Divergent series and memory of the initial condition in the long-time solution of some anomalous diffusion problems

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We consider various anomalous d-dimensional diffusion problems in the presence of an absorbing boundary with radial symmetry. The motion of particles is described by a fractional diffusion equation. Their mean-square displacement is given by $\langle r^2 \rangle \propto t^\gamma (0 < \gamma \le 1)$, resulting in normal diffusive motion if $\gamma = 1$ and subdiffusive motion otherwise. For the subdiffusive case in sufficiently high dimensions, divergent series appear when the concentration or survival probabilities are evaluated via the method of separation of variables. While the solution for normal diffusion problems is, at most, divergent as $t \to 0$, the emergence of such series in the long-time domain is a specific feature of subdiffusion problems. We present a method to regularize such series, and, in some cases, validate the procedure by using alternative techniques (Laplace transform method and numerical simulations). In the normal diffusion case, we find that the signature of the initial condition on the approach to the steady state rapidly fades away and the solution approaches a single (the main) decay mode in the long-time regime. In remarkable contrast, long-time memory of the initial condition is present in the subdiffusive case as the spatial part $\Psi_1(r)$ describing the long-time decay of the solution to the steady state is determined by a weighted superposition of *all* spatial modes characteristic of the normal diffusion problem, the weight being dependent on the initial condition. Interestingly, $\Psi_1(r)$ turns out to be independent of the anomalous diffusion exponent γ.

I. INTRODUCTION

Over the last few decades, the attitude of the scientific community toward fractional calculus has been changing rapidly. While for many years this discipline was regarded as a relatively arcane field of mathematics, more recently it is increasingly appreciated as a useful, at times even indispensable, tool for the study of a broad array of scientific problems in physics, biology, geology, engineering, economics, etc [1–5]. Fractional differential equations, and in particular, fractional diffusion equations have been successfully used to describe anomalous diffusion processes [2,4–12].

An important class of (normal and anomalous) diffusion problems are those with radial symmetry [6,13]. In this paper, we shall consider problems of this class in the presence of absorbing boundary conditions. This kind of boundary condition is characteristic of the subclass of so-called exit or escape problems, which find a wide application in biology and other disciplines and are the subject of the theory of first-passage processes [14,15]. Independently of whether the problem at hand makes it advisable to work with the forward or with the backward (adjoint) Smoluchowski equation, a route to the solution of the first-passage problem involves the use of an absorbing boundary condition which allows one to identify the exit process with an irreversible absorption step. In general, the resulting equations are not exactly solvable in dimensions $d > 1$; however, in the rather common situation where the system has radial symmetry the hope to find exact solutions for the resulting two-variable (spatial and temporal) problem is much more justified. In such cases the solution of the problem for this "two-body" system (i.e., the diffusing particle and the absorbing surface) may prove useful to devise suitable approximations for more complex many-body problems.

A known example of this is found in the so-called trapping problem, where one seeks to compute the survival probability of a diffusing particle in a d-dimensional sea of randomly distributed, static, and fully absorbing traps. This problem is amenable to exact analysis in the asymptotic, long-time regime [16,17]. Moreover, if the particle *and* the traps diffuse [10,18–22], the problem can still be tackled analytically, but the method involves the solution of *two* first-passage problems. In the first one asks what is the probability that a diffusing particle gets trapped by the perfectly absorbing surface of an *immobile* hypersphere when it starts diffusing from a point outside the hypersphere (this problem is also termed the "target problem" in the literature [15]). The second first-passage problem deals with exactly the same setting, except that the diffusive particle is initially located at an interior point of the hypersphere [23] (in what follows we shall refer to this problem as the "escape problem"). The d-dimensional trapping problem in which the particle and/or traps can be subdiffusive has recently been solved by means of the fractional diffusion formalism [12,22,24]. The long-time behavior of the solution turns out to be different from that of the corresponding normal diffusion problem in a rather surprising way. A similar surprising behavior is found in the long-time solutions of the problems considered in this paper. This shows that, in general, normal diffusion results are not immediately extendable to anomalous diffusion systems, which calls for a careful consideration of these anomalous diffusion problems. The usual reason for studying diffusion problems in dimensions $d > 3$ (as it is done in this paper) is that the dependence of physical phenomena on the dimension provides a better understanding of their behavior via additional insights on the role of the underlying geometry [4,15,25]. However, in some cases, the d-dimensional results with $d > 3$ can be directly useful: for

example, some N-particle diffusion problems in one dimension can be mapped into N-dimensional diffusion problems for a single particle (Chap. 8) [15].

The d-dimensional fractional diffusion equation for a spherically symmetric diffusive field $c(r,t)$ is

$$\frac{\partial c(r,t)}{\partial t} = K_\gamma \, _0D_t^{1-\gamma}\left(\frac{\partial^2 c(r,t)}{\partial r^2} + \frac{d-1}{r}\frac{\partial c(r,t)}{\partial r}\right), \quad (1)$$

where $c(r=|\vec{r}|,t)$ is the solution at $\vec{r}$, γ is the anomalous diffusion exponent, and K_γ is the anomalous diffusion coefficient. The limit $\gamma \to 1$ corresponds to ordinary normal diffusion. In what follows, we shall regard $c(r,t)$ as a particle concentration, but of course our results would be valid for any other physical quantity described by these equations. The nonlocal integrodifferential operator

$$_0D_t^{1-\gamma}c(r,t) = \frac{1}{\Gamma(\gamma)}\frac{\partial}{\partial t}\int_0^t dt' \frac{c(r,t')}{(t-t')^{1-\gamma}}, \quad (2)$$

is the Riemann-Liouville fractional derivative of $c(r,t)$ with respect to time. In the diffusive limit, Eq. (1) describes the spatiotemporal behavior of the concentration of continuous time random walkers (CTRW) when the probability distribution for the waiting time of the walkers between two successive steps follows the power-law decay $t^{-1-\gamma}$ at long times [5]. In this case, the mean-square displacement of each walker grows as $\langle r^2 \rangle \propto t^\gamma$ for large t.

