligible for sufficiently large values of $|x|$, one finds

$$\frac{d\langle x^n(t) \rangle}{dt} = D \sum_{m=0}^{\infty} a_m n(n+m-1) (\mu_0 t)^m \langle x^{n+2m-2} \rangle \quad (46)$$

with $a_0 = 1$, $a_1 = -2$, $a_2 = 2$, $a_3 = -4/3$, etc. Equation (46) can be written as

$$\begin{aligned} \frac{d}{dt} \langle x^n(t) \rangle = & D \sum_{m=0}^{\infty} \frac{(-1)^m (2\mu_0 t)^m}{m!} \{ \langle x^{2m+n-2} \rangle \\ & (2m+n)(2m+n-1) \\ & + \langle x^{2m+n} \rangle (2\mu_0 t) [3(2m+n+1) - 1] \\ & + 2 \langle x^{2m+n+2} \rangle (2\mu_0 t)^2 \}, \end{aligned} \quad (47)$$

for $n \geq 1$ (note that for $m = 0$ and $n = 1$ the term proportional to $2m+n-1$ is absent). For the time evolution of the first four integer-order moments, one has

$$\begin{aligned} \frac{d\langle x(t) \rangle}{dt} = & D[-2\mu_0 t \langle x(t) \rangle + 4\mu_0^2 t^2 \langle x^3(t) \rangle \\ & - 4\mu_0^3 t^3 \langle x^5(t) \rangle + \dots], \end{aligned} \quad (48)$$

$$\frac{d\langle x^2(t) \rangle}{dt} = D[2 - 8\mu_0 t \langle x^2(t) \rangle + 12\mu_0^2 t^2 \langle x^4(t) \rangle + \dots], \quad (49)$$

$$\frac{d\langle x^3(t) \rangle}{dt} = D[6\langle x(t) \rangle - 18\mu_0 t \langle x^3(t) \rangle + \dots], \quad (50)$$

$$\frac{d\langle x^4(t) \rangle}{dt} = D[12\langle x^2(t) \rangle - 32\mu_0 t \langle x^4(t) \rangle + \dots]. \quad (51)$$

This nonclosed hierarchy of equations can be solved iteratively to increasing order of powers of t . For example, assume that the initial distribution of particles $u(x, 0)$ has nonzero moments: $\langle x^n(0) \rangle \equiv \langle x_0^n \rangle \neq 0$. Then, one sees that

the rhs of Eq. (48) is $d\langle x(t) \rangle/dt = -2D\mu_0 t \langle x_0 \rangle + O(t^2)$ because $\langle x^n \rangle = O(1)$. Thus, $\langle x(t) \rangle = \langle x_0 \rangle - \mu_0 \langle x_0 \rangle D t^2 + O(t^3)$. We can improve this approximation by noting that the next-order correction contributed by the rhs of Eq. (48) stems from the term proportional to $\langle x^3 \rangle$ and is quadratic in time. This is because, from Eq. (50), we know that $\langle x^3(t) \rangle \approx \langle x_0^3 \rangle + O(t)$. Therefore, to order t^2 , Eq. (48) can be written as follows:

$$\frac{d\langle x(t) \rangle}{dt} = D[-2\mu_0 t \langle x_0 \rangle + 4\mu_0^2 t^2 \langle x_0^3 \rangle] + O(t^3). \quad (52)$$

Thus,

$$\langle x(t) \rangle = \langle x_0 \rangle - \mu_0 \langle x_0 \rangle D t^2 + \frac{4}{3} \mu_0^2 \langle x_0^3 \rangle D t^3 + O(t^4). \quad (53)$$

Other moments can be evaluated with the same procedure. For example, for the third-order moment, one finds

$$\langle x^3(t) \rangle = \langle x_0^3 \rangle + 6\langle x_0 \rangle D t - 9\mu_0 \langle x_0^3 \rangle D t^2 + O(t^3). \quad (54)$$

The result (53) for $\langle x(t) \rangle$ can be further improved by inserting Eqs. (53) and Eq. (54) into Eq. (48), and then taking into account that $\langle x^5 \rangle \approx \langle x_0^5 \rangle + O(t)$. This iterative procedure works also for even-order moments. In this way one finds

$$\langle x^2(t) \rangle = \langle x_0^2 \rangle + 2D t - 4\mu_0 \langle x_0^2 \rangle D t^2 + O(t^3) \quad (55)$$

and

$$\langle x^4(t) \rangle = \langle x_0^4 \rangle + 12\langle x_0^2 \rangle D t + O(t^2). \quad (56)$$

Improved expressions with an additional corrective term are given by

$$\begin{aligned} \langle x(t) \rangle = & \langle x_0 \rangle - \mu_0 \langle x_0 \rangle D t^2 + \frac{4}{3} \mu_0^2 \langle x_0^3 \rangle D t^3 \\ & + \left(\frac{13}{2} D \langle x_0 \rangle - \mu_0 \langle x_0^5 \rangle \right) D \mu_0^2 t^4 + O(t^5), \end{aligned} \quad (57)$$

$$\begin{aligned} \langle x^2(t) \rangle = & \langle x_0^2 \rangle + 2D t - 4\mu_0 \langle x_0^2 \rangle D t^2 \\ & + \left(4\mu_0 \langle x_0^4 \rangle - \frac{16}{3} D \right) \mu_0 D t^3 + O(t^4), \end{aligned} \quad (58)$$

$$\begin{aligned} \langle x^3(t) \rangle = & \langle x_0^3 \rangle + 6\langle x_0 \rangle D t - 9\mu_0 \langle x_0^3 \rangle D t^2 \\ & + \left(8\mu_0 \langle x_0^5 \rangle - 38D \langle x_0 \rangle \right) \mu_0 D t^3 + O(t^4), \end{aligned} \quad (59)$$

$$\langle x^4(t) \rangle = \langle x_0^4 \rangle + 12\langle x_0^2 \rangle D t + (12D - 16\mu_0 \langle x_0^4 \rangle) D t^2 + O(t^3). \quad (60)$$

By inspection, one easily notes that, at least up to the fourth-order moment, the leading correction to $\langle x^m \rangle$ arising from the domain growth takes the form $-m^2 \mu_0 \langle x_0^m \rangle D t^2$. We note the important role of the initial condition x_0 , as opposed to the case of a uniformly evolving domain. In the case of the first-order moment, when $\mu_0 > 0$, the term $-\mu_0 \langle x_0 \rangle D t^2$ reflects an accelerated motion towards the origin as a result of the confining effect of the domain growth in x space (for $\mu_0 < 0$, this motion is directed away from the origin).

One may wonder how many terms in Eq. (46) should be taken, and up to what order in t the x moments should be known, if one wants to find $\langle x^n \rangle$ up to order t^{k+1} , or equivalently, $d\langle x^n \rangle/dt$ up to order t^k . From Eq. (46) one can see that this is achieved if we know $\langle x^{n+2m-2} \rangle$ up to order t^{k-m} , that is, we have to know the $\langle x^{n-2} \rangle$ up to order t^k , $\langle x^n \rangle$ up to order t^{k-1} , etc., and finally $\langle x^{n+2k-2} \rangle$ up to order t^0 .

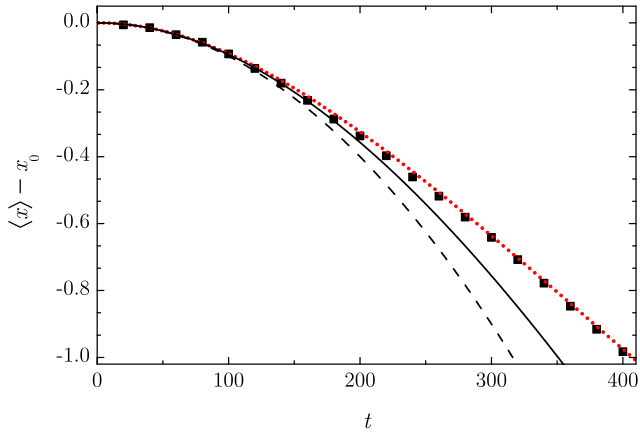


FIG. 2. $\langle x \rangle - x_0$ vs time for $\mu(x, t) = \mu_0 x^2$, $u(x, 0) = \delta(x - x_0)$, $x_0 = 20$, $D = 1/2$, and $\mu_0 = 10^{-6}$. The squares are simulation results. The dotted line corresponds to results obtained from the numerical solution of Eq. (43). The broken and solid lines are the analytical expressions to order t^2 and order t^3 , respectively, given in Eq. (53).

In Fig. 2 and Fig. 3 we compare the results from Eq. (53) and Eq. (55), respectively, with estimates of the moments obtained from simulations and from numerical solutions of Eq. (43). The simulation method for nonuniform domain evolution is a straightforward generalization of that described in Sec. III.E of Ref. [45] for the case of a uniformly evolving domain. We have taken the waiting time pdf and the jump length pdf used therein to perform the simulations.

