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The similarity group and anomalous diffusion equations

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Abstract. A number of distinct differential equations, known as generalized diffusion equations, have been proposed to describe the phenomenon of anomalous diffusion on fractal objects. Although all are constructed to correctly reproduce the basic subdiffusive property of this phenomenon, using similarity methods it becomes very clear that this is far from sufficient to confirm their validity. The similarity group that they all have in common is the natural basis for making comparisons between these otherwise different equations, and a practical basis for comparisons between the very different modelling assumptions that their solutions each represent. Similarity induces a natural space in which to compare these solutions both with one another and with data from numerical experiments on fractals. It also reduces the differential equations to (extra-) ordinary ones, which are presented here for the first time. It becomes clear here from this approach that the proposed equations cannot agree even qualitatively with either each other or the data, suggesting that a new approach is needed.

1. Introduction

Anomalous diffusion occurs in a multitude of physical or other phenomena [1]. It is normally characterized microscopically by a time-dependent distribution of particles in space where the distance, r, a particle has moved in time t from its starting point is

$$\langle r^2(t)\rangle \propto t^\gamma \qquad (1)$$

where $\gamma \neq 1$. Such deviation from the normal diffusion behaviour ($\gamma = 1$) has for instance been observed for hydrogen diffusion in amorphous metals [2], diffusion of water in biological tissues [3] or in disordered systems [4] more generally. It has also been discussed in conjunction with the growth of thin films on a solid surface [5] and with the important class of diffusion processes on fractal structures [6].

It is by no means clear that all these different phenomena are due to the same underlying mechanisms [1]. It could well be that in the case of, say, the anomalous diffusion of adsorbed molecules at liquid surfaces [7] ($\gamma > 1$) completely different rules apply than for the case of diffusion on a fractal ($\gamma < 1$). Nonetheless most attempts, linear [8–10] and nonlinear [11], as mathematical descriptions of anomalous diffusion, in the form of generalized diffusion equations, have been developed either explicitly or implicitly with simple diffusion on a fractal as the key application for consideration. This implicitly excludes cases where $\gamma > 1$. While that regime can be meaningful for some of those equations [12–15], it is not considered further here.

Although fruitful work has been carried out in the study of asymptotic properties and master equations [16–22], a detailed and comprehensive physical theory for generalized diffusion

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equations, in terms of the underlying fractal dynamics, has not emerged. Such a theory has proven to be much more difficult to construct than that of the classical diffusion case because there is no simple Gauss law to be used on a fractal to convert integrals to differential equations. That conversion is essential in the classical diffusion derivation, of course, as conservation in its simple differential equation form is then easily introduced. As this is not possible in the case of fractal dynamics the arguments behind these equations have been at times more heuristic and empirical than physical. They do not capture the full observed behaviour, even with the simplifying presumption of a single underlying mechanism. Furthermore, they each fail in different ways.

It has been difficult to establish a criterion to compare the relative merits and weaknesses of the solutions of these different equations and thus the merits of their accompanying reasoning, because of the substantial qualitative differences between the various equations and their solutions. Their probability densities change with time, making it seem necessary to compare solution surfaces. Thus few direct comparisons have been made, leaving each calculation isolated without a straightforward basis of comparison.

However, because of the scaling relationship between space and time implicit in (1), which all of these models share irrespective of whether the underlying mechanism is diffusion on a fractal or not, it is possible to compare probabilities in terms of a function of only one variable. This function is one factor, invariant under a similarity group, of the probability density function (PDF). We will call it the auxiliary function.

We show below that the auxiliary function contains all of the information that makes each distinct PDF unique. Furthermore, as it is a function of only one similarity variable, it is thus a solution of an ordinary (or fractional) differential equation instead of a partial (or partial extraordinary) differential equation. This ordinary differential equation is known in connection with similarity group methods as the *auxiliary* equation. It provides the necessary information from which to extract the original partial differential equation.

For the first time the auxiliary functions and the auxiliary equations for the four established generalized diffusion model equations are deduced below. It will become obvious that in each case the PDF is best presented as the auxiliary function plotted against the similarity variable. The theory introduced here makes it clear that this representation is best for all cases and that it is not unique for each model. Also for the first time all of the resulting auxiliary functions for the case of the Sierpinski gasket are plotted on the same graph, indicating the underlying differences in the PDFs between the different models. Furthermore this formal structure should apply to direct calculations of random walks on fractals as well. Even if the auxiliary function is a fractal in its own right, the similarity variable structure shows that walks on fractals conform to (1) as well, opening the door to comparing solutions of differential equations with numerical experiments. Thus data too are included in these direct comparison plots.