When seeking the solution of many normal diffusion problems by means of the method of separation of variables, one finds that the solution can be written as a linear superposition of exponentially decaying modes (eigenfunctions) $\psi_n(r)$:

$$c(r,t) = c(r,\infty) + \sum_{n=1}^\infty a_n \psi_n(r)\exp(-\lambda_n t), \quad (3)$$

where the eigenvalues λ_n satisfy $0 < \lambda_1 < \lambda_2 \ldots$ and where the specific initial condition of the problem is reflected in the corresponding specific set of coefficients $\{a_n\}$.

Similarly, if one applies this method to the fractional diffusion Eq. (1), it turns out that the time dependence is described by a Mittag-Leffler function $E_\gamma(\cdot)$ [1,5] rather than by an exponential function. Thus, the corresponding fractional solution reads [5,6]

$$c(r,t) = c(r,\infty) + \sum_{n=1}^\infty a_n E_\gamma(-\lambda_n t^\gamma)\psi_n(r). \quad (4)$$

When $\gamma \to 1$, $E_\gamma(-\lambda_n t^\gamma)$ becomes $\exp(-\lambda_n t^\gamma)$ and one recovers the solution of the normal diffusion problem (3). Using the asymptotic formula [26]

$$E_\gamma(-z) \approx \sum_{m=1}^\infty \frac{(-1)^{m+1}}{\Gamma(1-m\gamma)}z^{-m}, \quad z \to \infty, \quad (5)$$

one gets the long-time form of the solution

$$c(r,t) = c(r,\infty) + \sum_{n=1}^\infty \frac{(-1)^{n+1}}{\Gamma(1-n\gamma)}t^{-n\gamma}\Psi_n(r) \quad (6)$$

with

$$\Psi_n(r) = \sum_{k=1}^\infty a_k \lambda_k^{-n}\psi_k(r). \quad (7)$$

In the normal diffusion case described by Eq. (3), the small-n modes $\psi_n(r)$ corresponding to $n=1,2,\ldots$ can be interpreted as spatial patterns whose relative weight in the solution series becomes increasingly important in the course of the temporal evolution. For sufficiently long times one has $[c(r,t)-c(r,\infty)]/\exp(-\lambda_1 t) \propto \psi_1(r)$, i.e., the dominant decay mode is $\psi_1(r)$. Similarly, for the subdiffusive case the small-n modes $\Psi_n(r)$ corresponding to $n=1,2,\ldots$ can be interpreted as spatial patterns whose relative weight in the solution series (6) becomes increasingly important in the course of the temporal evolution. It therefore seems appropriate to term these functions $\Psi_n(r)$ as *long-time subdiffusive modes*. For sufficiently long times the dominant subdiffusive mode corresponding to $m=1$ is

$$[c(r,t)-c(r,\infty)]/t^{-\gamma} \propto \sum_{n=1}^\infty a_n \lambda_n^{-1}\psi_n(r) \equiv \Psi_1(r). \quad (8)$$

This result is very interesting; note that for normal diffusion problems the signature of the initial condition rapidly fades away because the weight of the eigenfunctions $\psi_n(r)$ rapidly becomes negligible for large values of n and in the end only the term proportional to $\psi_1(r)$ survives; however, in the subdiffusive case, the dominant long-time subdiffusion mode $\Psi_1(r)$ embodies the details of the initial condition, as it depends on the full set of coefficients $\{a_n\}$. This implies that, if somehow, $\Psi_1(r)$ (or any other subdiffusion mode, $\Psi_n(r)$) is known, then these coefficients $\{a_n\}$ can be obtained from $\Psi_1(r)$ using, as usual, the orthogonality properties of the eigenfunctions $\psi_k(r)$. Note, though, that the computation of the explicit form of $\Psi_n(r)$ from Eq. (7), i.e., the sum of a series of functions, is not an easy task in general (as illustrated by some representative examples in Sec. II).

A second remarkable aspect is that these "multimodal" functions $\Psi_n(r)$ do not depend on the specific value of γ as long as $\gamma < 1$, even for values of γ arbitrarily close to unity. However, an abrupt transition from multimodal to unimodal behavior takes place when switching from $\gamma < 1$ to $\gamma = 1$, Note that the above considerations on the long-time subdiffusive modes of the fractional diffusion Eq. (1) can be straightforwardly generalized to the long-time solutions of the fractional Fokker-Planck equation as the solution in this case is also of the form (4) [5,27].

In this paper, we will compute the long-time solution (or, equivalently, the long-time subdiffusive modes Ψ_n) for some typical fractional diffusion problems in the presence of an absorbing boundary with spherical symmetry. In such a case one has $\psi_n(r) = J_p(z_n r)$, where $J_p(z_n r)$ is the Bessel function of the first kind with $p = d/2 - 1$ and z_n is its n-th zero, i.e., $J_p(z_n) = 0$. As we will see, the route to the solution involves the evaluation of the function series

TABLE I. Numerical estimate of the series $S(d/2-1,1)$ obtained by summing the first 1000 and 1001 terms and comparison with the analytical value $2^{d/2-3}\Gamma(d/2)/d$ up to $d=8$.

d	1	2	3	4	5	6	7	8
1000	0.3133	0.1250	0.1044	0.1250	0.1878	0.3222	0.0448	−9.704
1001	0.3133	0.1250	0.1044	0.1250	0.1882	0.3445	1.2981	12.759
Ana.	0.3133	0.1250	0.1044	0.1250	0.1880	0.3333	0.6714	1.5000

$$\widetilde{S}(p,m;r) \equiv \sum_{j=1}^{\infty} \frac{z_j^{-2m-1}}{J_{p+1}(z_j)} J_p(z_j r). \quad (9)$$