For the special case where all the particles are initially placed at $x = 0$, one has $\langle x_0^n \rangle = 0$ for $n \geq 1$, $\langle x^n \rangle = 0$ for $n = \text{odd}$, and Eqs. (58) and (60) become

$$\langle x^2(t) \rangle = 2Dt - \frac{16}{3}\mu_0 D^2 t^3 + O(t^5), \quad (61)$$

$$\langle x^4(t) \rangle = 12D^2 t^2 + O(t^4). \quad (62)$$

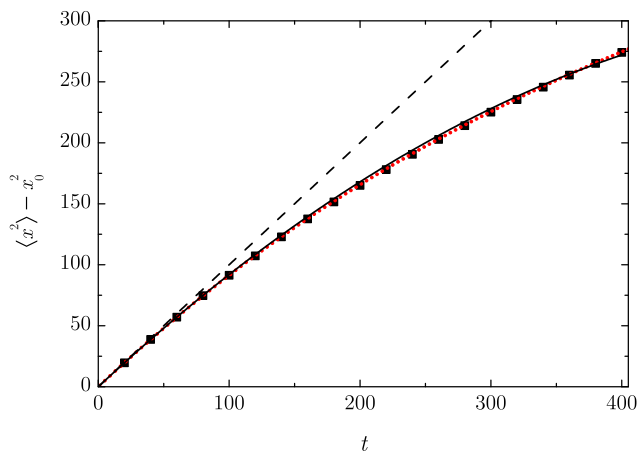


FIG. 3. $\langle x^2 \rangle - x_0^2$ vs time for $\mu(x, t) = \mu_0 x^2$, $u(x, 0) = \delta(x - x_0)$ with $x_0 = 20$, $D = 1/2$, and $\mu_0 = 10^{-6}$. The squares are simulation results. The dotted line corresponds to results obtained from the numerical solution of Eq. (43). The broken and solid lines are the analytical expressions to order t and order t^2 , respectively, given in Eq. (55). Note that the expression of order t is just the well-known expression for a static domain (case $\mu_0 = 0$).

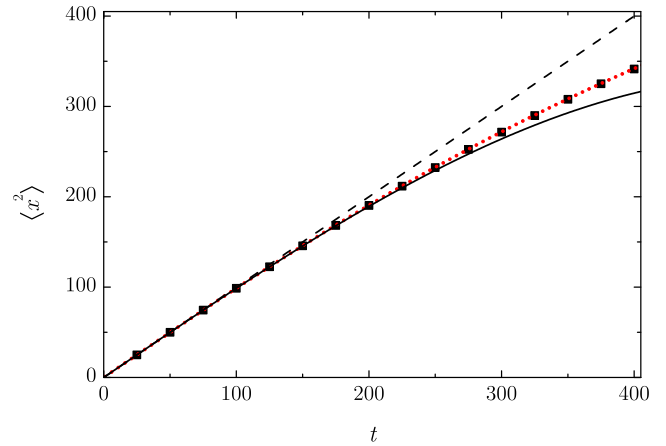


FIG. 4. $\langle x^2 \rangle$ vs time for $\mu(x, t) = \mu_0 x^2$, $u(x, 0) = \delta(x)$, $D = 1/2$, and $\mu_0 = 10^{-6}$. The squares are simulation results. The dotted line corresponds to results obtained from the numerical solution of Eq. (43). The broken and solid lines are the analytical expressions to order t (or equivalently, for a static domain) and order t^3 , respectively, given in Eq. (61).

The above findings highlight yet again the importance of the initial condition, to the extent that the time dependence of the leading correction to the second- and fourth-order moments is different than that obtained for the case $x_0 \neq 0$. For example, the short-time correction to leading order is cubic in the present case, and therefore weaker than the quadratic dependence obtained when $x_0 = 0$ [cf. Eq. (58)].

Comparisons between moment calculations and simulations for $\langle x^2(t) \rangle$, with the initial distribution of particles given by a Dirac δ function at $x = 0$, are shown in Fig. 4. It is noteworthy that $\langle x^2(t) \rangle$ does not scale linearly in time, as anticipated on a nonevolving domain. Note also that the moment calculations reproduce the numerical results with improved accuracy as the order is increased. For the case $x_0 = 0$, it is instructive to compare the result (61) with the case of a uniform exponential growth and contraction with $v(t) = \exp[\hat{\mu}_0 t]$. In this case, one has the exact result,

$$\langle x^2(t) \rangle_{\text{exp}} = 2D\tau(t) = D\hat{\mu}_0^{-1}(1 - e^{-2\hat{\mu}_0 t}), \quad (63)$$

valid for all times t . For short times this can be expanded as

$$\langle x^2(t) \rangle_{\text{exp}} = 2Dt - 2D\hat{\mu}_0 t^2 + O(t^3). \quad (64)$$

The correction (positive or negative) due to the domain evolution at early times is stronger in the uniform case, since it is proportional to t^2 .

Let us focus on the case of a growing domain. In contrast with the case $\mu(x, t) = \mu(x) = \mu_0 x^2$, for a uniform exponential growth the particle motion on the fixed domain experiences a strong confinement already for small excursions from the origin, typically corresponding to short travel times t . This is due to the aforementioned effective reduction of the diffusion coefficient on the fixed domain [cf. Eq. (44)]. Therefore, after a short time t , the correction to a pure diffusive motion is more important than in the case $\mu(x) \propto x^2$,

where the domain growth is practically zero at short distances from the origin and $\bar{v}(x, t) \approx 1$ in this regime [cf. Eq. (43)]. An analogous reasoning applies for the contracting case $\mu(x)$, $\hat{\mu}_0 < 0$.

Finally, it is also worth mentioning that, in the contracting case $\mu_0 < 0$, it is possible to obtain a hierarchy that is valid at all times, not only in the early-time regime. To this end, one uses a modified local growth rate $\bar{\mu}(x, t) = \mu_0 x^2 / (1 - \mu_0 x^2 t)$, with $\mu_0 < 0$. This yields $v(x, t)^{-1} = 1 - \mu_0 x^2 t$ for all times, whence the exact (albeit nonclosed) hierarchy

$$\begin{aligned} \frac{d\langle x^n(t) \rangle}{dt} = & Dn(n-1)\langle x^{n-2}(t) \rangle - 2n^2\mu_0 D t \langle x^n(t) \rangle \\ & + n(n+1)\mu_0^2 D t^2 \langle x^{n+2}(t) \rangle \end{aligned} \quad (65)$$

follows.

2. Moments of $u(y, t)$ for short times

The short-time moments of $u(x, t)$ can be employed to get the short-time moments of $u(y, t)$ by expanding $y^n = \bar{g}(x, t)^n$. For example, to first order in t one has $y^n = x^n + nt \int_0^x \bar{\mu}(z, 0) dz + O(t^2)$. In particular, for $\bar{\mu}(x, t) = \mu_0 x^2$, one finds

$$\langle y \rangle = \langle x \rangle + \frac{1}{3} \mu_0 t \langle x^3 \rangle + \frac{1}{10} \mu_0^2 t^2 \langle x^5 \rangle + O(\langle x^7 \rangle t^3) \quad (66a)$$

and

$$\langle y^2 \rangle = \langle x^2 \rangle + \frac{2}{3} \mu_0 t \langle x^4 \rangle + \frac{14}{45} \mu_0^2 t^2 \langle x^6 \rangle + O(\langle x^8 \rangle t^3). \quad (66b)$$

Then

$$\langle y(t) \rangle = \langle y_0 \rangle + \frac{1}{3} \mu_0 \langle y_0^3 \rangle t + \left(\mu_0 \langle y_0 \rangle D + \frac{\mu_0^2}{10} \langle y_0^5 \rangle \right) t^2 + O(t^3) \quad (67)$$

and

$$\begin{aligned} \langle y^2(t) \rangle = & \langle y_0^2 \rangle + (2D + \frac{2}{3} \mu_0 \langle y_0^4 \rangle) t + \frac{2}{45} (90 \mu_0 \langle y_0^2 \rangle D \\ & + 7 \mu_0^2 \langle y_0^6 \rangle) t^2 + O(t^3). \end{aligned} \quad (68)$$

It is worth noting that the leading correction to the first- and second-order moments has the same sign as μ_0 and is linear in time; therefore, it is stronger than the quadratic correction observed in the case of the x moments. In the case of the first-order moment, the leading correction can be interpreted as a deterministic drift of the form vt , with a velocity given by $v = \mu_0 \langle y_0^2 \rangle / 3$. Note that the diffusivity D does not appear in this term; indeed, the diffusive motion is a subleading correction to the dominant drift arising from the domain evolution.

In contrast, the leading contribution of the domain evolution to the second-order moment is of the same order as the intrinsic diffusive motion, leading to an apparent diffusivity $D + \mu_0 \langle y_0^4 \rangle / 3$ which describes particle spreading to dominant order.

For the case $y = 0$, insertion of Eqs. (61) and (62) into Eq. (66b) yields

$$\langle y^2(t) \rangle = 2Dt + \frac{8}{3} \mu_0 D^2 t^3 + O(t^5). \quad (69)$$

In Figs. 5 and 6 we compare these results with numerical estimates of the moments $\langle y^n \rangle$. These results have been

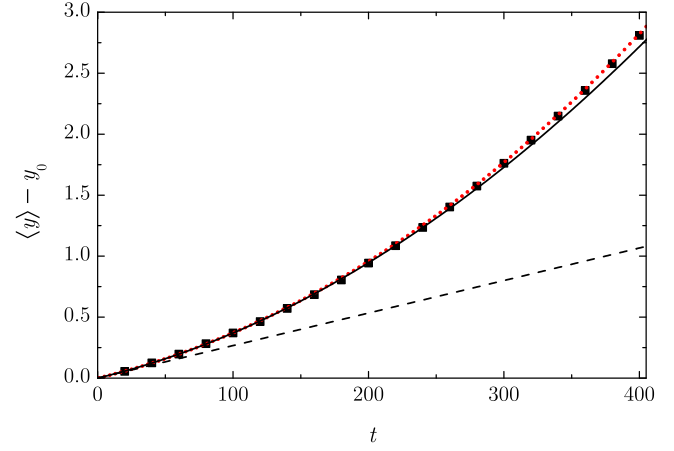


FIG. 5. $\langle y \rangle - y_0$ vs time for $\mu(x, t) = \mu_0 x^2$ and $u(y, 0) = \delta(y - y_0)$ with $y_0 = 20$, $D = 1/2$, and $\mu_0 = 10^{-6}$. The squares are simulation results. The dotted line is obtained from the numerical solution of Eq. (43). The broken and solid lines are the analytical expressions to order t and order t^2 , respectively, given in Eq. (67).

obtained by solving Eq. (43) numerically. From the numerical solution $u(x, t)$ one then finds $u(y = \bar{g}(x, t), t)$ and, from this function, $\langle y^n \rangle$.