2. Similarity group and probability density normalization

All of the differential equations posed [8–11] can be written in the form

$$\mathcal{L}P(r,t) = 0 \tag{2}$$

where $P(r,t)$ is the PDF induced by an underlying random walk process, and $\mathcal{L}$ is the (integro-) differential operator of the equation in question.

These equations are also invariant under a one-parameter similarity group, i.e. they are invariant under a scaling of the variables r and t:

$$r = \tilde{r}\lambda^{\beta} \qquad t = \tilde{t}\lambda$$

where λ is the scaling factor, and β is a value to be determined by the structure of $\mathcal{L}$. These equations introduce similarity variables, of which we select the one linear in r, $\eta \equiv r/t^{\beta}$. Similarity variables are also invariant under the group.

It follows that solutions may have the form $Q(\eta)$ provided that $Q(\eta)$ satisfies an equation $\mathcal{A}_\eta Q(\eta) = 0$, where $\mathcal{A}_\eta$ is an auxiliary (integro-) differential equation in one independent variable, η, induced by $\mathcal{L}$. However, while $Q(\eta)$ will satisfy (2), it cannot be a PDF because

$$1 \neq \int_\Sigma Q(\eta) c r^a \, \mathrm{d}r = t^{\beta(1+a)} \int_{\Sigma'} Q(\eta) c \eta^a \, \mathrm{d}\eta \tag{3}$$

where Σ is the domain of normalization in r space, Σ' is the corresponding domain in η coordinates and $cr^a \, \mathrm{d}r$ is the volume element of a spherical shell at r with the appropriate constants a and c.

This problem is easily solved if instead of solutions of the form of $Q(\eta)$, we seek solutions of the form $t^{-\beta(1+a)}G(\eta)$. Then

$$1 = \int_\Sigma P(r,t) c r^a \, \mathrm{d}r = t^{\beta(1+a)} \int_{\Sigma'} t^{-\beta(1+a)} G(\eta) c \eta^a \, \mathrm{d}\eta = \int_{\Sigma'} G(\eta) c \eta^a \, \mathrm{d}\eta \tag{4}$$

provided $G(\eta)$ satisfies $\mathcal{B}_\eta G(\eta) = 0$, where $\mathcal{B}_\eta$ is a new differential (or integro-differential) operator in one variable induced by $\mathcal{L}$.

If we suppose then that Gs may be found that are non-negative, then these will act as properly normalizable PDFs. We then conclude that $P(r,t)$ has the form

$$P(r,t) = t^{-\beta(1+a)} G(\eta). \tag{5}$$

With this $P(r,t)$ we may easily deduce a relation for the mean square displacement,

$$\langle r^2 \rangle = \int_\Sigma r^2 P(r,t) c r^a \, \mathrm{d}r = t^{2\beta} \int_{\Sigma'} G(\eta) c \eta^{a+2} \, \mathrm{d}\eta \tag{6}$$

which reduces to relation (1) if the parameters in $\mathcal{L}$ are set as $\beta = \gamma/2$, and the integral is taken as the constant of proportionality.

In order to obtain (6), very few restrictions were imposed on $\mathcal{L}$ other than the similarity group itself. So there is a broad class of (integro-) differential equations which agree with (1), far exceeding those found in the existing literature. Therefore compliance with (1) is far from sufficient to justify any particular anomalous diffusion equation proposed.

This is not to suggest that any author does claim that compliance with (1) is, in and of itself, sufficient. It simply means that more conditions (heuristic, empirical, physical or otherwise) are necessary to produce a specific equation. As we shall see below, while everyone agrees that (6) should hold, there is little consensus among the architects of generalized diffusion equations about other conditions to be desired. Some emphasize matching asymptotic behaviours, others care little for that and emphasize other aspects. This disagreement could only emerge because the equations have been proposed before a link to the direct microscopic physics is fully understood.

Nevertheless the similarity group need not just apply to a differential equation. It also must in principle apply to actual underlying dynamics on the fractal. This will in turn lead to an equation not unlike (6), where the integral would be generalized for the fractal argument, as is implied in [8].

This focuses the discussion onto the auxiliary function, $G(\eta)$, as it provides the natural invariant representation of the different PDFs. In the following we will refer to the auxiliary function in an invariant variable chosen to be proportional to r as the G-density function (GDF), as it will represent a time independent representation of the PDF. This leads to a direct static comparison of results of these various proposed equations.

3. Auxiliary functions and auxiliary equations for anomalous diffusion equations

In the following we calculate the auxiliary function $G(\eta)$ and the auxiliary equation for four anomalous diffusion equations. These functions and equations can be compared directly as they are all static and posed in the same space to represent the same phenomena.