We will also show how to evaluate the related numerical series

$$S(p,m) \equiv \sum_{j=1}^{\infty} \frac{z_j^{p-2m-1}}{J_{p+1}(z_j)}, \quad (10)$$

which appears in Sec. III when computing the survival probability (or fraction of nonabsorbed particles) in the aforementioned subdiffusive escape problem. It turns out that some of these series are divergent in spite of the fact that they represent well defined physical quantities. Thus, one of our main tasks in the present work will be to "regularize" such series, i.e., to assign them "sensible" values [28] compatible with the physics of the problem and coincident with those obtained by other methods. In order to sum $\widetilde{S}(p,m;r)$, we will regard this series as the Fourier-Bessel expansion of a function $f(r)$ which we will subsequently determine and identify with the physically correct value of $\widetilde{S}(p,m;r)$. To regularize the numerical series $S(p,m)$ we will use a procedure akin to the classical method of Abel summation. The latter uses the functions x^n as regulators of the sum $\sum_{n=0}^{\infty} a_n$ to obtain $f(x) = \sum_{n=0}^{\infty} a_n x^n$ and thus estimate $\sum_{n=0}^{\infty} a_n$ as $\lim_{x \to 1-} f(x)$. In contrast, the method employed in the present work uses the functions $\phi_n(x) = 2^p p! J_p(z_n x)/(z_n x)^p$ as regulators to obtain $g(x) = \sum_{n=0}^{\infty} a_n \phi_n(x)$, and thus estimate $\sum_{n=0}^{\infty} a_n$ as $\lim_{x \to 0+} g(x)$ [note that $\lim_{x \to 0+} \phi_n(x) = 1$].

Subdiffusion processes are only one out of many research areas in physics where divergent sums play a major role. The regularization techniques used in the present work may therefore be relevant beyond the specific problems considered here. For instance, the survival probability of a diffusing particle initially located at the center of a three-dimensional sphere whose surface is absorbing (3d escape problem) must obviously take the value unity at $t=0$. However, when obtained by separation of variables, the solution takes the form of an alternating series between 1 and −1 (Grandi's divergent series) multiplied by the factor 2. In order to obtain the "physically correct" value of 1/2 associated with this series it is necessary to resort to special summation methods [28]. A distinction between anomalous diffusion and normal diffusion is that such divergent series may appear not only in the early-time regime but also in the long-time regime. Beyond the above diffusive and subdiffusive problems, divergent series are quite common in perturbation methods [29]. Another

typical example is the analysis of the Casimir effect, where divergent series appear when one attempts to compute the force between two uncharged metallic plates *in vacuo* [30].

The paper is organized as follows. Section II is devoted to the sum of the series $S(p,m;x)$ and $S(p,m)$ by the procedure mentioned in the paragraph after Eq. (10). In Sec. III we present some spherically symmetric subdiffusion problems and show how the solution of the associated fractional diffusion equation leads to series of the form $S(p,m;x)$ and $S(p,m)$. We subsequently discuss the physics implied by the solution for the survival probability, and confirm the validity of our Fourier-Bessel regularization procedure via numerical simulations as well as an alternative method based on Laplace transform techniques. To conclude Sec. III, we discuss the long-time approach of the subdiffusive concentration profiles to the steady state and compare it to those for the normal diffusion case. Finally, Sec. IV summarizes the main conclusions of the work.

II. SUM OF THE SERIES $S(p,m)$ AND $\widetilde{S}(p,m;x)$

For odd-valued d, the Bessel functions can be written in terms of circular functions, and some sums $S(d/2-1,m)$ can be easily evaluated, e.g., $S(-1/2,1) = \sqrt{\pi/32}$ and $S(1/2,1) = \sqrt{\pi/288}$. However, for other values of d and m the evaluation is not trivial at all. Moreover, a closer inspection of the definition (10) of the series $S(p,m)$ reveals that it may become divergent. To see this, let us denote by s_j the j-th term of the series. The denominator of s_j decreases with increasing j and the absolute value of its numerator turns out to increase with j when $p-2m-1>0$ or, in terms of the dimension, when $d-4m-4>0$. Therefore, it is sure that $|s_j|$ will also increase with j when $d-4m-4>0$. Of course, this rule of thumb only leads to a crude overestimate $\widetilde{d}_c$ of the critical dimension d_c above which $S(d/2-1,m)$ becomes divergent: it is only an estimate because $|s_j|$ could grow with j, even if the absolute value of the numerator decreases with increasing j, if the denominator decreases even faster than the numerator. For instance, we carried out a brute-force term-by-term sum of $S(d/2-1,m)$ for $m=1$ and found that the series converges numerically only for $d \le d_c = 6$ (note that $\widetilde{d}_c = 8$ in this case). We show some of these numerical estimates in Table I.

As anticipated in the Introduction, we shall sum the numerical series $S(p,m)$ by making use of the regulator functions $\phi_j(x) = 2^p p! J_p(z_j x)/(z_j x)^p$. To this end, let us define the function series

$$S(p,m;x) \equiv \sum_{j=1}^{\infty} \frac{z_j^{p-2m-1}}{J_{p+1}(z_j)} \phi_j(x) = \frac{2^p p!}{x^p} \widetilde{S}(p,m;x). \quad (11)$$

Note that for $x \to 0^+$ the series $S(p,m;x)$ becomes identical with the numerical series $S(p,m)$. Also, the Fourier-Bessel

expansion of a given function $g(x)$ is defined as

$$g(x) \sim \sum_{j=1}^{\infty} c_j J_p(z_j x), \qquad (12)$$

where

$$c_j = \frac{2}{J_{p+1}^2(z_j)} \int_0^1 x g(x) J_p(z_j x) dx. \qquad (13)$$

Henceforth, the symbol $\sim$ will stand for a Fourier-Bessel expansion. Comparing Eq. (9) with Eq. (12) we can regard $\tilde{S}(p,m;x)$ as the Fourier-Bessel expansion of a continuous function $\tilde{f}(p,m;x)$ with coefficients

$$c_j \equiv c_j(p,m) = \frac{z_j^{-2m-1}}{J_{p+1}(z_j)}, \qquad (14)$$

i.e.,

$$\tilde{f}(p,m;x) \sim \tilde{S}(p,m;x). \qquad (15)$$

Defining

$$f(p,m;x) \equiv \frac{2^p p!}{x^p} \tilde{f}(p,m;x), \qquad (16)$$

we see from Eq. (11) that $f(p,m;x) \sim S(p,m;x)$. In order to assign $S(p,m)$ a value, we proceed as follows. First we determine $f(p,m;x)$ and then identify $S(p,m) = \lim_{x \to 0} S(p,m;x)$ with $\lim_{x \to 0} f(p,m;x)$, i.e.,

$$S(p,m) = \lim_{x \to 0} f(p,m;x) = \lim_{x \to 0} \frac{2^p p!}{x^p} \tilde{f}(p,m;x). \qquad (17)$$

(Even though we use the same symbol $S(p,m)$ to denote both the numerical series and its sum, its actual meaning should be clear from the context in which it is used.) The fact that this regularization procedure works (as will be shown below) is by no means surprising. Indeed, since $f(p,m;x)$ are polynomials (see Appendix B), the Fourier-Bessel expansion $S(p,m;x)$ of the function $f(p,m;x)$ is Cesàro-1 (C1) summable to $f(p,m;x)$ [31]. Therefore, assigning $\lim_{x \to 0} f(p,m;x)$ to $S(p,m)$ amounts to assigning the C1-sum of the series $S(p,m;x)$ in $x=0$ to $S(p,m)$. Furthermore, in the next section we shall demonstrate that the value yielded by our method coincides with the result of numerical simulations and with the value yielded by the solution of the corresponding subdiffusion problem in Laplace space.