As complementary information, we show the numerical plots of the $u(x, t)$ and $u(y, t)$ for $t = 400$ and $t = 2000$ in Figs. 7 and 8. The bimodal form of $u(x, t = 2000)$ shows the clear influence of the evolving domain on the distribution for the auxiliary domain.

As an aside we note that, in view of the relation

$$\begin{aligned} u(k, t) = \mathcal{F}\{u(x, t)\} &= \int_{-\infty}^{\infty} e^{-ikx} u(x, t) \\ dx &= \sum_{m=0}^{\infty} \frac{(-ik)^m}{m!} \langle x^m(t) \rangle, \end{aligned} \quad (70)$$

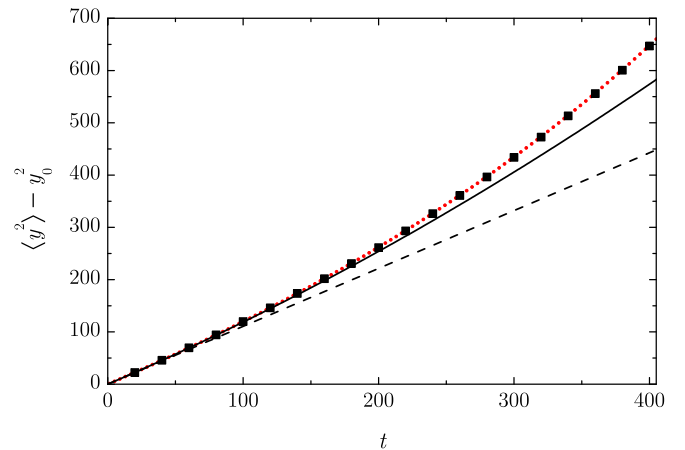


FIG. 6. $\langle y^2 \rangle - y_0^2$ vs time for $\mu(x, t) = \mu_0 x^2$ and $u(y, 0) = \delta(y - y_0)$ with $y_0 = 20$, $D = 1/2$, and $\mu_0 = 10^{-6}$. The dotted line is obtained from the numerical solution of Eq. (43). The broken and solid lines are the analytical expressions to order t and order t^2 , respectively, given in Eq. (68).

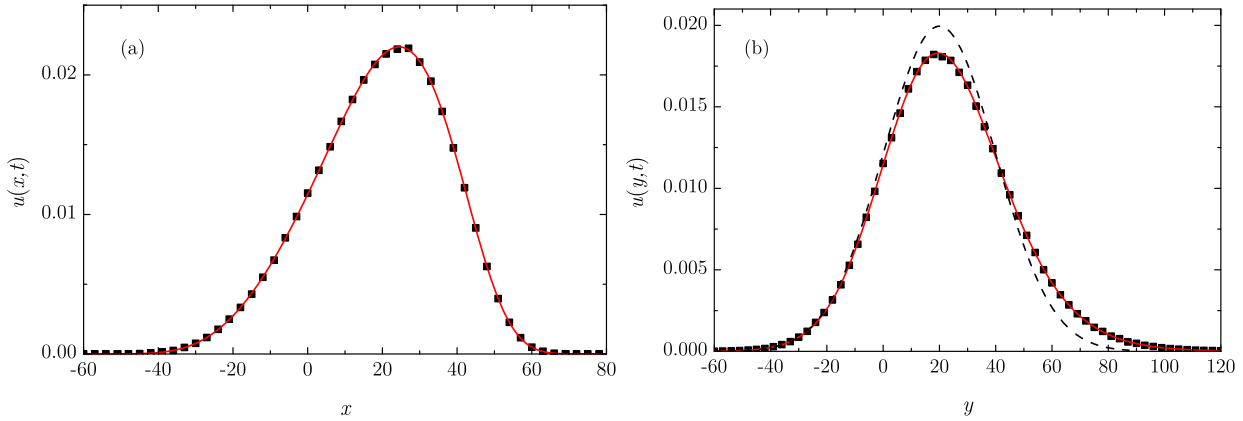


FIG. 7. (a) $u(x, t)$ and (b) $u(y, t)$ for $t = 400$, $D = 1/2$, $\mu_0 = 10^{-6}$, and $u(x, 0) = \delta(x - x_0)$ with $x_0 = 20$. This deterministic initial condition implies $u(x, t) = \rho(x, t)$. The solid lines represent the numerical solution of Eq. (43), whereas the squares are simulation results. The broken line corresponds to the solution for the static case ($\mu_0 = 0$).

the obtained expressions for the moments may be used to obtain an early-time approximation for the full Fourier-transformed probability density function by truncating the above series to different orders.

Finally, we note that the results obtained for the moments $\langle x^n \rangle$ in the absence of reactions, $\omega = \bar{\chi} = 0$, can be straightforwardly extended to include a pure death process with constant rate ($\bar{\omega} = \omega_0$, and $\bar{\chi} = 0$). This is done by noting that $\hat{u}(x, t)$ for this case and the corresponding solution $u(x, t)$ for the case without reactions, are related to one another by $\hat{u}(x, t) = u(x, t) \exp[-\omega_0 t]$. Therefore $\langle \hat{x}^n \rangle = \langle x^n \rangle \exp[-\omega_0 t]$, where $\langle \hat{x}^n \rangle$ and $\langle x^n \rangle$ are the moments associated with \hat{u} and u , respectively.

B. Subdiffusion

Subdiffusion can be obtained from CTRWs with a heavy-tailed power-law waiting time density [36]. The Mittag-Leffler density has been widely studied in this context. This is defined as

$$\psi(t) = \frac{t^{\alpha-1}}{\tau^\alpha} E_{\alpha,\alpha} \left[-\left(\frac{t}{\tau}\right)^\alpha \right], \tag{71}$$

where

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)} \tag{72}$$

is the Mittag-Leffler function.

Rather than substitute the corresponding memory kernel directly into the master equation, we first note a number of Laplace transform properties. Using the expression $\mathcal{L}[\psi(t)] \equiv \psi(s) = 1/(\tau^\alpha s^\alpha + 1)$ for the Laplace transform of the density (71) in Eq. (23), we obtain [59]

$$\mathcal{L}[K(t)] = \frac{s^{1-\alpha}}{\tau^\alpha}, \tag{73}$$

whence the result

$$\mathcal{L} \int_0^t K(t-t') Y(t') dt' = \frac{s^{1-\alpha}}{\tau^\alpha} \mathcal{L}[Y(t)] \tag{74}$$

follows by straightforward application of the convolution theorem for the Laplace transform.

We note, on the other hand, that

$$\mathcal{L}[_0\mathcal{D}_t^{1-\alpha} Y(t)] = s^{1-\alpha} \mathcal{L}[Y(t)], \tag{75}$$

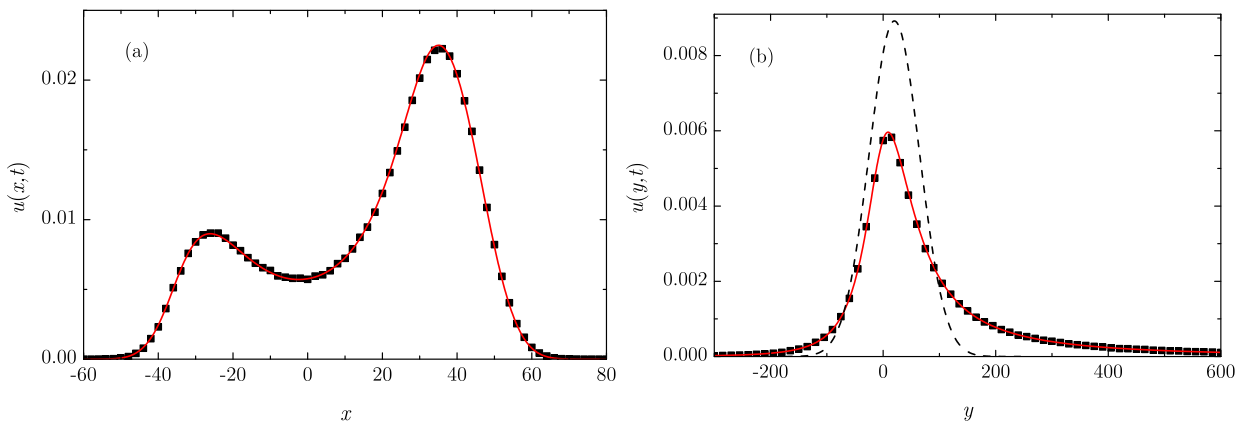


FIG. 8. (a) $u(x, t)$ and (b) $u(y, t)$ for $t = 2000$, $D = 1/2$, and $\mu_0 = 10^{-6}$ and $u(x, 0) = \delta(x - x_0)$ with $x_0 = 20$. The lines represent the numerical solution of Eq. (43), whereas the squares are simulation results. The broken line corresponds to the solution for the static case ($\mu_0 = 0$).

where $\mathcal{D}_t^{1-\alpha}Y(t)$ denotes the Grünwald-Letnikov fractional derivative of order $1 - \alpha$ of the function $Y(t)$. This operator is known to be equivalent to the Riemann-Liouville fractional derivative,

$${}_0\mathcal{D}_t^{1-\alpha}[Y(x, t)] = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{Y(x, t')}{(t-t')^{1-\alpha}} dt', \quad (76)$$

for sufficiently smooth functions [see, e.g., Eqs. (13)–(15) in Ref. [60]].