3.1. O'Shaughnessy and Procaccia

The equation [8]

$$\frac{\partial}{\partial t} P(r,t) = \frac{D_\mathrm{o}}{r^{d_\mathrm{f}-1}} \frac{\partial}{\partial r} r^{d_\mathrm{f}-d_\mathrm{w}+1} \frac{\partial}{\partial r} P(r,t) \tag{7}$$

is the oldest of the proposed equations for representing anomalous diffusion and it was the most meticulously constructed, with underlying dynamics on a Sierpinski gasket treated explicitly. Here d_w is the walk dimension and d_f is the fractal dimension, while D_o is a diffusion constant determined below.

The PDF, solving (7), given in [8], is

$$P(r,t) = P_\mathrm{o}(r,t) = \frac{d_\mathrm{w} \pi^{-\frac{d_\mathrm{f}}{2}} \Gamma(\frac{d_\mathrm{f}}{2})}{2\Gamma(\frac{d_\mathrm{f}}{d_\mathrm{w}})} (K_\mathrm{o} t)^{-\frac{d_\mathrm{f}}{d_\mathrm{w}}} \exp\left(-\frac{r^{d_\mathrm{w}}}{K_\mathrm{o} t}\right) \tag{8}$$

where $K_\mathrm{o} \equiv d_\mathrm{w}^2 D_\mathrm{o}$ and it was determined that

$$K_\mathrm{o} = \frac{4 W d_\mathrm{w}^2}{3 d_\mathrm{f}(d_\mathrm{w} - d_\mathrm{f})} \qquad W = \tfrac{1}{4}. \tag{9}$$

These values were set [8] by direct microscopic calculations on a Sierpinski gasket.

Equation (8) clearly has the form of (5) where $\beta = d_\mathrm{w}^{-1}$ and $a = d_\mathrm{f} - 1$, consistent with the volume element of [8]. Thus for [8] the auxiliary function, $G(\eta) = G_\mathrm{o}(\eta)$, is

$$G_\mathrm{o}(\eta) = \frac{d_\mathrm{w} \pi^{-\frac{d_\mathrm{f}}{2}} \Gamma(\frac{d_\mathrm{f}}{2})}{2\Gamma(\frac{d_\mathrm{f}}{d_\mathrm{w}})} K_\mathrm{o}^{-\frac{d_\mathrm{f}}{d_\mathrm{w}}} \exp\left(-\frac{\eta^{d_\mathrm{w}}}{K_\mathrm{o}}\right). \tag{10}$$

This function agrees well with numerical experiments for small r (see figure 1) but figure 2 shows that it has difficulty in the asymptotic regime as already mentioned in [4].

Naturally, (10) is a solution of the auxiliary equation (see table 1) which is produced by inserting (5) into the partial differential equation (7). The result is of second order in the single similarity variable η. Thus the PDE is reduced to an ODE in the framework of the similarity group.

3.2. Giona and Roman

Giona and Roman [9] proposed, through various heuristic arguments, a very different fractional-order partial differential equation,

$$\frac{\partial^{\frac{1}{d_\mathrm{w}}}}{\partial t^{\frac{1}{d_\mathrm{w}}}} P(r,t) = -\frac{D_\mathrm{g}}{r^{\frac{1}{2}(d_\mathrm{s}-1)}} \frac{\partial}{\partial r} (r^{\frac{1}{2}(d_\mathrm{s}-1)} P(r,t)) \tag{11}$$

which nonetheless satisfies the same similarity group as did (7). Here $d_\mathrm{s} = 2d_\mathrm{f}/d_\mathrm{w}$ and D_g is an adjustable diffusion-like constant, which was not set in [9].

That work, in contrast to [8], focused on asymptotics. While the Laplace transform was calculated there, only asymptotic approximations of the PDF were given directly. Giona and Roman also deduced an integral representation of the inverse Laplace transform with which they performed numerical computations to determine the PDF in a range of cases.