Our final goal in this section will be to devise a procedure to compute $\tilde{f}(p,m;x)$ and thus obtain finite values for $S(p,m)$. The Fourier-Bessel expansion of $\tilde{f}(p,m;x)$ is given in terms of the coefficients (14). Using the well-known relation [31]

$$\frac{x^p}{2} \sim \sum_{j=1}^{\infty} \frac{z_j^{-1}}{J_{p+1}(z_j)} J_p(z_j x), \qquad (18)$$

together with Eqs. (9) and (15) we find $\tilde{f}(p,0;x) = x^p/2$. Therefore, from Eq. (17) we see that $S(p,0) = 2^{p-1} p!$. In or-

der to compute $\tilde{f}(p,m;x)$ for $m \geq 1$ we first note that, as shown in Appendix A,

$$x^p \int_x^1 \frac{du}{u^{2p+1}} \int_0^u dv\, v^{2p+1} \tilde{f}(p,m;v) \sim \sum_{j=1}^{\infty} \frac{1}{z_j^2} c_j(p,m) J_p(z_j x). \qquad (19)$$

Also, one sees from the definition (14) that the relation

$$c_j(p,m+1) = \frac{1}{z_j^2} c_j(p,m), \qquad (20)$$

holds. Therefore, the left-hand side of Eq. (19) defines a function whose Fourier-Bessel expansion is $\tilde{S}(p,m+1;x)$, i.e.,

$$\tilde{f}(p,m+1;x) = x^p \int_x^1 \frac{du}{u^{2p+1}} \int_0^u dv\, v^{p+1} \tilde{f}(p,m;v), \qquad (21)$$

or, in a more symmetric form,

$$f(p,m+1;x) = \int_x^1 \frac{du}{u^{2p+1}} \int_0^u dv\, v^{2p+1} f(p,m;v). \qquad (22)$$

This relation allows one to generate the $f(p,m;x)$'s recursively from $f(p,0;x) = 2^{p-1} p!$. In fact, it is possible to prove (see Appendix B) that

$$f(p,m;x) = \frac{(-1)^m (p!)^2 x^{2m}}{2^{2m+1-p} m! (m+p)!} - \sum_{k=1}^{m} \frac{(-1)^k p!}{2^{2k} k! (k+p)!} f(p,m-k;x) \qquad (23)$$

so that $f(p,m;x)$ is a polynomial of degree $2m$. From the above recursion we get, for example,

$$f(p,1;x) = 2^{p-1} p! \frac{1-x^2}{4(1+p)}, \qquad (24)$$

and

$$f(p,2;x) = 2^{p-1} p! \frac{3+p-2(2+p)x^2+(1+p)x^4}{32(1+p)^2(2+p)}. \qquad (25)$$

Taking the limit $x \to 0^+$ in Eq. (23) and using the definition (17) gives

$$S(p,m) = p! \sum_{k=1}^{m} \frac{(-1)^{k+1}}{2^{2k} k! (k+p)!} S(p,m-k), \qquad (26)$$

with $S(p,0) = 2^{p-1} p!$.

III. THREE SUBDIFFUSION PROBLEMS WHERE THE SERIES $S(p,m)$ AND $\tilde{S}(p,m;x)$ APPEAR

As anticipated in the Introduction, in the present section we shall consider the subdiffusive version of three standard d-dimensional diffusion problems whose solution involves the Bessel series $S(p,m)$ or $\tilde{S}(p,m;x)$. The three problems considered have spherical symmetry and an absorbing sur-

face, i.e., a surface on which the solution $c(r,t)$ must be zero at any time t.

A. Survival probability of a subdiffusive particle starting at the center of a hypersphere with absorbing surface

The numerical Bessel series $S(p,m)$ appears in the first problem we shall consider, namely, the calculation of the probability (survival probability) $W(R,t)$ that a subdiffusive particle starting at the center of a d-dimensional hypersphere of radius R has not reached its absorbing surface by time t [13,23,24]. This problem was addressed, but only partially solved, in the appendix of Ref. [24]. In this section we solve it in full. The solution for this subdiffusive version of the escape problem can be found by separation of variables (or eigenfunction method) [32]. For a generic initial concentration $c(r,0)=c_0(r)$ one gets

$$c(r,t) = \sum_{j=1}^{\infty} a_j r^{1-d/2} J_{d/2-1}(z_j r/R) E_\gamma\left[-\left(\frac{z_j}{R}\right)^2 K_\gamma t^\gamma\right]. \quad (27)$$

(more details can be found in the appendix of [24]). By virtue of the orthogonality properties for the Bessel functions $\int_0^1 x J_\alpha(z_j x) J_\alpha(z_m x) dx = J_{\alpha+1}^2(z_j)\delta_{m,j}/2$, the coefficients a_j can be expressed as

$$a_j = \frac{2}{R^2 J_{d/2}^2(z_j)} \int_0^R r^{d/2} c_0(r) J_{d/2-1}(z_j r/R) dr. \quad (28)$$