Comparing Eq. (74) with Eq. (75), we find that for a Mittag-Leffler memory kernel one has

$$\int_0^t K(t-t')Y(t') dt' = \frac{1}{\tau^\alpha} {}_0\mathcal{D}_t^{1-\alpha}Y(t). \quad (77)$$

Consequently, the auxiliary CTRW master equation, Eq. (33), can be written as

$$\begin{aligned} & \frac{\partial \bar{u}(x, t)}{\partial t} \\ &= \frac{\Delta y^2 \bar{v}(x, t)^{-2}}{2\tau^\alpha} \left\{ \frac{\partial^2}{\partial x^2} \left[\bar{\sigma}(x, t, 0) {}_0\mathcal{D}_t^{1-\alpha} \frac{\bar{u}(x, t)}{\bar{\sigma}(x, t, 0)} \right] \right. \\ & \quad \left. - \left[\int_0^t \frac{\partial \bar{\mu}(x, s)}{\partial x} ds \right] \frac{\partial}{\partial x} \left[\bar{\sigma}(x, t, 0) {}_0\mathcal{D}_t^{1-\alpha} \frac{\bar{u}(x, t)}{\bar{\sigma}(x, t, 0)} \right] \right\} \\ & \quad - [\bar{\mu}(x, t) + \bar{\omega}(x, t)]\bar{u}(x, t) + \bar{\chi}(x, t) + O(\Delta y^3). \end{aligned} \quad (78)$$

We consider the diffusion limit, $\Delta y \rightarrow 0$ and $\tau \rightarrow 0$ with

$$D_\alpha = \lim_{\Delta y, \tau \rightarrow 0} \frac{\Delta y^2}{2\tau^\alpha}, \quad (79)$$

and then

$$\begin{aligned} \frac{\partial \bar{u}(x, t)}{\partial t} &= D_\alpha \bar{v}(x, t)^{-2} \left\{ \frac{\partial^2}{\partial x^2} \left[\bar{\sigma}(x, t, 0) {}_0\mathcal{D}_t^{1-\alpha} \frac{\bar{u}(x, t)}{\bar{\sigma}(x, t, 0)} \right] \right. \\ & \quad \left. - \left[\int_0^t \frac{\partial \bar{\mu}(x, s)}{\partial x} ds \right] \frac{\partial}{\partial x} \left[\bar{\sigma}(x, t, 0) {}_0\mathcal{D}_t^{1-\alpha} \frac{\bar{u}(x, t)}{\bar{\sigma}(x, t, 0)} \right] \right\} \\ & \quad - [\bar{\mu}(x, t) + \bar{\omega}(x, t)]\bar{u}(x, t) + \bar{\chi}(x, t). \end{aligned} \quad (80)$$

Equation (80) can be rewritten as

$$\begin{aligned} \frac{\partial \bar{u}(x, t)}{\partial t} &= D_\alpha \bar{v}(x, t)^{-1} \frac{\partial}{\partial x} \left\{ \bar{v}(x, t)^{-1} \frac{\partial}{\partial x} \left[\bar{\sigma}(x, t, 0) {}_0\mathcal{D}_t^{1-\alpha} \right. \right. \\ & \quad \left. \left. \times \frac{\bar{u}(x, t)}{\bar{\sigma}(x, t, 0)} \right] \right\} \\ & \quad - [\bar{\mu}(x, t) + \bar{\omega}(x, t)]\bar{u}(x, t) + \bar{\chi}(x, t) \end{aligned} \quad (81)$$

or, in terms of the ensemble density of particles on the fixed domain, $u(x, t) = \bar{v}(x, t)\bar{u}(x, t)$, as

$$\begin{aligned} \frac{\partial u(x, t)}{\partial t} &= D_\alpha \frac{\partial}{\partial x} \left\{ \bar{v}(x, t)^{-1} \frac{\partial}{\partial x} \left[\bar{v}(x, t)^{-1} \right. \right. \\ & \quad \left. \left. \times e^{-\int_0^t \bar{\omega}(x, s) ds} {}_0\mathcal{D}_t^{1-\alpha} \frac{u(x, t)}{e^{-\int_0^t \bar{\omega}(x, s) ds}} \right] \right\} \\ & \quad - \bar{\omega}(x, t)u(x, t) + \bar{\chi}(x, t)\bar{v}(x, t), \end{aligned} \quad (82)$$

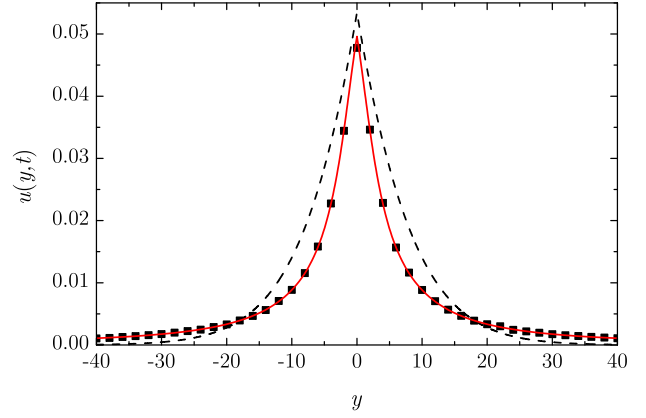


FIG. 9. Numerical solution $u(y, t)$ (solid line) and simulation results (squares) for $\alpha = 1/2$, $D_\alpha = 1/2$, $\mu_0 = 10^{-5}$, $\omega(x, t) = \omega_0 = 5 \times 10^{-5}$, and $u(x, 0) = \delta(x)$. The broken line is the corresponding solution for the case of a static domain.

where we have used the relationship

$$\bar{\sigma}(x, t, 0) = \bar{\theta}(x, t, 0)\bar{v}(x, t)^{-1} = e^{-\int_0^t \bar{\omega}(x, s) ds} \bar{v}(x, t)^{-1}.$$

Equations (80), (81), and (82) are the main results of this second part of this paper. They are the reaction subdiffusion equations, in fixed domain coordinates, for particles undergoing subdiffusion with reactions, on a growing domain. Similar to the case with standard diffusion, solutions to these equations at position x and time t can be mapped to provide the concentrations of diffusing particles with reactions on a growing domain at position y and time t .

For the case $\omega(x, t) = \omega(t)$ one finds a simpler expression in terms of $u^*(x, t) = u(x, t)e^{\int_0^t \bar{\omega}(s) ds}$,

$$\begin{aligned} \frac{\partial u^*(x, t)}{\partial t} &= D_\alpha \left\{ \frac{\partial}{\partial x} \bar{v}(x, t)^{-1} \frac{\partial}{\partial x} \left[\bar{v}(x, t)^{-1} {}_0\mathcal{D}_t^{1-\alpha} u^*(x, t) \right] \right\} \\ & \quad + \bar{\chi}(x, t)\bar{v}(x, t)e^{-\int_0^t \bar{\omega}(x, s) ds}. \end{aligned} \quad (83)$$

In general, Eq. (82) cannot be solved exactly, but one can resort to numerical methods instead. For example, in Fig. 9 we show the numerical solution of Eq. (82) for a particular yet representative case. The solution has been obtained by means of a straightforward extension of the fractional Crank-Nicolson method described in Ref. [61] (see Appendix C).

Moments of $u(x, t)$ for short times

We proceed here in the same way as for the case of standard diffusion. For example, assume that we have an expansion of the form $\mu(x, t) = \mu_0 x^2$, and no reactions. Then it is easy to see that the hierarchy of moment equations obtained for subdiffusion is recovered from that in Sec. IV A 1, Eqs. (46)–(51), by simply replacing $\langle x^n(t) \rangle$ with ${}_0\mathcal{D}_t^{1-\alpha} \langle x^n(t) \rangle$ and D with D_α . The iterative procedure for solving this hierarchy of equations is also similar to that employed in Sec. IV A 1. The first two

equations for odd-order moments are [cf. Eqs. (48) and (50)]

$$\begin{aligned} \frac{d\langle x(t) \rangle}{dt} &= D_\alpha [-2\mu_0 t {}_0\mathcal{D}_t^{1-\alpha} \langle x(t) \rangle \\ &\quad + 4\mu_0^2 t^2 {}_0\mathcal{D}_t^{1-\alpha} \langle x^3(t) \rangle - 4\mu_0^3 t^3 {}_0\mathcal{D}_t^{1-\alpha} \langle x^5(t) \rangle + \dots], \end{aligned} \quad (84)$$

$$\frac{d\langle x^3(t) \rangle}{dt} = D_\alpha [6 {}_0\mathcal{D}_t^{1-\alpha} \langle x(t) \rangle - 18\mu_0 t {}_0\mathcal{D}_t^{1-\alpha} \langle x^3(t) \rangle + \dots]. \quad (85)$$

To order t^0 we have $\langle x^n(t) \rangle = \langle x^n \rangle(0) \equiv \langle x_0^n \rangle$, and so Eq. (84) can be approximated, to order t^α , by

$$\begin{aligned} \frac{d\langle x(t) \rangle}{dt} &= -2\mu_0 t D_\alpha {}_0\mathcal{D}_t^{1-\alpha} \langle x_0 \rangle + o(t^\alpha) \\ &= -2\mu_0 D_\alpha \langle x_0 \rangle \frac{t^\alpha}{\Gamma(\alpha)} + o(t^\alpha). \end{aligned} \quad (86)$$

Here we have used the fact that ${}_0\mathcal{D}_t^{1-\alpha} 1 = t^{\alpha-1}/\Gamma(\alpha)$, which is a special case of the more general result

$${}_0\mathcal{D}_t^{1-\alpha} t^\beta = \frac{\Gamma(1+\beta)}{\Gamma(\alpha+\beta)} t^{\alpha+\beta-1}. \quad (87)$$