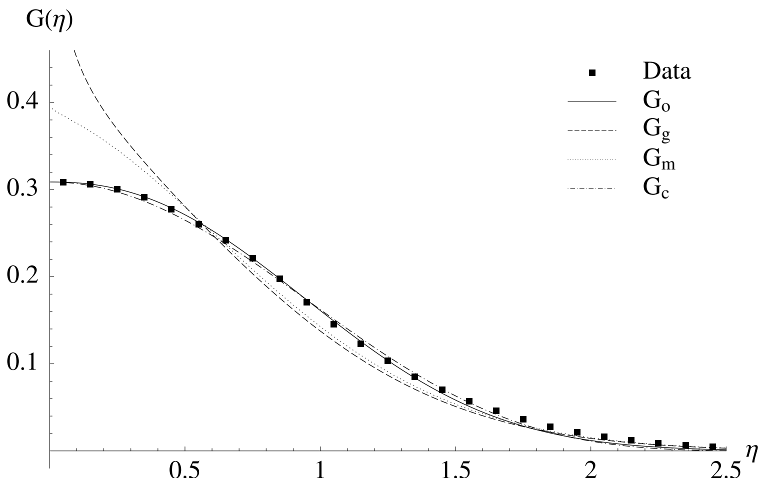

Figure 1. GDF versus η for solutions of four different equations: the full curve represents G_{o} while the dashed one shows G_{g}. Note that in the latter case G_{g} is singular at $\eta = 0$, and its constant is chosen to achieve the same asymptotics as G_{m}. The dotted curve represents G_{m}, and the one with dashes and dots G_{c}. G_{c} becomes strictly zero outside the domain of the plot, and K_{c} is set so that $G_{\mathrm{c}}(0) = G_{\mathrm{o}}(0)$. All of these GDFs are compared with data (filled squares) resulting from a simulation of a diffusion process on a Sierpinski gasket.

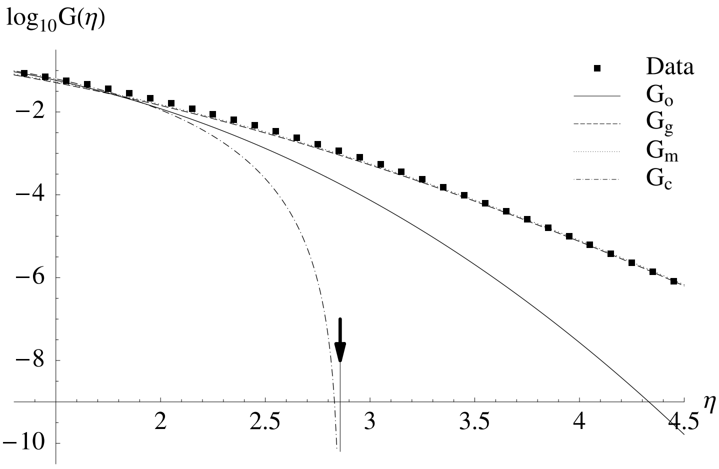

Figure 2. Logarithm of GDF versus η for larger η. The arrow denotes where G_{c} (dash–dotted curve) has its zero and where it is set to zero for larger η. Clearly G_{o} (full curve) differs from G_{g} (dashed curve) and G_{m} (dotted curve) asymptotically, but G_{g} does agree closely with G_{m} (which has identical asymptotics) even in this intermediate regime.

We can determine the PDF explicitly in terms of established functions. These functions, which belong to the class of H-functions [23], permit us to perform the inverse transform directly, providing an explicit alternative to the integral representation:

$$P_{\mathrm{g}}(r,t) = \frac{d_{\mathrm{w}}\pi^{-\frac{d_{\mathrm{f}}}{2}}\Gamma(\frac{d_{\mathrm{f}}}{2})}{2\Gamma(d_{\mathrm{f}} - \frac{1}{2}(d_{\mathrm{s}}-1))}(K_{\mathrm{g}}t)^{-\frac{d_{\mathrm{f}}}{d_{\mathrm{w}}}} H^{1,0}_{1,1}\left(\frac{r^{d_{\mathrm{w}}}}{K_{\mathrm{g}}t}\,\middle|\, \begin{matrix}(1-\frac{d_{\mathrm{f}}}{d_{\mathrm{w}}},1)\\ (-\frac{1}{2}(d_{\mathrm{s}}-1), d_{\mathrm{w}})\end{matrix}\right) \tag{12}$$

where $K_{\mathrm{g}} \equiv D_{\mathrm{g}}^{d_{\mathrm{w}}}$.

As in section 3.1, this PDF has the form of (5) with a and β having the same values as before. This in turn leads to an auxiliary function, $G(\eta) = G_{\mathrm{g}}(\eta)$, of the form

$$G_{\mathrm{g}}(\eta) = \frac{d_{\mathrm{w}}\pi^{-\frac{d_{\mathrm{f}}}{2}}\Gamma(\frac{d_{\mathrm{f}}}{2})}{2\Gamma(d_{\mathrm{f}} - \frac{1}{2}(d_{\mathrm{s}} - 1))} K_{\mathrm{g}}^{-\frac{d_{\mathrm{f}}}{d_{\mathrm{w}}}} H_{1,1}^{1,0}\left(\frac{\eta^{d_{\mathrm{w}}}}{K_{\mathrm{g}}}\,\middle|\, \begin{matrix}(1-\frac{d_{\mathrm{f}}}{d_{\mathrm{w}}}, 1)\\ (-\frac{1}{2}(d_{\mathrm{s}}-1), d_{\mathrm{w}})\end{matrix}\right). \tag{13}$$