For the present case where one deals with a single point particle starting from the center of the hypersphere one has $c(r,0)=s_d^{-1}(r)\delta_+(r)$, where $\delta_+(r)$ is the slightly modified Bessel function with $\int_0^R \delta_+(r)dr=1$, and $s_d(r)=2\pi^{d/2}r^{d-1}/\Gamma(d/2)$ is the surface of a d-dimensional hypersphere of radius r. In this case Eq. (27) becomes

$$c(r,t) = \sum_{j=1}^{\infty} \left(\frac{z_j}{2R}\right)^{d/2-1} \frac{r^{1-d/2}}{\pi^{d/2}R^2 J_{d/2}^2(z_j)} J_{d/2-1}\left(\frac{z_j r}{R}\right)$$
$$\times E_\gamma\left[-\left(\frac{z_j}{R}\right)^2 K_\gamma t^\gamma\right]. \quad (29)$$

Using the asymptotic expansion (5), one gets for long times

$$c(r,t) = \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{\Gamma(1-m\gamma)}\left(\frac{R^2}{K_\gamma t^\gamma}\right)^m \Psi_m(r), \quad (30)$$

where the long-time subdiffusion modes are

$$\Psi_m(r) = \frac{(2r)^{1-d/2}}{\pi^{d/2}R^{d/2+1}} \sum_{j=1}^{\infty} \frac{z_j^{d/2-2m-1}}{J_{d/2}^2(z_j)} J_{d/2-1}\left(\frac{z_j r}{R}\right). \quad (31)$$

The survival probability $W(R,t)$ we are interested in straightforwardly follows as

$$W(R,t) = \int_0^R s_d(r) c(r,t) dr$$
$$= \frac{2^{2-d/2}}{\Gamma(d/2)} \sum_{j=1}^{\infty} \frac{z_j^{d/2-2}}{J_{d/2}(z_j)} E_\gamma\left[-\left(\frac{z_j}{R}\right)^2 K_\gamma t^\gamma\right]. \quad (32)$$

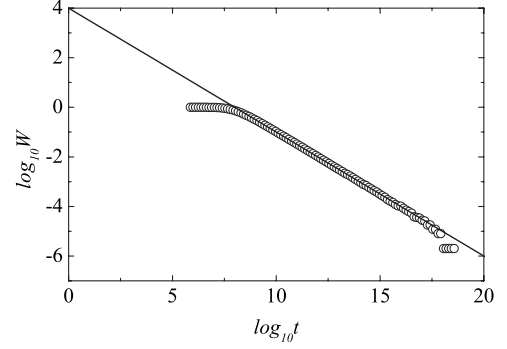To obtain the long-time survival probability (long-time reac-

FIG. 1. Simulation results (symbols) for the survival probability of a subdiffusive particle with diffusion exponent $\gamma=0.5$ in an eight-dimensional sphere of radius $R=100$ with absorbing surface. The particle starts moving from the center of the hypersphere. We carried out 5×10^5 realizations. The solid line $\log_{10} W = 4 - \frac{1}{2}\log_{10} t$ is obtained from the exact asymptotic prediction given by Eq. (36).

tion kinetics) we insert the asymptotic expansion (5) of the Mittag-Leffler function into Eq. (32):

$$W(R,t) \approx \frac{2^{2-d/2}}{\Gamma(d/2)} \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{\Gamma(1-m\gamma)}\left(\frac{R^2}{K_\gamma t^\gamma}\right)^m \sum_{j=1}^{\infty} \frac{z_j^{d/2-2m-2}}{J_{d/2}(z_j)}, \quad (33)$$

or, using Eq. (10),

$$W(R,t) \approx \frac{2^{2-d/2}}{\Gamma(d/2)} \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{\Gamma(1-m\gamma)}\left(\frac{R^2}{K_\gamma t^\gamma}\right)^m S(d/2-1,m). \quad (34)$$

where the values of the coefficients $S(d/2-1,m)$ can be evaluated by means of Eq. (26). In particular, the first two terms are explicitly given by the result

$$W(R,t) = \frac{1}{2d\Gamma(1-\gamma)}\frac{R^2}{K_\gamma t^\gamma} - \frac{4+d}{8d^2(2+d)\Gamma(1-2\gamma)}\left(\frac{R^2}{K_\gamma t^\gamma}\right)^2$$
$$+ O\left(\frac{R^2}{K_\gamma t^\gamma}\right)^3. \quad (35)$$

When the subdiffusive particle is described by means of the CTRW model [14] with the Pareto waiting time distribution $\psi(t)=\gamma/(1+t)^{1+\gamma}$, the diffusion constant becomes $K_\gamma=1/[2d\Gamma(1-\gamma)]$, and the leading term of the asymptotic survival probability nicely simplifies to

$$W(R,t) \approx \frac{R^2}{t^\gamma}. \quad (36)$$

In Fig. 1 we compare this prediction with simulation results for $d=8$. We chose this value of the dimension because we know that in this case the series $S(3,1)$ used to compute the numerical coefficient of the leading term of $W(R,t)$ in Eq. (34) is divergent (see Table I) in spite of the fact that it must be associated with a finite physical value. The simulations were carried out using a CTRW model with Pareto waiting times and the anomalous diffusion exponent $\gamma=1/2$. As one

can see, the agreement between theory and simulation is excellent.

It is interesting to note that the result (35) might have been obtained in a different way. Indeed, one can show that the Laplace transform $\hat{W}(R,u) = \int_0^\infty W(R,t)e^{-ut}dt$ of the survival probability in the above problem reads

$$\hat{W}(R,u) = \frac{1}{u} - \frac{2^{1-d/2}}{u} \frac{(u^\gamma R^2/K_\gamma)^{(d/2-1)/2}}{\Gamma(d/2)I_{d/2-1}(\sqrt{u^\gamma R^2/K_\gamma})}. \quad (37)$$

This result is essentially obtained by taking the Laplace transform of the adjoint fractional diffusion equation, integrating over the interior of the hypersphere, and solving the resulting equation with the pertinent boundary condition (this procedure is described in detail in Ref. [12] for a subdiffusive version of the target problem). Note that this result for the anomalous diffusion case could have been obtained from the normal diffusion case by performing the simple replacement $u \rightarrow u^\gamma$ in the expression for $u\hat{W}(R,u)$ [8,14]. At this point we can use the series expansion of the Bessel function $I_{d/2-1}$ [33] to write Eq. (37) as

$$\hat{W}(R,u) = \frac{1}{u} - \frac{1}{u} \frac{1}{\Gamma(d/2)} \left[\sum_{k=0}^\infty \frac{(R^2/4K_\gamma)^k}{k!\Gamma(d/2+k)} u^{k\gamma} \right]^{-1}, \quad (38)$$

or, equivalently, as

$$u\hat{W}(R,u) = \frac{1}{2d} \frac{R^2 u^\gamma}{K_\gamma} - \frac{(d+4)}{8(d+2)d^2} \left(\frac{R^2 u^\gamma}{K_\gamma} \right)^2 + \mathcal{O}\left(\frac{R^2 u^\gamma}{K_\gamma} \right)^3. \quad (39)$$

Inverting term-by-term this expression, we immediately recover the asymptotic large-t behavior predicted by Eq. (35).