The integration of Eq. (86) yields

$$\langle x(t) \rangle = \langle x_0 \rangle - \frac{2\mu_0 \langle x_0 \rangle}{(1+\alpha)\Gamma(\alpha)} D_\alpha t^{1+\alpha} + o(t^{1+\alpha}). \quad (88)$$

Similarly, one finds

$$\langle x^3(t) \rangle = \langle x_0^3 \rangle + \frac{6\langle x_0 \rangle}{\Gamma(1+\alpha)} D_\alpha t^\alpha + o(t^\alpha). \quad (89)$$

We can improve these approximations in an iterative way. For example, from the approximations in Eqs. (88) and (89), we find that the equation for $d\langle x \rangle/dt$ to order $t^{1+\alpha}$ is

$$\begin{aligned} \frac{d\langle x(t) \rangle}{dt} &= -2\mu_0 D_\alpha t {}_0\mathcal{D}_t^{1-\alpha} \langle x_0 \rangle \\ &\quad + 4\mu_0^2 D_\alpha t^2 {}_0\mathcal{D}_t^{1-\alpha} \langle x_0^3 \rangle + o(t^{1+\alpha}). \end{aligned} \quad (90)$$

Taking into account Eq. (87) and integrating the resulting equations, we easily find the first-order moment up to order $t^{2+\alpha}$:

$$\begin{aligned} \langle x(t) \rangle &= \langle x_0 \rangle - \frac{2\mu_0 \langle x_0 \rangle D_\alpha}{(1+\alpha)\Gamma(\alpha)} t^{1+\alpha} + \frac{4\mu_0^2 \langle x_0^3 \rangle D_\alpha}{(2+\alpha)\Gamma(\alpha)} t^{2+\alpha} \\ &\quad + o(t^{2+\alpha}). \end{aligned} \quad (91)$$

It is easy to see that the insertion of Eqs. (88) and (89) into Eq. (84) leads to an equation for $d\langle x \rangle/dt$ to order $t^{1+2\alpha}$, which would in turn lead to an expression for the first-order moment to order $t^{2+2\alpha}$, and so on.

Let us briefly discuss the difference in behavior between the normal diffusive and the subdiffusive case. From Eq. (91), we immediately see that the leading correction to the case of a static domain is of the order $t^{1+\alpha}$, i.e., stronger than the quadratic correction predicted by Eq. (57). This reflects the fact that the domain growth plays a more dominant role when the intrinsic particle motion is subdiffusive rather than diffusive. The result corresponding to normal diffusion is recovered in the limit $\alpha \rightarrow 1$.

The short-time behavior of even-order moments can be obtained in a similar way. The equations for the first two even-order moments are [cf. Eqs. (49) and (51)]

$$\begin{aligned} \frac{d\langle x^2(t) \rangle}{dt} &= D_\alpha [2 {}_0\mathcal{D}_t^{1-\alpha} \langle x_0^2 \rangle - 8\mu_0 t {}_0\mathcal{D}_t^{1-\alpha} \langle x^2(t) \rangle \\ &\quad + 12\mu_0^2 t^2 {}_0\mathcal{D}_t^{1-\alpha} \langle x^4(t) \rangle + \dots], \end{aligned} \quad (92)$$

$$\frac{d\langle x^4(t) \rangle}{dt} = D_\alpha [12 {}_0\mathcal{D}_t^{1-\alpha} \langle x^2(t) \rangle - 32\mu_0 t {}_0\mathcal{D}_t^{1-\alpha} \langle x^4(t) \rangle + \dots]. \quad (93)$$

To order $t^{-1+\alpha}$, the equation for $\langle x^2 \rangle$ reads

$$\frac{d\langle x^2(t) \rangle}{dt} = 2D_\alpha {}_0\mathcal{D}_t^{1-\alpha} 1 + o(t^{-1+\alpha}), \quad (94)$$

so that

$$\langle x^2(t) \rangle = \langle x_0^2 \rangle + \frac{2D_\alpha}{\Gamma(1+\alpha)} t^\alpha + o(t^\alpha). \quad (95)$$

Note that, to this order, the expansion plays no role.

Assume that all the subdiffusive particles are initially placed at $x = 0$. In this case $\langle x_0^n \rangle = 0$ for $n \geq 1$. Inserting this expression into Eq. (93), one sees that the equation for $d\langle x^4 \rangle/dt$ to order $t^{-1+2\alpha}$ takes the form

$$\frac{d\langle x^4(t) \rangle}{dt} = \frac{24}{\Gamma(2\alpha)} D_\alpha^2 t^{-1+2\alpha} + o(t^{-1+2\alpha}). \quad (96)$$

Consequently,

$$\langle x^4(t) \rangle = \frac{24D_\alpha^2}{\Gamma(1+2\alpha)} t^{2\alpha} + o(t^{2\alpha}). \quad (97)$$

An improved differential equation for $\langle x^2(t) \rangle$ can be obtained by taking advantage of the fact that we now know a more accurate expression for $\langle x^2(t) \rangle$ [cf. Eq. (95)] which can be inserted into Eq. (92). The resulting equation is

$$\frac{d\langle x^2(t) \rangle}{dt} = \frac{2D_\alpha}{\Gamma(\alpha)} t^{-1+\alpha} - \frac{16D_\alpha^2 \mu_0}{\Gamma(2\alpha)} t^{2\alpha} + o(t^{2\alpha}). \quad (98)$$

Note that, to this order, it is not necessary to include the moment $\langle x^4(t) \rangle$ (and, *a fortiori*, higher order moments), since the contribution coming from this term will be at least of order $t^{1+3\alpha}$. The integration of Eq. (98) yields

$$\langle x^2(t) \rangle = \frac{2D_\alpha}{\Gamma(1+\alpha)} t^\alpha - \frac{16D_\alpha^2 \mu_0}{(1+2\alpha)\Gamma(2\alpha)} t^{1+2\alpha} + o(t^{1+2\alpha}). \quad (99)$$

The main term is simply the standard exact expression for the mean-square displacement of a subdiffusive particle evolving on a static domain. In Fig. 10 we compare the approximation given by Eq. (99) with results obtained by numerical integration and by random walk simulations. From Eq. (99), one clearly sees that the leading correction introduced by the domain evolution is of the order $t^{1+2\alpha}$, as opposed to the cubic correction characteristic of the normal diffusive case [cf. Eq. (61)]. Once again, the limit $\alpha \rightarrow 1$ yields the result for normal diffusion.

The short-time behavior of the moments of $u(y, t)$ for subdiffusion is readily obtained by the method already used in the normal diffusive case. Note that Eqs. (66a)–(66b) continue to

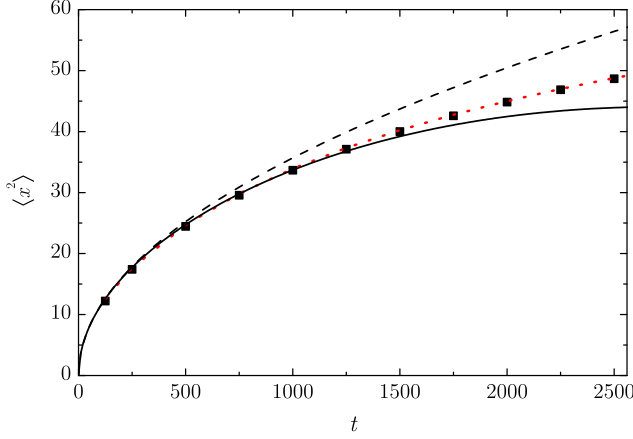


FIG. 10. $\langle x^2 \rangle$ vs time for $\mu(x, t) = \mu_0 x^2$, $u(x, 0) = \delta(x)$, and $\mu_0 = 10^{-6}$ for subdiffusive particles with $\alpha = 1/2$ and $D_\alpha = 1/2$. The dotted line represents numerical results, whereas the squares are simulation results. The broken line corresponds to the static case, i.e., to the main term in Eq. (98), whereas the solid line corresponds to the analytical short-time approximation given by the full equation (98).

hold in the subdiffusive case. Inserting Eqs. (89), (91), (97), and (99) into Eqs. (66a)–(66b), we find

$$\begin{aligned} \langle y(t) \rangle &= \langle y_0 \rangle + \frac{1}{3} \mu_0 \langle y_0^3 \rangle t + \frac{2\mu_0 \langle y_0 \rangle}{\Gamma(2 + \alpha)} D_\alpha t^{1+\alpha} \\ &\quad + \frac{\mu_0^2}{10} \langle y_0^5 \rangle t^2 + o(t^2) \end{aligned} \quad (100)$$

for $y_0 \neq 0$. Note that the linear drift term already encountered in the normal diffusive case remains dominant. For $y_0 = 0$, one has

$$\langle y^2 \rangle = \frac{2D_\alpha}{\Gamma(1 + \alpha)} t^\alpha + \frac{16\mu_0 D_\alpha^2}{\Gamma(2 + 2\alpha)} t^{1+2\alpha} + o(t^{1+2\alpha}), \quad (101)$$

implying that the first correction arising from the domain evolution is proportional to $t^{1+2\alpha}$, and thus more important than the cubic correction given by Eq. (69).

V. REACTION DIFFUSION EQUATIONS AND REACTION SUBDIFFUSION EQUATIONS IN GROWING DOMAIN COORDINATES FOR GROWING DOMAIN PROBLEMS

In the preceding section we derived the evolution equations for the diffusion limits of the master equations for an auxiliary CTRW with standard diffusion, and with subdiffusion. The auxiliary CTRW was defined as a CTRW on a fixed domain, with variable jump lengths, corresponding to a CTRW on an evolving domain with fixed nearest-neighbor jump lengths. The evolution equations were obtained in the coordinate system of the fixed domain. In this section we obtain the corresponding evolution equations in the coordinate system of the evolving domain by mapping the equations Eq. (40) for standard diffusion and Eq. (80) for subdiffusion back to the growing domain. It is important to note that this is largely a formality. The governing equations are easier to solve for the auxiliary process on the fixed domain.