As above, an auxiliary equation may be obtained. It is displayed in table 1. However, the fractional derivatives in time would produce new integral operators when using the new variable η, which is not linear in t. Instead, η is linear in r, and it was used because it allowed $G(\eta)$ to have straightforward interpretations in terms of the original PDF. Nonetheless no new integral operators are introduced into the auxiliary equation by using another similarity variable linear in t, $\tau \equiv \eta^{-d_{\mathrm{w}}}$, such that $G(\eta) = F(\tau)$. Inserting $P(r,t) = t^{-d_{\mathrm{f}}/d_{\mathrm{w}}}F(\tau)$ into (11) leads to the auxiliary equation listed in table 1. There is only one independent variable, τ, in the result, making this an (extra-) ordinary differential equation. An auxiliary equation for this unusual fractional type has been deduced previously [12].

One complication with (12) and (13) is that they are singular at the origin, as mentioned in [9]. To see this singularity, the H-function can be expanded in a series [23] about $\eta = 0$. This gives a series expansion for $G_{\mathrm{g}}(\eta)$ illustrating the small-η behaviour:

$$G_{\mathrm{g}}(\eta) = a_0\eta^{-\frac{1}{2}(d_{\mathrm{s}}-1)} + \sum_{\nu=1}^{\infty} a_\nu \eta^{\nu-\frac{1}{2}(d_{\mathrm{s}}-1)} \tag{14}$$

where

$$a_0 = \frac{\pi^{-\frac{d_{\mathrm{f}}}{2}}\Gamma(\frac{d_{\mathrm{f}}}{2})}{2\Gamma(d_{\mathrm{f}} - \frac{1}{2}(d_{\mathrm{s}}-1))\Gamma(1 - \frac{d_{\mathrm{f}}}{d_{\mathrm{w}}} + \frac{d_{\mathrm{s}}-1}{2d_{\mathrm{w}}})} K_{\mathrm{g}}^{-\frac{d_{\mathrm{f}}}{d_{\mathrm{w}}} + \frac{d_{\mathrm{s}}-1}{2d_{\mathrm{w}}}}. \tag{15}$$

As $(d_{\mathrm{s}} - 1)/2 > 0$, the leading term is clearly singular at the origin. This is depicted in figure 1.

While this might be regarded as unusual behaviour in a physical sense, it does not prevent the function from being a formally correct PDF as it remains positive and normalizable despite the singularity. Furthermore, probability is always measured over some volume element, so the singularity would never show up in practice. However, this singularity may be spurious as such behaviour is not unknown among fractional-order differential equations when the wrong null space has come into play [24]. Even so, as seen in figure 2, the correct asymptotics sought in [9] show themselves even for moderate η.

3.3. Metzler, Glöckle and Nonnenmacher

Metzler *et al* [10] developed, following [13], an equation that aimed to improve on (11) but with some of the qualities of (7). It was

$$\frac{\partial^{\frac{2}{d_{\mathrm{w}}}}}{\partial t^{\frac{2}{d_{\mathrm{w}}}}} P(r,t) = \frac{D_{\mathrm{m}}}{r^{d_{\mathrm{s}}-1}}\frac{\partial}{\partial r} r^{d_{\mathrm{s}}-1}\frac{\partial}{\partial r}P(r,t) \tag{16}$$

where D_{m} is a diffusion-like constant [25] inserted into the equation to allow comparisons with (computer) experiments. Metzler *et al* have implicitly set this to unity, assuming dimensionless quantities.

Equation (16) has been solved [10, 25] to yield the PDF

$$P_{\mathrm{m}}(r,t) = \frac{d_{\mathrm{w}}\pi^{-\frac{d_{\mathrm{f}}}{2}}}{2\Gamma(1 + \frac{d_{\mathrm{f}}}{2} - \frac{d_{\mathrm{f}}}{d_{\mathrm{w}}})}(K_{\mathrm{m}}t)^{-\frac{d_{\mathrm{f}}}{d_{\mathrm{w}}}} H_{1,2}^{2,0}\left(\frac{r^{d_{\mathrm{w}}}}{K_{\mathrm{m}}t}\,\middle|\, \begin{matrix}(1-\frac{d_{\mathrm{f}}}{d_{\mathrm{w}}}, 1)\\ (0, \frac{d_{\mathrm{w}}}{2}), (1-\frac{d_{\mathrm{f}}}{d_{\mathrm{w}}}, \frac{d_{\mathrm{w}}}{2})\end{matrix}\right) \tag{17}$$

where $K_{\rm m} \equiv D_{\rm m}^{\frac{d_{\rm w}}{2}}$. Accordingly we find the GDF,

$$G_{\rm m}(\eta) = \frac{d_{\rm w}\pi^{-\frac{d_{\rm f}}{2}}}{2\Gamma(1+\frac{d_{\rm f}}{2}-\frac{d_{\rm f}}{d_{\rm w}})} K_{\rm m}^{-\frac{d_{\rm f}}{d_{\rm w}}} H_{1,2}^{2,0}\left(\frac{\eta^{d_{\rm w}}}{K_{\rm m}}\,\middle|\, \begin{matrix} (1-\frac{d_{\rm f}}{d_{\rm w}}, 1) \\ (0, \frac{d_{\rm w}}{2}), (1-\frac{d_{\rm f}}{d_{\rm w}}, \frac{d_{\rm w}}{2}) \end{matrix}\right). \quad (18)$$