B. Homogeneous distribution of particles inside a hypersphere with absorbing surface

The physical system in our second example is the same as in the previous one, except that we now consider a homogeneous initial concentration of particles $c(r,0) = c_0$ [13,34]. Using

$$\int_0^R r^{d/2} J_{d/2-1}\left(\frac{z_j r}{R} \right) dr = \frac{R^{d/2+1} J_{d/2}(z_j)}{z_j}, \quad (40)$$

in Eq. (28) and inserting the resulting expression into Eq. (27) one easily finds

$$c(r,t)/c_0 = 2(r/R)^{1-d/2} \sum_{j=1}^\infty \frac{J_{d/2-1}(z_j r/R)}{z_j J_{d/2}(z_j)} E_\gamma[-(z_j/R)^2 K_\gamma t^\gamma]. \quad (41)$$

For long times, one can use the expansion Eq. (5) in Eq. (41) and get

$$c(r,t)/c_0 = \sum_{m=1}^\infty \frac{(-1)^{m+1}}{\Gamma(1-m\gamma)} \left(\frac{R^2}{K_\gamma t^\gamma} \right)^m \Psi_m(r), \quad (42)$$
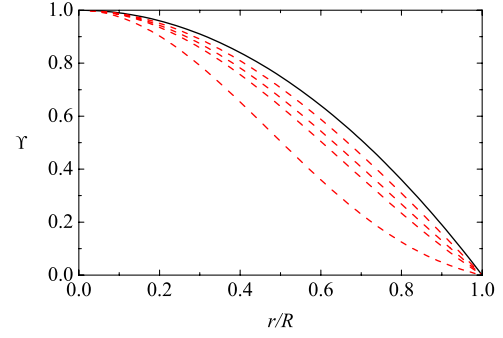

FIG. 2. (Color online) Profile of the long-time asymptotically dominant mode $\Upsilon(r)$ for anomalous diffusion (solid line) and normal diffusion (dashed lines). The dashed lines correspond to $d = 1,2,3,8$ with increasing dimensionality from top to bottom. In order to facilitate the comparison, all curves have been rescaled so as to take the value unity at the origin.

where, upon use of the definitions (9) and (15), the long-time subdiffusion modes can be written in closed form in terms of the functions $\tilde{f}(p,m;x)$:

$$\Psi_m(r) = 2(r/R)^{1-d/2} \tilde{f}(d/2-1,m;r/R). \quad (43)$$

Regarding the behavior of the long-time dominant mode, one sees that it satisfies $c(r,t)/\varphi(t) \propto \Upsilon(r)$, where $\varphi(t) = \exp[-z_1 K t^\gamma/R^2]$ for normal diffusion and $\varphi(t) = 1/(K t^\gamma/R^2)$ for anomalous diffusion. Most remarkably, one has $\Upsilon(r) = \psi_1(r) = (r/R)^{1-d/2} J_{d/2-1}(z_1 r/R)$ for normal diffusion and [see Eq. (24)]

$$\Upsilon(r) = \Psi_1(r) \propto f(d/2-1,1;r/R) \propto 1 - r^2/R^2, \quad (44)$$

for anomalous diffusion, i.e., the concentration profile at late times $\Psi_1(r)$ is different from that of the normal diffusion case and its form *does not* depend either on the dimension d or on γ. In conclusion, a minute amount of subdiffusivity in the particle motion is seen to destroy the form $(r/R)^{1-d/2} J_{d/2-1}(z_1 r/R)$ of the long-time normal diffusion mode and leads to the subdiffusive form $1 - r^2/R^2$ which holds for *any* $\gamma < 1$. In Fig. 2 we show a comparative plot of the long-time profiles $\Upsilon(r)$ induced by normal diffusion ($\gamma = 1$) and by anomalous diffusion ($\gamma < 1$) for different values of d.

The aforementioned singular long-time behavior of the solution with respect to γ is not an exclusive feature of the escape problem. A similar behavior has also been observed when calculating the survival probability of a diffusing particle in a sea of mobile traps. In Refs. [10,21,22,24] it is shown that the survival probability displays a crossover between two different asymptotic regimes: for $\gamma = 1$ one has a Donsker-Varadhan decay law characteristic of the trapping problem (where a mobile particle can be annihilated upon contact with immobile traps), while for $\gamma < 1$ one has Bramson-Lebowitz behavior associated to the target problem (where an immobile particle or "target" surrounded by mobile traps is annihilated upon contact with the latter) [24].

C. Source of particles inside a hypersphere with absorbing surface

The setting of our third and last example consists of a homogeneous source of particles of strength Q placed in a hypersphere of radius R with absorbing surface [13,34] and zero initial concentration of particles. The temporal evolution of the concentration is described by the reaction-subdiffusion equation [34]

$$\frac{\partial c(r,t)}{\partial t} = K_{\gamma\,0} D_t^{1-\gamma} \left(\frac{\partial^2 c(r,t)}{\partial r^2} + \frac{d-1}{r} \frac{\partial c(r,t)}{\partial r} + Q \right). \quad (45)$$

The solution reads

$$\frac{K_\gamma c(r,t)}{QR^2} = \frac{1 - r^2/R^2}{2d} - 2\left(\frac{r}{R}\right)^{1-d/2}$$

$$\times \sum_{j=1}^{\infty} \frac{J_{d/2-1}(z_j r/R)}{z_j^3 J_{d/2}(z_j)} E_\gamma\left(-\frac{z_j^2 K_\gamma t^\gamma}{R^2}\right). \quad (46)$$

