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Fractional diffusion: exact representations of spectral functions

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Abstract. For all the relevant transformed spaces, i.e. Fourier, Laplace and Fourier–Laplace, we present *exact* solutions of a fractional diffusion equation, describing random transport on fractals. The potential importance of such spectral representations lies in their applications to interpreting experimental measurements of anomalous diffusion processes. In contrast to the well known asymptotic results, the exact representations provide a much broader basis for comparison with data.

Relaxation (Schiessel *et al* 1995) as well as diffusion (Havlin and Ben-Avraham 1987) processes in complex systems show deviations from the standard (Debye or Fickean) laws, respectively. Substituting for the Markovian nature, a straightforward way to incorporate memory effects is the modification of the corresponding differential equations by use of fractional calculus, modelling memory as a long (Lévy) tail. Anomalous diffusion is characterized via the mean square displacement

$$\langle r^2(t)\rangle \propto t^{2/d_w} \tag{1}$$

deviating from the 'normal' linear dependence on time, if the anomalous diffusion exponent, d_w, differs from 2. For diffusion on fractals one finds $d_w > 2$. The returning probability of a random walker to the origin is decaying like

$$P(r=0,t) \propto t^{-d_s/2} \tag{2}$$

where $d_s = 2d_f/d_w$ is the spectral (fracton) dimension; d_f is the fractal dimension of the underlying structure. Much effort has been spent on obtaining the asymptotic shape of the position probability density $P(r,t)$ displayed by a random walker. The asymptotes under discussion are of stretched exponential nature:

$$P_i(r,t) \sim t^{-d_s/2}\xi^{\alpha_i}\exp\left(-c_i\xi^{u_i}\right) \tag{3}$$

where the connection to the different models is given in table 1. $\xi = rt^{-1/d_w}$ is the unequivocal similarity variable. Regarding α arbitrary, the case Gen is the most general model which may be discussed on the basis of equation (3), for the case $u = d_w/(d_w-1)$. A detailed discussion of the power law prefactor ξ^{α_i} may be found in Roman and Alemanyi (1994), Roman (1995). The influence of the number of configurations, taken into account in the averages, on $P(r,t)$ is investigated in Bunde and Draeger (1995).

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Table 1. Asymptotic parameters for the various models discussed (cf equation (3)): OP (O'Shaugnessy and Procaccia 1985), KZB (Klafter *et al* 1991, Roman and Alemanyi 1994), M (Metzler *et al* 1994, see also Schneider and Wyss 1989 and Giona and Roman 1992) and Gen.

	α_i	u_i
OP	0	d_w
KZB	$(d_f - d_w/2)/(d_w - 1)$	$d_w/(d_w - 1)$
M	0	$d_w/(d_w - 1)$
Gen	$(d_f - Dd_w/2)/(d_w - 1)$	$d_w/(d_w - 1)$

Table 2. Identification of the occurring parameters (see equation (4)) for the different models discussed.

	M	KZB	Gen	OP
Θ	0	0	0	$d_w - 2$
γ	$2/d_w$	$2/d_w$	$2/d_w$	1
D	d_s	1	D	d_f

To account for the scaling power ξ^{α_i} in equation (3), let us regard the generalized diffusion equation (Metzler *et al* 1994 with $\alpha = 0$)

$$\frac{\partial^\gamma P(r,t)}{\partial t^\gamma} = r^{1-D}\frac{\partial}{\partial r} r^{D-1} r^{-\Theta}\frac{\partial}{\partial r} P(r,t) \tag{4}$$

which involves a fractional t-derivative of order γ, a modified Laplacian operator with fractal order D, and $r^{-\Theta}$ being a possibly non-constant diffusion coefficient. Some comments on equation (4) and its connection to CTRW are given by Shlesinger (1995). The solution procedure of equation (4), shown in Metzler *et al* (1994), remains valid and the propagator is given, in terms of Fox's H-functions:

$$P(r,t) = \frac{A}{t}\left(r^{\frac{2+\Theta}{2}}\right)^{\frac{2}{\gamma}-\frac{2d_f}{2+\Theta}} H^{20}_{12}\left[\frac{r^{(2+\Theta)/\gamma}}{(2+\Theta)^{2/\gamma}t}\,\middle|\, \begin{matrix} (0,1) \\ \left(1-\frac{1}{\gamma}+\frac{d_f-D}{2+\Theta},\frac{1}{\gamma}\right),\left(\frac{d_f}{2+\Theta}-\frac{1}{\gamma},\frac{1}{\gamma}\right)\end{matrix}\right] \tag{5}$$