Using the same conventions and reasoning as in section 3.2 for fractional-order auxiliary equations, we find the auxiliary equation in the function $F(\tau)$ for (16) (see table 1), which is a second-order extraordinary differential equation in τ.

The GDF in this case, like that of Giona and Roman, emphasizes asymptotics, but does not agree so well with the numerical experiment for small η (see figure 1). Note particularly that the slope of (18) is negative at the origin. This does not change on adjusting $D_{\rm m}$, which means that these curves, all being normalized, cannot agree even with careful tuning.

In a subsequent paper Metzler and Nonnenmacher [26] have considered alternative parameter values to match slightly different asymptotics found in the literature (see, e.g., [17]) with the solution of their generalized diffusion equation. While alternative parameter values could also allow some flexibility to face the problem at the origin, it would be at the price of deteriorated asymptotics, contrary to the goals of these papers.

3.4. Compte and Jou

Compte and Jou [11] take a different approach, inspired by nonequilibrium thermodynamics, but nonetheless producing an equation invariant under the similarity group. Asymptotics are not matched. The result is not of fractional order; rather it is nonlinear:

$$\frac{\partial}{\partial t} P(r,t) = \frac{q D_{\rm c} d_{\rm f}}{d_{\rm w}+d_{\rm f}-2} \frac{1}{r^{d_{\rm f}-1}} \frac{\partial}{\partial r} r^{d_{\rm f}-1} \frac{\partial}{\partial r} (P(r,t))^{\frac{d_{\rm w}+d_{\rm f}-2}{d_{\rm f}}} \quad (19)$$

where the constants $D_{\rm c}$, and q from [11], are subsequently rolled together into $K_{\rm c}$ so that $K_{\rm c} \equiv q D_{\rm c}$. The PDF is offered in the paper by Compte and Jou, from which the GDF, $G(\eta)$, is extracted, in the same manner as in the preceding sections. Nevertheless it has some unusual properties:

$$G(\eta) = G_{\rm c}(\eta) = b K_{\rm c}^{-\frac{d_{\rm f}}{d_{\rm w}}} [a^2 - K_{\rm c}^{-\frac{2}{d_{\rm w}}} \eta^2]_+^{\frac{d_{\rm f}}{d_{\rm w}-2}} \quad (20)$$

where the notation $[\cdot]_+$ is defined as

$$[u]_+ = \begin{cases} u & \text{if} \quad u > 0 \\ 0 & \text{otherwise} \end{cases}$$

and

$$b = \left(\frac{d_{\rm w}-2}{2d_{\rm w}d_{\rm f}}\right)^{\frac{d_{\rm f}}{d_{\rm w}-2}} \qquad a = \left(\frac{d_{\rm w}\Gamma(\frac{d_{\rm w}d_{\rm f}}{2d_{\rm w}-4})}{2b\pi^{\frac{d_{\rm f}}{2}}\Gamma(\frac{d_{\rm f}}{d_{\rm w}-2})}\right)^{\frac{d_{\rm w}-2}{d_{\rm w}d_{\rm f}}}.$$

Note that this result only holds for the case $d_{\rm w} > 2$.

The usual introduction of $G(\eta)$ into (19) leads to a nonlinear ordinary differential equation in $G_{\rm c}(\eta)$ listed in table 1.

The most unusual property of these is that the boundary of non-zero probability spreads out in r-space at a rate limited by η. This is consistent with (1) of course but it is far from necessary. This is most clearly seen in a similarity space plot of equation (20), where, for values of η larger than a critical value, $\eta_{\rm c} = a K_{\rm c}^{1/d_{\rm w}}$, $G_{\rm c}$ is strictly zero. Of course this means that the direct solution is no longer real and positive beyond the critical value, requiring the grafting together of two solutions of (19). Figure 2 shows its incorrect asymptotic behaviour for a Sierpinski gasket.

