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Lie symmetry solutions for anomalous diffusion

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Abstract

An anomalous diffusion equation is solved by the method of Lie symmetries. The nonlinear diffusion equation includes fractal dimensions and power-law dependence on the radial variable and the diffusion function. The Lie symmetries, appropriate boundary and initial conditions and a first integral replace an ansatz that was previously used to find a class of analytic solutions. The mean-squared displacement of the diffusion varies in time t by an exponent that is easily found by the Lie symmetries and boundary conditions.

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1. Introduction

Anomalous diffusion has recently been the topic of extensive research but it has a long history [1–28]. The criterion for anomalous diffusion is that the mean-squared displacement does not grow linearly in time. Many physical, chemical or biological processes cannot be described by the linear diffusion equation derived for Brownian motion. Anomalous diffusion has been found to occur in fluid turbulence, seepage of liquid into a porous body, diffusion on fractals, turbulent plasmas and many other systems [1–27]. Applications and a short history of anomalous diffusion appear in the review article on a fractional dynamics approach to anomalous diffusion [22]. A more traditional theoretical approach to anomalous diffusion has been to alter the Brownian motion diffusion equation (concentration, temperature, etc) with a spatial, temporal or diffusion function-dependent diffusion coefficient [1, 3, 5, 7–9, 14, 21, 23, 27]. The most common dependence of the diffusion coefficient has been on the diffusion function. In the traditional approach, boundary conditions were customarily used and a set sometimes stated [9, 21]. There are several modern approaches but less attention to boundary and initial conditions is found in these approaches. Statistical methods such as the continuous-time random walk models or the generalized master equation alter the statistical foundation of the Brownian motion diffusion equation and include memory effects [6, 13, 18]. A thermostatistical foundation of anomalous diffusion [12, 16, 19] has been based on a generalized entropy introduced by Tsallis [12]. The inclusion of fractal geometry in the transport of fractals has been modelled by fractional calculus [11, 15, 16, 18, 20, 22, 26] as well as by modified diffusion equations [10, 15, 16, 18–20, 24, 25]. Modern approaches to diffusion have been developed concurrently with the use of Lie symmetries to solve partial differential equations (PDEs) [9, 21, 27–31]. Most Lie group symmetry analyses of nonlinear diffusion equations have not included boundary and initial conditions although there are exceptions [9, 21, 28].

The procedure adopted here is to combine aspects of the different approaches to anomalous diffusion. The generalized nonlinear diffusion equation includes fractal dimensions and a diffusion coefficient that depends on the radial variable and the diffusion function. Lie group symmetry analysis is used to solve the nonlinear differential equation but the boundary and initial conditions play an essential role in that solution. The contributions of this paper to anomalous diffusion are next stated. The solutions of a generalized, nonlinear diffusion equation [19, 20, 24, 25] are reported here. The new results include the derivation of an analytical solution [24, 25] found previously by an ansatz. That analytical result is derived here by a systematic method based on the determination of Lie symmetries with boundary and initial conditions. The solution method for which the norm conservation does not hold is discussed with a mixed use of Lie symmetries and phase plane analysis. Finally, the mean-squared displacement dependence on time is reported for three sets of boundary and initial conditions in terms of three parameters of the nonlinear diffusion equation [9, 21].

2. Nonlinear diffusion equation

A generalized nonlinear diffusion equation that includes an effective fractal dimension d and a diffusion coefficient that is a power-law function of the diffusion function ρ that is a function of r and t and the spatial variable r is studied. The diffusion equation [24, 25] is

$$\frac{\partial \rho}{\partial t} = \frac{K_0}{r^{d-1}} \frac{\partial}{\partial r} \left(r^{d-1-\theta} \frac{\partial \rho^{\nu}}{\partial r} \right) \tag{1}$$

where the radial coordinate is r and the time is t. The diffusion coefficient $K = K_0 \nu r^{\theta} \rho^{\nu-1}$ where θ and ν are the power-law constants and K_0 is a constant. The ρ-dependence of the diffusion coefficient has been incorporated into the term $\partial\rho/\partial r$ so that equation (1) is of the form in [24, 25]. The angular-dependent term of the diffusion equation has been neglected. Equation (1) is a generalization of a diffusion equation found for fractal geometry where K is a function of r only [10] and the traditional nonlinear diffusion equation with K depending on ρ only [1, 3–5, 7, 9, 21, 28].

The boundary and initial conditions used here are based on those for one-dimensional diffusion equations [9, 21] and for equations in several dimensions [3, 4]. The first two conditions hold for all three sets

$$\rho(r, 0) = 0, \qquad r > 0. \tag{2a}$$

$$\rho(\infty, t) = 0, \qquad t > 0. \tag{2b}$$

The second condition may hold at a moving boundary and is zero ahead of the moving boundary. Three possibilities for a third boundary condition are added. These conditions depend on the physical conditions for the problem. The first is an instantaneous point source or unit pulse. It may be expressed as a delta function but is here expressed in its integral form. It is also termed the norm conservation.

$$\Omega_d \int_0^{\infty} \rho(r, t) r^{d-1}\, \mathrm{d}r = k_1 \tag{3a}$$

where k_1 is a constant and the d-dimensional solid angle is $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$. Another boundary condition is the clamped diffusion function where ρ is suddenly raised from 0 to a fixed value k_2

$$\rho(0, t) = k_2, \qquad t > 0. \tag{3b}$$

The clamped flux boundary condition completes the trio

$$K_0 r^{d-1-\theta} \left. \frac{\partial \rho^{\nu}}{\partial r} \right|_{r=0} = k_3. \tag{3c}$$

We are assuming the initial surface is a plane in one dimension but a point otherwise. The boundary and initial conditions for equation (1) must collapse to an appropriate set for an ordinary differential equation (ODE) found by the Lie symmetry method; otherwise a solution is not found by this method.