We recall that the space coordinate y on the evolving domain can be represented by $\bar{g}(x, t)$, and we have defined

functions on the growing domain, $\zeta(y, t) = \zeta(\bar{g}(x, t), t) = \bar{\zeta}(x, t)$ in terms of functions on the fixed domain using the mapping (5). In this way we identify the following:

$$u(y, t) = \bar{u}(x, t), \quad (102)$$

$$\mu(y, t) = \bar{\mu}(x, t), \quad (103)$$

$$v(y, t) = \bar{v}(x, t) = \frac{\partial \bar{g}(x, t)}{\partial x} = e^{\int_0^t \bar{\mu}(x, s) ds}, \quad (104)$$

$$\eta(y, t) = \bar{\eta}(x, t) = \frac{\partial \bar{g}(x, t)}{\partial t} = \int_0^x \bar{\mu}(z, t) e^{\int_0^t \bar{\mu}(z, s) ds} dz. \quad (105)$$

Many results can now be obtained in a straightforward way from simple chain rules, for example,

$$\frac{\partial \bar{\mu}(x, t)}{\partial x} = \frac{\partial \mu(y, t)}{\partial y} v(y, t). \quad (106)$$

Note that

$$\begin{aligned} \frac{\partial \bar{v}(x, t)}{\partial x} &= \left[\int_0^t \frac{\partial \bar{\mu}(x, s)}{\partial x} ds \right] e^{\int_0^t \bar{\mu}(x, s) ds} \\ &= \left[\int_0^t \frac{\partial \bar{\mu}(x, s)}{\partial x} ds \right] \bar{v}(x, t) \end{aligned} \quad (107)$$

and

$$\frac{\partial \bar{v}(x, t)}{\partial x} = \left[\frac{\partial v(y, t)}{\partial y} \right] \frac{\partial y}{\partial x} = \left[\frac{\partial v(y, t)}{\partial y} \right] \bar{v}(x, t), \quad (108)$$

so that

$$\int_0^t \frac{\partial \bar{\mu}(x, s)}{\partial x} ds = \frac{\partial v(y, t)}{\partial y}. \quad (109)$$

We also note that

$$\frac{\partial \bar{v}(x, t)}{\partial t} = \bar{\mu}(x, t) e^{\int_0^t \bar{\mu}(x, s) ds} = \bar{\mu}(x, t) \bar{v}(x, t), \quad (110)$$

and then

$$\frac{\partial \bar{v}(x, t)}{\partial t} = \mu(y, t) v(y, t). \quad (111)$$

Partial derivatives, with respect to time, of functions on the fixed domain are replaced with material derivatives of the corresponding functions on the growing domain. Thus, if $\zeta(y, t) = \bar{\zeta}(x, t)$, then

$$\frac{\partial \bar{\zeta}(x, t)}{\partial t} = \frac{\partial \zeta(y, t)}{\partial t} + \frac{\partial \zeta(y, t)}{\partial y} \frac{\partial y}{\partial t}. \quad (112)$$

Finally in this preamble we note the following result, obtained by combining Eqs. (111) and (112),

$$\mu(y, t) = \frac{1}{v(y, t)} \left[\frac{\partial v(y, t)}{\partial t} + \frac{\partial v(y, t)}{\partial y} \eta(y, t) \right]. \quad (113)$$

A. Standard diffusion

Using the results presented earlier in Sec. V, it is now straightforward to transform the evolution equation for the auxiliary process with standard diffusion, Eq. (38), to an evolution equation in the coordinates of the evolving domain.

There are various ways to express the resulting equation,

$$\frac{\partial u(y, t)}{\partial t} = D \frac{\partial^2 u(y, t)}{\partial y^2} - \eta(y, t) \frac{\partial u(y, t)}{\partial y} - [\mu(y, t) + \omega(y, t)]u(y, t) + \chi(y, t), \quad (114)$$

or

$$\begin{aligned} \frac{\partial u(y, t)}{\partial t} = & D \frac{\partial^2 u(y, t)}{\partial y^2} - \eta(y, t) \frac{\partial u(y, t)}{\partial y} \\ & + \left[\frac{1}{\sigma(y, t)} \frac{\partial \sigma(y, t)}{\partial t} + \frac{\partial \sigma(y, t)}{\partial y} \eta(y, t) \right] u(y, t) \\ & + \chi(y, t), \end{aligned} \quad (115)$$

or

$$\begin{aligned} \frac{\partial u(y, t)}{\partial t} = & D \frac{\partial^2 u(y, t)}{\partial y^2} - \eta(y, t) \frac{\partial u(y, t)}{\partial y} \\ & - \left[\frac{1}{v(y, t)} \frac{\partial v(y, t)}{\partial t} + \frac{1}{v(y, t)} \frac{\partial v(y, t)}{\partial y} \eta(y, t) \right] u(y, t) \\ & - \omega(y, t)u(y, t) + \chi(y, t). \end{aligned} \quad (116)$$

$$\begin{aligned} \frac{\partial u(y, t)}{\partial t} = & D \frac{\partial^2 u(y, t)}{\partial y^2} - \eta(y, t) \frac{\partial u(y, t)}{\partial y} \\ & - \left[\frac{1}{v(y, t)} \frac{\partial v(y, t)}{\partial t} + \frac{1}{v(y, t)} \frac{\partial v(y, t)}{\partial y} \eta(y, t) \right] u(y, t) \\ & - \omega(y, t)u(y, t) + \chi(y, t). \end{aligned} \quad (117)$$

B. Subdiffusion

We now carry out the transformation of the evolution equation for the auxiliary process with standard diffusion, Eq. (80), to an evolution equation in the coordinates of the evolving domain. In this transformation, the fractional derivatives with respect to time of functions on the fixed domain are replaced with comoving fractional derivatives on the evolving domain, defined as [47]

$$\begin{aligned} {}_0^g \mathcal{C}_t^{1-\alpha} f(y, t) = & \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t f(\bar{g}(\bar{g}^{-1}(y, t), t'), t') \\ & \times (t - t')^{\alpha-1} dt'. \end{aligned} \quad (118)$$

The evolution equation for subdiffusion with reactions on the evolving domain can now be written as

$$\begin{aligned} \frac{\partial u(y, t)}{\partial t} = & D_\alpha \frac{\partial^2}{\partial y^2} \left\{ \sigma(y, t, 0) {}_0^g \mathcal{C}_t^{1-\alpha} \left[\frac{u(y, t)}{\sigma(y, t, 0)} \right] \right\} \\ & - \eta(y, t) \frac{\partial u(y, t)}{\partial y} \\ & - [\mu(y, t) + \omega(y, t)]u(y, t) + \chi(y, t). \end{aligned} \quad (119)$$

Equation (119) is a major result of the paper. It provides a general evolution equation that can be employed to describe the space and time concentration of a system of particles that are undergoing subdiffusive transport, with mean-square displacement growing as t^α , with particle deaths occurring at rate $\omega(y, t)$, particle births occurring at rate $\chi(y, t)$, on a domain $y \in [0, L(t)]$ that is evolving as $y = \bar{g}(x, t)$ at time t from each initial location $x \in [0, L]$. The quantities, $\eta(y, t)$ and $\mu(y, t)$ are well defined in terms of the growth function $\bar{g}(x, t)$ via

$$\eta(y, t) = \bar{\eta}(x, t) = \frac{\partial \bar{g}(x, t)}{\partial t}$$

and

$$\mu(y, t) = \bar{\mu}(x, t) = \frac{\partial}{\partial t} \log \left(\frac{\partial y}{\partial x} \right),$$

and $\sigma(y, t, 0) = \bar{\sigma}(x, t, 0)$ includes contributions from the growth function and the death rate via

$$\sigma(x, 0, t) = e^{-\int_0^t \bar{\mu}(x, s) ds} e^{-\int_0^t \bar{\omega}(x, s) ds}. \quad (120)$$

In practical terms this evolution equation on the growing domain would rarely be solved, instead it is more straightforward to solve the evolution equation for the formulation of the auxiliary process on the fixed domain, Eq. (82).

Note that if we take the limit as $\alpha \rightarrow 1$ in Eq. (119), we recover the equation for standard diffusion with reactions on an evolving domain, Eq. (114). Note also that if the growth rate is zero, $\bar{\mu}(x, t) = 0$, then $\eta(y, t) = 0$ and $y = x$, and Eq. (119) reduces to the equation for subdiffusive transport with reactions on a fixed domain [6,7], i.e.,

$$\begin{aligned} \frac{\partial u(x, t)}{\partial t} = & D_\alpha \frac{\partial^2}{\partial x^2} \left\{ \theta(x, t, 0) {}_0 \mathcal{D}_t^{1-\alpha} \left[\frac{u(x, t)}{\theta(x, t, 0)} \right] \right\} \\ & - \omega(x, t)u(x, t) + \chi(x, t). \end{aligned} \quad (121)$$

Finally we note that if there are no reactions, then Eq. (119) reduces to

$$\begin{aligned} \frac{\partial u(y, t)}{\partial t} = & D_\alpha \frac{\partial^2}{\partial y^2} \left\{ e^{-\int_0^t \bar{\mu}(\bar{g}^{-1}(y, t), s) ds} {}_0^g \mathcal{C}_t^{1-\alpha} \left[\frac{u(y, t)}{e^{-\int_0^t \bar{\mu}(\bar{g}^{-1}(y, t), s) ds}} \right] \right\} \\ & - \eta(y, t) \frac{\partial u(y, t)}{\partial y} \\ & - \mu(y, t)u(y, t). \end{aligned} \quad (122)$$

This is in agreement with Eq. (40) in Ref. [47] in the special case of uniform growth where $\mu(y, t) = r$ and $y(x, t) = xe^{rt}$ so that $\eta(y) = ry$.