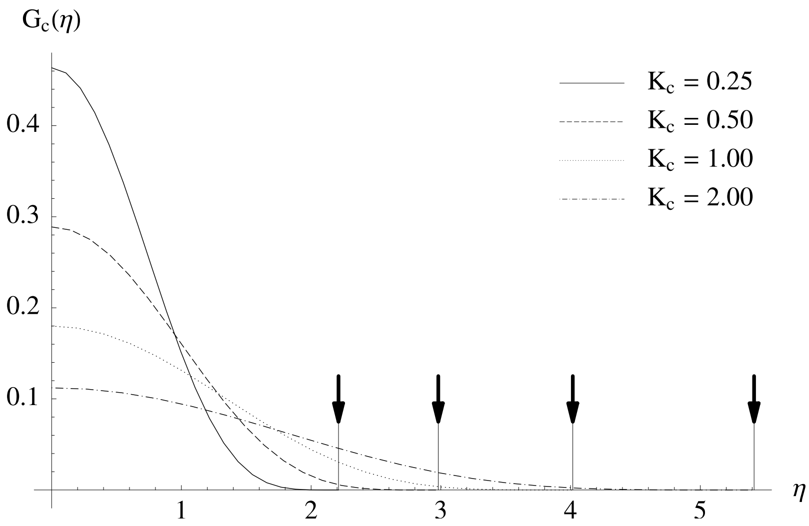

Figure 3. *G*DF versus η for the case of G_c for several values of K_c. Note that the plot is stopped for $\eta > \eta_c$, that is where $G_c = 0$. η_c is indicated for each value of K_c by an arrow. It is clear that η_c grows with decreasing K_c.

4. Comparing auxiliary equations and their solutions in similarity space

In this section we compare the different auxiliary differential equations to highlight some of their similarities and differences. In table 1 the four different equations are presented in such a way that the coefficient of the highest derivative (second order) is at the left-hand end, followed by the first-order coefficient. The zeroth-order derivative is given at the right-hand end. The fractional derivatives are placed between the first- and the zeroth-order terms as their exponents, $1/d_w$ and $2/d_w$, are between zero and one for the fractal case $d_w > 2$.

We first note that, unlike the others, (g) has no second-order derivative. A closer look reveals that compared with (m) the first-order term of (g) is just a kind of 'square root' of the second-order term of (m). Such a relation is not unexpected as the PDE (11) that led to (g) was referred to as a 'halved' diffusion equation before [10].

The nonlinearity of (c) sets it apart from the other equations, but it is interesting to see that for $d_w = 2$ the nonlinearity completely vanishes and (c) and (o) agree with $K_c = D_o$ (remember $K_o = d_w^2 D_o$).

From the point of view of a master equation approach to the time development of the probability on the underlying fractal a linear differential equation seems preferable. Thus the question remains which mechanism should be responsible for the nonlinearity.

The solutions of these auxiliary equations are compared with data from a numerical simulation of diffusion on a Sierpinski gasket as described in [8]. The probability densities for many different times are gathered and averaged in η-space to get rid of their fractal properties.

In order to compare the different *G*DFs with these data the diffusion constants have to be set. In the case of O'Shaugnessy and Procaccia K_o was fixed directly by microscopic analysis. However, in the case of Compte and Jou the value of K_c was not set and the solution is sensitive to its value. To see this, a number of values of K_c were used to plot G_c in figure 3. Note that in figure 1 we set K_c so that $G_c(0) = G_o(0)$ to take advantage of the effectiveness of $G_o(\eta)$ in representing the numerical experiment. There is of course no hope of adjusting K_c to match behaviours at large η beyond η_c.

Table 1. Auxiliary differential equations for anomalous diffusion processes. They are deduced from the PDE proposed by (o) O'Shaughnessy and Procaccia, (g) Giona and Roman, (m) Metzler *et al* and (c) Compte and Jou by inserting $P(r,t) = t^{-d_\mathrm{f}/d_\mathrm{w}} G(\eta)$ or $P(r,t) = t^{-d_\mathrm{f}/d_\mathrm{w}} F(\tau)$. The function $F(\tau) = G(\eta)$ is introduced for the fractional PDEs to retain the fractional derivative using the variable τ linear in t rather than η linear in r. Note that all these equations are (fractional) ODEs compared with the original (fractional) PDEs.