with A being the normalization constant. The occurring parameters may now be reduced by considering the conditions (1)–(3). One thus arrives at the identification of the parameters for the different models listed in table 2. The model Gen leaves α open, according to the discussion in Roman (1995), and embraces the more special models M and KZB. The single restriction for D is that it must reduce to the Euclidean dimension d if the standard Fickean case ($d_w \to 2$, $d_f \to d \in \mathbb{N}$) shall be recovered. For $\alpha = u(d_s/2 - D/2)$, as suggested in Klafter *et al* (1991), one is led to the peculiar constraint that D must equal 1 for the standard Fickean pendant. The reason is shown below.

The advantage of the present approach involving H-functions which may seem rather complicated is, that equation (4) can be solved in closed form, and the spectral functions can also be calculated *exactly*. Thus, one can find access to more than only the $\xi \gg 1$ asymptote: to the $\xi \ll 1$ and the transition region. The exact solutions for $P(r,t)$ and its spectral functions provide increased information for comparison with experimental or computer data. We do not hesitate mentioning that the presented equation (4) remains valid, even in the intermediate ultradiffusive regime in between standard ($d_w = 2$) and ballistic ($d_w = 1$) transport (West *et al* 1996).

Table 3. Asymptotic expansions for the different transform domains where $H^{m,n}_{p,q}(z) = \mathcal{O}(z^c)$ for $z \ll 1$ and $H^{m,n}_{p,q}(z) = \mathcal{O}(z^d)$ for $z \gg 1$. Here, $\mathcal{O}$ denotes the Landau symbol.

	z	c	d
$P^*(k,t)$	$kt^{\gamma/(2+\Theta)}$	0	$\max(-d_f, -2-\Theta+D-d_f)$
$r^{\tilde{d}-(2+\Theta)/\gamma}\tilde{P}(r,s)$	$r^{(2+\Theta)/\gamma}s$	$\gamma \min\left(1-\frac{1}{\gamma}+\frac{d_f-D}{2+\Theta}, \frac{d_f}{2+\Theta}-\frac{1}{\gamma}\right)$	$z^{\gamma(\alpha-1/2)/2}\exp -dz^{\gamma/2}$
$s\tilde{P}^*(k,s)$	$ks^{-\gamma/(2+\Theta)}$	0	$\max(-d_f, -2-\Theta+D-d_f)$

The modified Laplacian in equation (4) may be written as $(\mathrm{d}V_{\text{eff}}/\mathrm{d}r)^{-1}\partial/\partial r(\mathrm{d}V_{\text{eff}}/\mathrm{d}r)\,\partial/\partial r$, involving the *effective volume* V_{eff} as sensed by the wiggling random walker. Identifying $V_{\text{eff}} \propto r^D$, $D < d_f$ suggests that the walker senses a smeared-out structure. Thus, it is a matter of importance to have at hand adequate information—either by simulations or by very precise experimental measurements—on the 'true' shape of $P(r,t)$, i.e. which D is significant for the actually underlying structure, see also Roman (1995) in this connection. As our closed form solution for $P(r,t)$ includes the $\xi \ll 1$ and the *transition region* towards $\xi \gg 1$ it should be significantly better for comparisons with data than the mere stretched exponential asymptote, or the asymptotic power-laws in the transformed spaces.

For the discussion of the asymptotic probability density in the Laplace domain, let us first consider the Gaussian position probability density

$$P(r,t) = (2\pi t)^{-d/2}\exp\left(-\frac{r^2}{4t}\right) \tag{6}$$

in $d \in \mathbb{N}$ dimensions, and its Laplace transform

$$\tilde{P}(r,s) = \pi^{-d/2}r^{(2-d)/2}s^{(d-2)/4}K_{d/2-1}(rs^{1/2}) \sim r^{(1-d)/2}s^{(d-3)/4}\exp -rs^{1/2} \tag{7}$$

which involves the Bessel function K. Guyer's result (Guyer 1984) in the Laplace domain

$$\tilde{P}_{\text{Guy}} \sim s^{d_s/2-1}\exp -ars^{1/d_w} \tag{8}$$

upon which Klafter *et al* (1991) base their research, it does not include the prefactor $(rs^{1/2})^{(1-d)/2}$ before the exponential in comparison with equation (7). But the models previously labelled OSP, M, and Gen reduce exactly to the Laplace transformed Gaussian, equation (7). Especially for the model Gen one finds

$$\tilde{P}(r;s) \propto (rs^{1/d_w})^{1-D/2}s^{d_s/2-1}K_{1-D/2}(rs^{1/d_w}) \sim (rs^{1/d_w})^{(1-D)/2}s^{d_s/2-1}\exp(-rs^{1/d_w}). \tag{9}$$