VI. EXAMPLE

In this section, we will show how our formalism could be used for describing a specific reaction-diffusion process occurring in a growing surface. In order to apply the equations in this paper, it is necessary to have explicit expressions for the domain growth function $\bar{\mu}(x, t)$ and the birth and death rates $\bar{\chi}(x, t)$ and $\bar{\omega}(x, t)$. As an illustration we consider a population with logistic growth dynamics, spreading along an evolving interface whose height $h(r, t)$ above a horizontal baseline $r \in [0, L]$ is given by

$$\frac{\partial h(r, t)}{\partial t} = v + \lambda \left\{ 1 + \frac{1}{2} \left[\frac{\partial h(r, t)}{\partial r} \right]^2 \right\}. \quad (123)$$

In this model, v represents a vertical growth rate parameter, λ represents a surface normal growth rate parameter, and it is assumed that the height is a slowly varying function of r , i.e., $\partial h / \partial r \ll 1$. This surface growth model has been used to model laminations in growing stromatolites [53,54]. The application considered here could model the lateral spread of microbicides on the surface of a growing stromatolite. In the application to stromatolite growth the height would typically be measured in mm and the growth rates v and λ would be measured in millimeters per year.

The arc length along the interface is given by

$$s(r, t) = \int_0^r \sqrt{1 + \left[\frac{\partial h(r', t)}{\partial r'} \right]^2} dr'. \quad (124)$$

The initial fixed domain coordinate $x \in [0, L_0]$ can then be defined as

$$x = s(r, 0), \quad (125)$$

and the evolving domain coordinate $y \in [0, L(t)]$ is given as

$$y(x, t) = s(r(x), t). \quad (126)$$

Note that Eq. (125) defines $r(x)$ used in Eq. (126). The growth rate $\bar{\mu}(x, t)$ can then be obtained by differentiating Eq. (4) with respect to x , taking the logarithm, and differentiating with respect to t ,

$$\bar{\mu}(x, t) = \frac{\partial}{\partial t} \log \left(\frac{\partial y}{\partial x} \right). \quad (127)$$

In logistic growth a population with number density $u(x, t)$, representing the number per mm, evolves via

$$\frac{\partial u(x, t)}{\partial t} = \gamma u(x, t) \left[1 - \frac{u(x, t)}{u_0} \right], \quad (128)$$

where u_0 is the threshold carrying capacity and γ is a net per capita growth rate. This then identifies

$$\bar{\chi}(x, t) = \gamma u(x, t) \quad \text{and} \quad \bar{\omega}(x, t) = \frac{\gamma u(x, t)}{u_0}. \quad (129)$$

The expressions for $\bar{\mu}(x, t)$, $\bar{\omega}(x, t)$, and $\bar{\chi}(x, t)$ can be employed in the evolution equations of $u(x, t)$ with standard diffusion, Eq. (42), or subdiffusion, Eq. (82), and the solutions $u(x, t)$ can be mapped onto corresponding locations y at time t on the evolving domain using Eq. (126). The solutions of Eq. (42) or Eq. (82) could be obtained using numerical methods such as a modification of the fractional Crank-Nicolson of Ref. [61] or a modification of the discrete time random walk algorithm presented in Ref. [62].

VII. SUMMARY AND OUTLOOK

In this paper we have derived evolution equations for a system undergoing diffusion and reactions on an arbitrarily evolving one-dimensional domain. Evolution equations have been obtained for both standard diffusion and subdiffusion. The evolution equations were obtained from the following sequence of steps. First we identified a general mapping between the initial fixed domain and the evolving domain. We then derived master equations for an auxiliary CTRW on a fixed domain with birth and death processes, corresponding to a CTRW with unbiased fixed length steps on a growing domain with birth and death processes. We considered particular waiting time densities, corresponding to standard diffusion in one case and subdiffusion in another, and we obtained diffusion limits of the master equations for the auxiliary process on the fixed domain. We then mapped the governing equations back to the evolving domain.

Interesting behavior arises already in the case of a uniformly evolving domain, even in the absence of reactions. As we have shown, mapping the normal diffusive dynamics onto the initial fixed domain results in rescaled Brownian motion, i.e., Brownian motion with a time-dependent diffusion coefficient. As pointed out in Ref. [31], this process is often used as a fitting model for experimental data without physical

justification, but here we see that it emerges naturally from our formalism for a random walk on a uniformly evolving domain.

Having derived the governing equations for arbitrarily evolving domains, we then developed an iterative method for obtaining analytic expressions for short-time moments for standard diffusion and for subdiffusion on an evolving domain. We showed that the moments calculated in this way compared favorably with moment evaluations obtained from numerical solutions of the governing equations, and from numerical simulations of the processes.

Beyond this quantitative agreement, let us briefly enumerate some key features of the underlying physics. We have seen that the short-time behavior of the moments in the absence of reactions is characterized by the strong influence of the initial condition.

In this paper, we have largely focused on particular case $\mu = \mu_0 x^2$ (with $\mu_0 > 0$, say) which lends itself particularly well to analytical treatment. In terms of x coordinates, when a particle starts away from $x = 0$, it is dragged towards the origin in an accelerated fashion. In the case of normal diffusion, the behavior of $\langle x^2 \rangle$ is characterized by a correction to the standard contribution $2Dt$ which is quadratic in time and which also contains the diffusion coefficient D . When the particle starts at the origin, the correction to the diffusive contribution is quadratic rather than cubic. For any starting point $y_0 \neq 0$, the behavior of $\langle y(t) \rangle$ is characterized by a linear correction which does not depend on the diffusivity D . The apparent diffusivity in y coordinates is also modified by an additive contribution that stems from the domain evolution. In the subdiffusive case, the corrections associated with the domain evolution are stronger, since the relative influence of subdiffusive transport is less important than that of Brownian diffusion.

As an application we considered how a diffusion process in an evolving domain corresponding to surface growth, above a horizontal baseline, driven by constant vertical growth and surface normal growth could be described in terms of the formalism developed in this paper. The coordinates for the evolving domain represent the arc length along the surface in this application. Our KPZ-like approach is a suitable starting point to describe layer-by-layer deposition in stromatolites. In addition to this specific application, we have already mentioned in the Introduction some systems where both diffusive transport and inhomogeneous domain growth are at play. A general framework for applications would require extensions in higher spatial dimensions, consideration of different boundary conditions, inclusion of forces, and inclusion of stochastic fluctuations.

Given the importance of boundary conditions for applications, we would like to briefly discuss their role in problems involving diffusion in growing domains. The mathematical treatment of boundary conditions follows the same lines as in the case of a static domain. If the boundary coincides with the limiting surface of the physical domain, it will evolve with the same scale factor; such a boundary becomes static when mapping the problem onto the auxiliary fixed domain, and the subsequent implementation of the boundary condition in x coordinates can take place in the same manner as on a static domain. In some situations of interest, though, the boundary could be static, implying that one would have a

moving boundary in x coordinates. In such cases, sticking to a description in terms of x coordinates would require solving a problem with a time-dependent boundary condition. In general, such problems are more difficult than problems with static boundaries; on the other hand, the effect of time dependent boundary conditions (the so-called ‘‘Stefan problem’’) has been the object of comprehensive studies in the literature (see, e.g., Refs. [63–65]). Of course, one could still use static boundaries if one chose to work with y coordinates instead. However, as we have seen in Sec. V, the price to pay is that the corresponding reaction-diffusion equations are much more complicated than those derived in Sec. IV for the auxiliary domain.

We close by noting that the results obtained in the present work may also be relevant for the study of encounter-controlled reactions in nonuniformly evolving domains. Consider, for example, two pulses describing two diffusing particles that evolve on a domain with expansion rate $\mu \propto x^2$. Further, assume that these particles react instantaneously upon encounter. Strictly speaking, the computation of the reaction rate is a first-passage problem, but an approximation based on the overlap of the two pulses (defined via the respective pulse widths and second-order moments) may yield acceptable results for a suitable parameter choice. If the initial separation is small enough, the reaction rate will be dominated by the short-

time regime, and some of our results might prove useful. As we have seen, for a given initial separation, the reaction rate may display significant differences depending on the initial location of the pulses with respect to the origin. More generally, the study of first passage problems in nonuniformly evolving domains may be of interest for biological applications, as we explained in the Introduction when discussing the model of Ref. [52]. Further examples are target and trapping problems, such as the subdiffusive trapping problem studied in Ref. [66]. An extension of the results available in the literature for the case of a static domain may unveil interesting effects arising from the interplay between intrinsic transport and domain evolution.