(o)	$\eta^{2-d_\mathrm{w}}\, G_\mathrm{o}''(\eta)$	$+$	$\left\{(d_\mathrm{f} - d_\mathrm{w} + 1)\eta^{1-d_\mathrm{w}} + \frac{d_\mathrm{w}}{K_\mathrm{o}}\eta\right\}\, G_\mathrm{o}'(\eta)$			$+$	$\frac{d_\mathrm{f} d_\mathrm{w}}{K_\mathrm{o}}\, G_\mathrm{o}(\eta)$	$=$	0
(g)			$\left(K_\mathrm{g}^{\frac{1}{d_\mathrm{w}}}\, d_\mathrm{w}\tau\right)\, F_\mathrm{g}'(\tau)$	$-$	$\tau^{\frac{d_\mathrm{f}}{d_\mathrm{w}}} \frac{\partial^{\frac{1}{d_\mathrm{w}}}}{\partial\tau^{\frac{1}{d_\mathrm{w}}}} \left(\tau^{-\frac{d_\mathrm{f}}{d_\mathrm{w}}}\, F_\mathrm{g}(\tau)\right)$	$-$	$\frac{K_\mathrm{g}^{\frac{1}{d_\mathrm{w}}}}{2}(d_\mathrm{s} - 1)\, F_\mathrm{g}(\tau)$	$=$	0
(m)	$\left(K_\mathrm{m}^{\frac{1}{d_\mathrm{w}}}\, d_\mathrm{w}\tau\right)^2\, F_\mathrm{m}''(\tau)$	$+$	$K_\mathrm{m}^{\frac{2}{d_\mathrm{w}}}\, d_\mathrm{w}(d_\mathrm{w} - d_\mathrm{s} + 2)\tau\, F_\mathrm{m}'(\tau)$	$-$	$\tau^{\frac{d_\mathrm{f}}{d_\mathrm{w}}} \frac{\partial^{\frac{2}{d_\mathrm{w}}}}{\partial\tau^{\frac{2}{d_\mathrm{w}}}} \left(\tau^{-\frac{d_\mathrm{f}}{d_\mathrm{w}}}\, F_\mathrm{m}(\tau)\right)$			$=$	0
(c)	$G_\mathrm{c}''(\eta)$	$+$	$\left\{\frac{d_\mathrm{f} - 1}{\eta} + \frac{\eta}{K_\mathrm{c} d_\mathrm{w}}(G_\mathrm{c}(\eta))^{\frac{2-d_\mathrm{w}}{d_\mathrm{f}}} + \frac{d_\mathrm{w} - 2}{d_\mathrm{f}}\frac{G_\mathrm{c}'(\eta)}{G_\mathrm{c}(\eta)}\right\}\, G_\mathrm{c}'(\eta)$			$+$	$\frac{d_\mathrm{f}}{K_\mathrm{c} d_\mathrm{w}}\, (G_\mathrm{c}(\eta))^{\frac{2-d_\mathrm{w}+d_\mathrm{f}}{d_\mathrm{f}}}$	$=$	0

We note (figure 1) that for small to medium values of η $G_c(\eta)$ and $G_o(\eta)$ are both very close to the numerical data, demonstrating that similar behaviours can arise from quite different functions and quite different equations, but both GDFs are unable to cover the right asymptotic behaviour of the probability density on a fractal as figure 2 shows most clearly.

For each of the fractional diffusion equations, (g) and (m), the constant was set to match the asymptotics. As it turns out from asymptotic expansions [23] of (13) and (18), the values of K_m and K_g are closely related via $K_g = K_m/5$. We found that $K_m \approx 1.11$ shows the best agreement with the asymptotic data (see figure 2). Although the functions G_m and G_g are designed to have good asymptotics, they clearly have significant problems in matching the data for small η (figure 1). Evidently good asymptotics are not enough.

5. Concluding remarks

It has been shown here that conforming to (1) is far from sufficient to confirm the correctness of an equation purporting to describe anomalous diffusion. Indeed it is clear from section 2 that the class of equations for which it does hold is much larger than the examples (often heuristically obtained) of section 3 might suggest.

Even so, the equations in section 3, notwithstanding the fact that they all satisfy the same similarity group, are very different indeed. Two are of fractional order, with one having a singular GDF. One of integer order is nonlinear, having a PDF with a moving outer envelope outside which there is no probability. This envelope expands according to relation (1).

Exploiting the similarity group allows these seemingly unlike equations and the functions comprising their solutions to be compared as static functions of one variable. The similarity space in which this is done provides a basis not only for comparing such solutions with each other, but also for comparing solutions with the results of numerical experiments. It is clear that while solutions have similar general properties of decreasing outward, they are all qualitatively different in significant ways, and none agrees with numerical experiment, suggesting that new approaches are needed.

This analysis shows that the search for equations needs only be performed in one independent variable, as this automatically guarantees that (1) is satisfied. The auxiliary equations (table 1) presented show us how such reduced equations actually appear. It is, however, also clear, as O'Shaughnessy and Procaccia warned from the beginning, that the PDF (thus the GDF) will be itself a fractal, so direct analysis using continuous differential equations will be doomed when attempting to treat the full GDF and not just an averaged one (as done here) from numerical experiments.

Instead of looking for *ad hoc* envelopes and averages of probability densities on fractals there may be ways around this problem particularly suited to similarity space. This will be the topic of a forthcoming paper.

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