For a proper description in Laplace space equation (9) should therefore be preferred to equation (8). It is exactly the choice of (8) instead of (9) that causes the failure of the KZB model to reduce to the transformed Gaussian for any integer dimension but 1.

Physical measurements mostly reveal not $P(r,t)$ but some spectral function, e.g. the Fourier transformed spectral density $P^*(k,t)$. Especially for these spectral functions relatively large ranges are experimentally accessible. It is there, where the transition region described by our results, significantly enhances the accuracy of data fits, a fact well known from asymptotic fractals. Therefore, we present the general integral transforms of (5) in closed form. This is made possible by use of the H-function (see appendix). Below, A denotes the appropriate normalization constant. The asymptotic behaviour of the calculated functions is summarized in table 3. All the occurring H-functions may be represented in a computable form by simply inserting the parameters into equation (A2). This can be done conveniently with a `Mathematica` program.

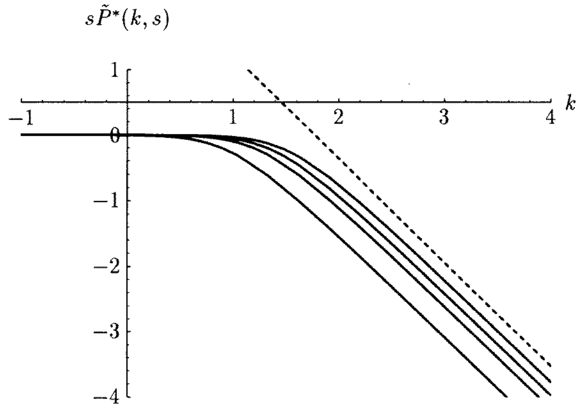

Figure 1. Fourier–Laplace transform $\tilde{P}^*(k,s)$ for $s = 100$, 500, 1000, 2000 (bottom to top) and $d_f = 1.58$, $d_w = 2.32$ in log–log representation. The broken line indicates the long-tail power law $\sim k^{-d_f}$. Note the late inset of the asymptotic power-law behaviour.

The fractal Fourier transform (see appendix) of $P(r,t)$, equation (5), is given by

$$P^*(k,t) = AH^{12}_{23}\left[(2+\Theta)^{2/(2+\Theta)}kt^{\gamma/(2+\Theta)}\left|\begin{matrix}\left(\frac{D-d_f}{2+\Theta},\frac{1}{2+\Theta}\right),\left(1-\frac{d_f}{2+\Theta},\frac{1}{2+\Theta}\right)\\ \left(0,\frac{1}{2}\right),\left(0,\frac{\gamma}{2+\Theta}\right),\left(-\frac{1}{2},\frac{1}{2}\right)\end{matrix}\right.\right]. \tag{10}$$

The Laplace transform of $P(r,t)$, equation (5), can either be written in terms of modified Bessel functions (Metzler *et al* 1994) or directly be expressed by the corresponding H-function:

$$\tilde{P}(r,s) = Ar^{(2+\Theta)/\gamma-d_f}H^{20}_{02}\left[\frac{r^{(2+\Theta)/\gamma}s}{(2+\Theta)^{2/(2+\Theta)}}\left|\left(1-\frac{1}{\gamma}+\frac{d_f-D}{2+\Theta},\frac{1}{\gamma}\right),\left(\frac{d_f}{2+\Theta}-\frac{1}{\gamma},\frac{1}{\gamma}\right)\right.\right]. \tag{11}$$

Finally, the Fourier–Laplace transform of equation (5) turns out to be

$$\tilde{P}^*(k,s) = \frac{A}{s}H^{12}_{22}\left[(2+\Theta)^{2/(2+\Theta)}ks^{-\gamma/(2+\Theta)}\left|\begin{matrix}\left(\frac{D-d_f}{2+\Theta},\frac{1}{2+\Theta}\right),\left(1-\frac{d_f}{2+\Theta},\frac{1}{2+\Theta}\right)\\ \left(0,\frac{1}{2}\right),\left(-\frac{1}{2},\frac{1}{2}\right)\end{matrix}\right.\right]. \tag{12}$$

It is worth mentioning that the reduction of this function to the standard Fickean case is accomplished easily for the H-function, using its standard properties.