Using Eqs. (5), (9), and (15), one arrives at the long-time result

$$\frac{K_\gamma c(r,t)}{QR^2} = \frac{1 - r^2/R^2}{2d} - \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{\Gamma(1-m\gamma)} \left(\frac{R^2}{K_\gamma t^\gamma}\right)^m \Psi_m(r), \quad (47)$$

where the long-time subdiffusion modes can again be written in closed form in terms of the functions $\tilde{f}(p,m;x)$:

$$\Psi_m(r) = 2(r/R)^{1-d/2} \tilde{f}(d/2-1, m+1; r/R). \quad (48)$$

If one only retains the leading term of the analytic expression describing the approach to the stationary profile, one obtains

$$\left[\frac{K_\gamma c(r,t)}{QR^2} - \frac{1}{2d}(1 - r^2/R^2) \right] / \varphi(t) \propto \Upsilon(r). \quad (49)$$

Here, one has $\Upsilon(r) = \psi_1(r) = (r/R)^{1-d/2} J_{d/2-1}(z_1 r/R)$ when $\gamma = 1$ (as in our previous example of Sec. III B) and

$$\Upsilon(r) = \Psi_1(r) \propto f(d/2-1, 2; r/R) \propto 4 + d - 2(d+2)(r/R)^2 + d(r/R)^4, \quad (50)$$

in the anomalous diffusion case $(0 < \gamma < 1)$ [cf. Eq. (25)]. Note that the form of the dominant subdiffusion mode $\Psi_1(r)$ describing the decay to the stationary concentration profile depends on the dimension d, as opposed to the example in the previous subsection [cf. Eq, (44)]. In Fig. 3 we show a comparison of the long-time profiles $\Upsilon(r)$ for $d = 1, 2, 3$, and 8. In spite of the different analytic expressions for $\Upsilon(r)$, the similarity between the diffusive and the subdiffusive profiles is remarkable, especially in lower dimensions. This suggests that the impact of memory effects is smaller in the presence of a particle source than in its absence.
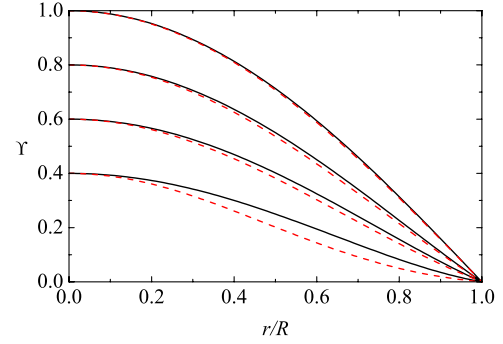

FIG. 3. (Color online) Form of the long-time dominant decay mode $\Upsilon(r)$ for anomalous diffusion (solid lines) and normal diffusion (dashed lines) in the particle source problem. The solid and dashed lines correspond to $d = 1, 2, 3, 8$ with increasing dimensionality from top to bottom. In order to facilitate the comparison, the respective profiles have been normalized to take the values 1, 0.8, 0.6, and 0.4 at $r = 0$.

IV. CONCLUSIONS

We have considered the long-time solution $c(r,t)$ of fractional diffusion problems with anomalous diffusion exponent $\gamma < 1$ (subdiffusion problems). To find this solution is tantamount to finding the "long-time subdiffusion modes" $\Psi_n(r)$ as the solution can be expressed as a weighted superposition of $\Psi_n(r)$, the weight being proportional to $t^{-n\gamma}$. Remarkably, the functions $\Psi_n(r)$ do not depend on γ, but depend on the details of the initial condition as they are linear superpositions of *all* normal diffusive modes $\psi_n(r)$ needed to construct the initial condition. This has a remarkable consequence: it is well-known that for normal diffusion the influence of the initial conditions on the solution rapidly fades away and at long times only the first normal diffusion mode $\psi_1(r)$ survives; similarly, in the equivalent subdiffusion problem, at long times only the first subdiffusion mode $\Psi_1(r)$ survives, but note that even for very long times the form of the initial condition plays a key role in the subdiffusive solution as the particular form of $\Psi_1(r)$ depends on the initial condition. Finally, as the long-time dominant behavior of the solution is described by $\Psi_1(r)$ for the subdiffusion case $(\gamma < 1)$ and by $\psi_1(r)$ for the normal diffusion solution $(\gamma = 1)$, and because $\Psi_1(r)$ is independent of γ, we find that an interesting crossover occurs when switching from $\gamma < 1$ to $\gamma = 1$ in the long-time solution.

In this paper, we have studied in detail the long-time solution $c(r,t)$ of two fractional d-dimensional subdiffusion problems with radial symmetry and a hyperspherical absorbing surface. In the first problem, there is an initial homogeneous concentration of particles. In the second, there is a homogeneous source of particles in a medium initially devoid of particles. The solution is given in terms of the long-time subdiffusion modes $\Psi_n(r)$ which take the form of Fourier-Bessel series $S(d/2-1, n; r)$ whose coefficients involve both Bessel functions and their zeros: $S(p,n;r) \equiv \sum_{j=1}^{\infty} z_j^{-2n-1} J_p(z_j r) / J_{p+1}(z_j)$. These series may become divergent in sufficiently high dimensions, so that regularization methods are needed to recover their correct values. We have been able to sum these series, and have shown that $S(p,n;r)$,

i.e., $\Psi_n(r)$, is given by a polynomial $f(p,n,r)$ of degree $2n$. These polynomials can easily be computed by means of the recursive formula (23). For the two examples considered, and especially in the first example, the difference between the dominant normal diffusive mode and the dominant sub-diffusive mode becomes increasingly large as d increases.

The third problem we have considered is the so-called escape problem of a single particle initially located at the center of a d-dimensional hypersphere of radius R with absorbing surface. Here we are interested in the survival probability $W(R,t)$ of the particle. In the solution of this problem there again appears a (numerical) series $S(d/2-1,n)$ whose coefficients involve both Bessel functions and their zeros: $S(p,n) \equiv \sum_{j=1}^{\infty} z_j^{p-2n-1}/J_{p+1}(z_j)$. As in the previous examples, such series are divergent in sufficiently high dimensions, and regularization methods are again necessary to sum them. They were summed by means of a procedure based on the use of Bessel functions as regulators. These sums can be computed recursively by means of the formula (26).