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APPENDIX A: AUXILIARY FIXED DOMAIN MASTER EQUATION DERIVATION

The master equation is obtained by differentiating Eq. (20) with respect to time. To avoid problems with the discontinuity in the arrival rate density at $t = 0$ we write [11]

$$\bar{q}(x, t|x_0, 0) = \delta(x - x_0)\delta(t - 0^+) + \bar{q}^+(x, t|x_0, 0) \quad (\text{A1})$$

and then

$$\bar{\rho}(x, t|x_0, 0) = \Phi(t)\bar{\sigma}(x, t, 0)\delta_{x,x_0} + \int_0^t \Phi(t - t')\bar{\sigma}(x, t, t')\bar{q}^+(x, t'|x_0, 0) dt', \quad (\text{A2})$$

where $\bar{q}^+(x, t|x_0, 0)$ is right continuous at $t = 0$. We now use Leibniz rule and the results $\Phi(0) = 1$, $\bar{\sigma}(x, t, t) = 1$ and $\partial\Phi(t - t')/\partial t = -\psi(t - t')$ to differentiate under the integral sign, arriving at

$$\begin{aligned} \frac{\partial\bar{\rho}(x, t|x_0, 0)}{\partial t} &= -\psi(t)\bar{\sigma}(x, t, 0)\delta_{x,x_0} - \Phi(t)[\bar{\mu}(x, t) + \bar{\omega}(x, t)]\bar{\sigma}(x, t, 0)\delta_{x,x_0} \\ &\quad + \bar{q}^+(x, t|x_0, 0) - \int_0^t \psi(t - t')\bar{\sigma}(x, t, t')\bar{q}^+(x, t'|x_0, 0) dt' \\ &\quad - \int_0^t \Phi(t - t')[\bar{\mu}(x, t) + \bar{\omega}(x, t)]\bar{\sigma}(x, t, t')\bar{q}^+(x, t'|x_0, 0) dt'. \end{aligned} \quad (\text{A3})$$

This can be simplified using Eqs. (19), (A2), (20), and (A1) to arrive at

$$\begin{aligned} \frac{\partial\bar{\rho}(x, t|x_0, 0)}{\partial t} &= \int_0^{L_0} \lambda(x, x', t) \int_0^t \psi(t - t')\bar{\sigma}(x', t, t')\bar{q}(x', t'|x_0, 0) dt' dx' \\ &\quad - \int_0^t \psi(t - t')\bar{\sigma}(x, t, t')\bar{q}(x, t'|x_0, 0) dt' \\ &\quad - [\bar{\mu}(x, t) + \bar{\omega}(x, t)]\bar{\rho}(x, t|x_0, 0). \end{aligned} \quad (\text{A4})$$

We now wish to replace the terms involving q with terms involving ρ . Without loss of generality we can define a kernel $K(t - t')$ such that

$$\int_0^t \psi(t - t')\bar{q}(x, t'|x_0, 0)\bar{\sigma}(x, t, t') dt' = \int_0^t K(t - t')\bar{\rho}(x, t'|x_0, 0)\bar{\sigma}(x, t, t') dt', \quad (\text{A5})$$

and then we can write Eq. (A4) as

$$\begin{aligned} \frac{\partial \bar{\rho}(x, t|x_0, 0)}{\partial t} &= \int_0^{L_0} \lambda(x, x', t) \int_0^t K(t-t') \bar{\sigma}(x', t, t') \bar{\rho}(x', t'|x_0, 0) dt' dx' \\ &\quad - \int_0^t K(t-t') \bar{\sigma}(x, t, t') \bar{\rho}(x, t'|x_0, 0) dt' \\ &\quad - [\bar{\mu}(x, t) + \bar{\omega}(x, t)] \bar{\rho}(x, t|x_0, 0). \end{aligned} \quad (\text{A6})$$

Using the semigroup property

$$\bar{\sigma}(x, t, 0) = \bar{\sigma}(x, t, t') \bar{\sigma}(x, t', 0) \quad (\text{A7})$$

in Eq. (A5), and taking the Laplace transform $\mathcal{L}[\cdot]$ with respect to time in the resulting equation, we obtain

$$\mathcal{L}[\psi(t)] \mathcal{L} \left[\frac{\bar{q}(x, t|x_0, 0)}{\bar{\sigma}(x, t, 0)} \right] = \mathcal{L}[K(t)] \mathcal{L} \left[\frac{\bar{\rho}(x, t|x_0, 0)}{\bar{\sigma}(x, t, 0)} \right]. \quad (\text{A8})$$

On the other hand, we can also divide both sides of Eq. (13) by $\bar{\sigma}(x, t, 0)$ and take the Laplace transform to find

$$\mathcal{L} \left[\frac{\bar{\rho}(x, t|x_0, 0)}{\bar{\sigma}(x, t, 0)} \right] = \mathcal{L}[\Phi(t)] \mathcal{L} \left[\frac{\bar{q}(x, t|x_0, 0)}{\bar{\sigma}(x, t, 0)} \right]. \quad (\text{A9})$$

Comparing Eq. (A8) and Eq. (A9), we obtain the result (23).

APPENDIX B: NONUNIFORM NEAREST-NEIGHBOR STEPS ON A FIXED DOMAIN

Here we relate nearest-neighbor jump lengths of a fixed size Δy on the growing domain to corresponding jump lengths ϵ^+ and ϵ^- for the auxiliary CTRW on the original fixed domain. The jump lengths on the ϵ^+ and ϵ^- were defined in Sec. IV by the relations $y - \Delta y = \bar{g}(x - \epsilon^-, t)$ and $y + \Delta y = \bar{g}(x + \epsilon^+, t)$. Taking into account that $y = \bar{g}(x, t)$, we can rewrite these expressions as

$$\pm \Delta y = \bar{g}(x \pm \epsilon^\pm, t) - \bar{g}(x, t). \quad (\text{B1})$$

We now take Taylor series expansions around the point x and retain leading order terms in ϵ^+ and ϵ^- to arrive at

$$\Delta y = \epsilon^\pm \bar{g}_x(x, t) \pm \frac{(\epsilon^\pm)^2}{2} \bar{g}_{xx}(x, t) + O[(\epsilon^\pm)^3]. \quad (\text{B2})$$

We can now solve the above quadratic approximations for ϵ^+ and ϵ^- , noting that both terms must vanish when $\Delta y = 0$, to arrive at

$$\epsilon^\pm \approx \frac{\mp \bar{g}_x(x, t) \pm \bar{g}_x(x, t) \sqrt{1 + \frac{2\bar{g}_{xx}(x, t)}{\bar{g}_x(x, t)^2} \Delta y}}{\bar{g}_{xx}}. \quad (\text{B3})$$

We now expand each of these terms as a series expansion in powers of Δy , arriving at

$$\epsilon^\pm = \frac{\Delta y}{\bar{g}_x(x, t)} \mp \frac{\bar{g}_{xx}(x, t)}{2\bar{g}_x(x, t)^3} \Delta y^2 + O(\Delta y^3). \quad (\text{B4})$$

Finally, using Eq. (4) we obtain Eqs. (34).

APPENDIX C: NUMERICAL METHOD FOR THE SOLUTION OF THE FRACTIONAL REACTION-DIFFUSION EQUATION IN GROWING DOMAINS

In what follows, we describe the numerical finite difference method used to solve the fractional Fokker-Planck equation

obtained in Sec. IV. This is exemplified for Eq. (80), which we first rewrite as $\partial_t \bar{u}(x, t) = G(x, t)$.

In any finite-difference method, one discretizes the variables in time and space. Let us denote by Δt and Δx the respective time and spatial discretization steps. The discretized functions will be hereafter denoted by $f_j^{(m)} \equiv f(x_j, t_m)$, where $m = 0, 1, \dots, M$ and $j = -J, -J+1, \dots, 0, \dots, J-1, J$. In the weighted average finite difference scheme employed in the present work, we replace the fractional partial differential equation $\partial_t \bar{u}(x, t) = G(x, t)$ with the following discretized version [61]:

$$\begin{aligned} \frac{\bar{u}_j^{(m+1)} - \bar{u}_j^{(m)}}{\Delta t} &= \zeta G(x_j, t_m) + (1 - \zeta) G(x_j, t_{m+1}) \\ &\equiv \zeta G_j^{(m)} + (1 - \zeta) G_j^{(m+1)}, \end{aligned} \quad (\text{C1})$$

where $\zeta \in (0, 1)$ is the weighting parameter determining the convergence and stability of the algorithm. In this paper, we take $\zeta = 1/2$, which corresponds to the so-called Crank-Nicolson method [61]. We still have to approximate the continuous differential operators appearing in $G(x, t)$ by expressions in terms of finite differences. We use standard approximations for the ordinary derivatives, namely, the two-point centered formula for the first-order spatial derivative, and the three-point centered formula for the second-order spatial derivative. The fractional derivative ${}_0\mathcal{D}_t^{1-\alpha}$ is approximated by the Grünwald-Letnikov formula [59,61]

$${}_0\mathcal{D}_t^{1-\alpha} f(x, t) \Big|_{x_j, t_m} \approx (\Delta t)^{\alpha-1} \sum_{k=0}^m w_k^{(1-\alpha)} f_j^{(m-k)}, \quad (\text{C2})$$

where the parameters $w_k^{(1-\alpha)}$ can be obtained from the recursive equation

$$w_k^{(1-\alpha)} = \left(1 - \frac{2-\alpha}{k}\right) w_{k-1}^{(1-\alpha)}, \quad k = 1, 2, \dots \quad (\text{C3})$$

with $w_0^{(1-\alpha)} = 1$. The resulting difference equation can be rearranged as

$$b_{j-1}^{(m+1)}\bar{u}_{j-1}^{(m+1)} + b_j^{(m+1)}\bar{u}_j^{(m+1)} + b_{j+1}^{(m+1)}\bar{u}_{j+1}^{(m+1)} = R, \quad (\text{C4})$$

where $b_j^{(m+1)}$ is a quantity depending on the functions \bar{v} , $\bar{\mu}$, and $\bar{\omega}$, as well as on Δt and Δx . The term R on the right-hand

side also depends on the (approximate) numerical values of the solutions $\bar{u}(x, t_n)$ at times t_n smaller than t_{m+1} , i.e., at times t_n with $n = 0, \dots, m$. Equation (C4) is a tridiagonal system which can be efficiently solved by means of the well-known Thomas algorithm.

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