Consulting table 2 one observes that, due to the choice of the volume element in the fractal Fourier transform, both P^* and $\tilde{P}^*$ show a horizontal asymptote, i.e. constant behaviour for $\xi \ll 1$. Thus, it is a reasonable generalization of the standard case and underlines the significance of the (k,s)-space. Figure 1 shows $\tilde{P}^*$ as an example. The inserted long-tail asymptote visualizes the relatively late inset of the calculated behaviour. This again shows the great importance of the knowledge of the transition region.

In this paper, ambiguities of existing theories have been discussed and a *new suggestion for the Laplace transform* of $P(r,t)$ has been presented. For the first time *exact solutions for the spectral functions* have been stated and given in a computable form. Nevertheless, real existing experimental evidence on the occurrence of the coupling of static space (d_f) and dynamics (d_w) in a fractional diffusion process is still outstanding. Taken from the formal mathematical manipulations, the presented exact solutions are the basis for reliable numerical investigations of experimental data.

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Appendix. Fox's H-function and fractal Fourier transform

Fox's H-function is defined in terms of a Mellin–Barnes-type integral, its mathematical definition and properties are compiled in Mathai and Saxena (1978). For a given H-function

$$H_{pq}^{mn}(z) = H_{pq}^{mn}\left[z \mid \begin{matrix} (a_1, A_1), (a_2, A_2), \ldots, (a_p, A_p) \\ (b_1, B_1), (b_2, B_2), \ldots, (b_q, B_q) \end{matrix}\right] \tag{A1}$$

the series expansion reads

$$H_{pq}^{mn}(z) = \sum_{h=1}^{m}\sum_{\nu=a}^{\infty} \frac{\prod_{j=1,\, j\neq h}^{m} \Gamma(b_j - B_j(b_h+\nu)/B_h)}{\prod_{j=m+1}^{q} \Gamma(1 - b_j + B_j(b_h+\nu)/B_h)} \times \frac{\prod_{j=1}^{n} \Gamma(1 - a_j + A_j(b_h+\nu)/B_h)}{\prod_{j=n+1}^{p} \Gamma(a_j - A_j(b_h+\nu)/B_h)} \frac{(-1)^{\nu} z^{(b_h+\nu)/B_h}}{\nu! B_h}. \tag{A2}$$

Applying integral transforms to a given H-function results in very convenient relations which only affect the occurring parameters (Glöckle and Nonnenmacher 1993).

To get an explicit expression for the Fourier transform on fractals one can rewrite the definition of a spherical N-dimensional ($N \in \mathbb{N}$) Fourier transform by use of the surface of the corresponding unit-hypersphere

$$\mathcal{F}_{(N)}\{f(r); q\} = (2\pi)^{-N/2} S_N(1) \int \mathrm{d}r\, r^{N-1} f(r) \frac{\sin qr}{qr} \tag{A3}$$

where $S_N(R) = 2\pi^{N/2} R^{N-1}/\Gamma(N/2)$ is well known from statistical mechanics. For a fractal hypersphere this relation is now—heuristically—generalized (Takayasu 1984) and usually written as $S_{\mathrm{f}}(R) = 2\pi^{d_f/2} R^{d_f-1}/\Gamma(d_f/2)$ so that a fractal volume element $\mathrm{d}V_{\mathrm{f}} = 2\pi^{d_f/2} r^{d_f-1}/\Gamma(d_f/2)\,\mathrm{d}r$ is recovered. Thus, the fractal Fourier transform is defined as

$$\mathcal{F}_{\mathrm{f}}\{f(r); q\} = (2\pi)^{-N/2} \frac{2\pi^{d_f/2}}{\Gamma(d_f/2)} q^{-1} \mathcal{F}_S\left\{r^{d_f-2} f(r); q\right\}. \tag{A4}$$

The fractal Fourier transform can be expressed by an ordinary Fourier sine transform.

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