In view of the results in Ref. [34], we expect that some of the techniques employed here may be relevant not only for subdiffusion problem ($\gamma < 1$), but also for diffusion-wave equations where $1 \leq \gamma \leq 2$. This is certainly a promising avenue for future research.

ACKNOWLEDGMENTS

APPENDIX A: RECURSION RELATION FOR THE FOURIER-BESSEL COEFFICIENTS OF $\tilde{f}(p,m;x)$

The Fourier-Bessel coefficients of the m-th order function $\tilde{f}(p,m;x)$ are given by Eq. (14). Our goal is to show that the Fourier-Bessel coefficients of the function

$$\tilde{f}(p,m+1;x) = x^p \int_x^1 \frac{du}{u^{2p+1}} \int_0^u dv\, v^{p+1}\tilde{f}(p,m;v), \quad \text{(A1)}$$

satisfy the recursion relation (20). Making the change of variable $y = z_j x$, the Fourier-Bessel coefficients $c_j(p,m)$ of $\tilde{f}(p,m;v)$ can be expressed as follows:

$$c_j(p,m) = \frac{2}{J_{p+1}^2(z_j)} \int_0^1 x\tilde{f}(p,m;x)J_p(z_jx)dx. \quad \text{(A2)}$$

Thus, they can be written as $c_j(p,m) = 2z_j^{-2}\hat{c}_j(p,m)/J_{p+1}^2(z_j)$ with

$$\hat{c}_j(p,m) = \int_0^{z_j} yJ_p(y)\tilde{f}(p,m;y/z_j)dy. \quad \text{(A3)}$$

Therefore, to prove Eq. (20) is equivalent to proving $\hat{c}_j(p,m+1) = \hat{c}_j(p,m)/z_j^2$. Using $y^{p+1}J_p(y) = d[y^{p+1}J_{p+1}(y)]/dy$, one can rewrite Eq. (A3) as

$$\hat{c}_j(p,m+1) = \int_0^{z_j} \frac{d}{dy}[y^{p+1}J_{p+1}(y)]y^{-p}\tilde{f}(p,m+1;y/z_j)dy. \quad \text{(A4)}$$

Integrating by parts, the boundary terms are seen to vanish since, by Eq. (A1), $\lim_{x\to 1}\tilde{f}(p,m+1;x) = 0$. Next, inserting Eq. (A1) into the resulting expression we find

$$\hat{c}_j(p,m+1) = z_j^p \int_0^{z_j} dy\frac{J_{p+1}(y)}{y^p}\int_0^{y/z_j} dv\, v^{p+1}\tilde{f}(p,m;v). \quad \text{(A5)}$$

We can now make use of the relation $J_{p+1}(y)/y^p = -d[J_p(y)/y^p]/dy$ in the integrand and integrate by parts one more time. Once again, the boundary terms are seen to vanish: when y tends to z_j one trivially has $J_p(y) \to 0$ and when y goes to 0 one has $y^{-p}J_p(y)\int_0^{y/z_j}dv\,v^{p+1}\tilde{f}(p,m;v) \to 0$. The reason is that the prefactor of the integral goes to a constant because of the behavior of the Bessel functions for small arguments; the integral itself goes to zero as the integration interval shrinks, because the functions $\tilde{f}(p,m;v)$ are well-behaved polynomials. Thus, one is finally left with the identity $\hat{c}_j(p,m+1) = \hat{c}_j(p,m)/z_j^2$, as we aimed to show.

APPENDIX B: RECURSION RELATION FOR $f(p,m;x)$

Using a more formal language, one can rewrite Eq. (22) as

$$f(p,m+1;x) = \Lambda[f(p,m;x)], \quad \text{(B1)}$$

where we have presented the operator

$$\Lambda[f(p,m;x)] = \int_x^1 du\frac{1}{u^{2p+1}}\int_0^u dv\, v^{2p+1}f(p,m;v). \quad \text{(B2)}$$

Using the recursion relation (B1) repeatedly, we find

$$\Lambda[f(p,m;x)] = \Lambda^m[f(p,0;x)]. \quad \text{(B3)}$$

Since $f(p,0;x) = 2^{p-1}p!$, we get

$$f(p,m;x) = \Lambda^m(2^{p-1}p!) = 2^{p-1}p!\Lambda^m(1). \quad \text{(B4)}$$

We can now show by induction that

$$\Lambda^m(1) = \frac{(-1)^m p! x^{2m}}{2^{2m}m!(m+p)!} - \sum_{k=1}^{m}\frac{(-1)^k p!}{2^{2k}k!(k+p)!}\Lambda^{m-k}(1) \quad \text{(B5)}$$

holds for all $m \in \mathbb{N}$. For $m=1$ one can easily show by integration that the statement is correct:

$$\Lambda(1) = \frac{1-x^2}{2(2+2p)} \quad \text{(B6)}$$

Assuming that the statement holds for $m-1$, and taking into account that $\Lambda(x^{2m-2}) = (1-x^{2m})/[4m(m+p)]$ and $\Lambda^0(1) = 1$, one finds

$$\Lambda^m(1) = \Lambda[\Lambda^{m-1}(1)]$$

$$= \frac{(-1)^{m-1}p!\Lambda(x^{2m-2})}{2^{2m-2}(m-1)!(m-1+p)!}$$

$$- \sum_{k=1}^{m-1} \frac{p!(-1)^k}{2^{2k}k!(k+p)!}\Lambda^{m-k}(1)$$

$$= -\frac{(-1)^m p!\Lambda^0(1)}{2^{2m}m!(m+p)!} + \frac{(-1)^m p!x^{2m}}{2^{2m}m!(m+p)!}$$

$$- \sum_{k=1}^{m-1} \frac{(-1)^k p!}{2^{2k}k!(k+p)!}\Lambda^{m-k}(1)$$

$$= \frac{(-1)^m p!x^{2m}}{m!(m+p)!2^{2m}} - \sum_{k=1}^{m} \frac{(-1)^k p!}{2^{2k}k!(k+p)!}\Lambda^{m-k}(1),$$

as we intended to show. Multiplying Eq. (B5) by $2^{p-1}p!$ and making use of the representation (B4), Eq. (23) follows.

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