Analytic solutions of equation (1) have been reported in which an ansatz for $\rho(r, t)$ is proposed as a more general form of the equilibrium function from a generalized entropy [12, 16, 19, 24, 25]. From the form of that solution one could expect that Lie symmetries of the nonlinear PDE (1) can be used to find the analytic solutions. A differential equation is invariant under Lie group symmetries if the form of the differential equation is unchanged under the Lie group transformation. The total number of independent and dependent variables of a PDE that is invariant under a one-parameter Lie group transformation can be reduced by 1. The order of an ordinary differential equation (ODE) that is invariant under a one-parameter Lie group transformation can be reduced by 1. With enough Lie group symmetries a solution can be found.

3. Lie symmetry solutions of nonlinear diffusion equation

The Lie group symmetries of the nonlinear diffusion equation (1) can be determined in several ways: (1) the classical method with an extended group generator [5, 7, 14, 28–31] (2) the solution of the group generator by a computer program such as LIE [32] or (3) by the use of finite transformations [9, 21, 28]. The computer program LIE is not suitable for the general form of equation (1), but it is possible that other computer programs might be suitable. The third approach is presented as it is sufficient for use here. Equation (1) is invariant under translations in time and two stretching transformations

$$\bar{t} = t + \gamma. \tag{4a}$$

$$\bar{t} = \alpha^n t, \qquad \bar{\rho} = \alpha^p \rho, \qquad \bar{r} = \alpha^s r. \tag{4b}$$

The Lie group transformations constitute a three-parameter group as only two of the parameters n, p and s are independent. The two-parameter group of stretching transformations is chosen since it involves the two independent variables and one dependent variable and hence enables us to reduce equation (1) to an ODE. The time translation symmetry, equation (4a), is hidden once the reduction to two similarity variables is made and does not enter into the solution of the diffusion equation. The resultant solutions are pure similarity solutions. The parameters in equation (4b) are fixed by the differential equation and the third condition (3a), (3b) or (3c). We rewrite equation (1) in the new variables and require that α factors out of the equation. This yields the parameter relation

$$p(1 - \nu) + s(\theta + 2) = n. \tag{5}$$

We next form invariant quantities such that

$$\rho^n(r, t) = t^p R\left(\frac{r^n}{t^s}\right). \tag{6}$$

Here, the invariant quantities are found from equation (4*b*) such that the combinations of the barred variables have the same form as the combinations of the original variables where the factors of alpha cancel. The relation in equation (6) can also be found by integrating the characteristic (differential) equations with the invariant surface condition [7]. We set here $n = 1$ since only two of the three parameters n, p and s are independent. Substitution of equation (6) into equation (1) gives the second-order ordinary differential equation (OED)

$$K_0 \frac{\mathrm{d}}{\mathrm{d}z}\left(z^{d-1-\theta}\frac{\mathrm{d}R^{\nu}}{\mathrm{d}z}\right) + s z^{\frac{p}{s}+d}\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{R}{z^{p/s}}\right) = 0. \tag{7}$$

Here, $z = r/t^s$ and $R = R(z)$. The explicit dependence on t has cancelled out of equation (7); three variables have reduced to two. The boundary and initial conditions (2*a*), (2*b*) and (3*a*) reduce to

$$R(\infty) = 0. \tag{8a}$$

$$\Omega_d t^{p+sd}\int_0^{\infty} R(z)z^{d-1}\,\mathrm{d}z = k_1. \tag{8b}$$

For this first set clearly $p + sd = 0$ in equation (8*b*) is required for k_1 to be a constant. The boundary and initial conditions in equation (1) have reduced to two boundary conditions for the second-order ODE. The parameters p and s from equation (5) with $n = 1$ and $p + sd = 0$ give

$$s = \frac{1}{d(\nu-1)+\theta+2}, \qquad p = \frac{-d}{d(\nu-1)+\theta+2}. \tag{9}$$

Also with $p + sd = 0$, equation (7) can be expressed as a total derivative or a first integral exists. As a result, a first-order ODE is found

$$K_0 z^{d-1-\theta}\frac{\mathrm{d}R^{\nu}}{\mathrm{d}z} + s z^d R = C_1. \tag{10}$$

We did not need to use a symmetry to reduce the order of the second-order ODE but the stretching symmetry of equation (7) is lost in equation (10) [33]. It can be recovered if the integration constant $C_1 = 0$ where that choice is required to recover a previous result [24]. Setting $C_1 = 0$, we find that equation (10) is solved by separation of variables to give the analytic solution

$$\rho(r,t) = t^p\left[C_2 - \frac{s(1-q)}{K_0\nu(\theta+2)}\left(\frac{r}{t^s}\right)^{\lambda}\right]^{1/(1-q)} \tag{11}$$

with the notation $\lambda = \theta + 2$, $\nu - 1 = 1 - q$ [24]. The constant C_2 can be computed by substituting $R(z)$ in the norm conservation condition, equation (8*b*), and is B^{-2} as given in equations (13) and (14) in [24] where $k_1 = \rho_0$ and $K_0 = D$. Now as $z \to \infty$ is required by the boundary condition, equation (8*a*), if $q > 1$ for the superdiffusion regime but z is finite for $R(z) = 0$ for $q < 1$ for the subdiffusion regime. The diffusion has a sharp boundary in the subdiffusion regime at $z = b$ as determined from equation (11) where $R(z) = 0$ for $z \geqslant b$.

4. New solutions of the generalized diffusion equation

Other solutions than those in equation (11) are possible. First, we consider nonzero C_1 in equation (10) but find for the cases investigated that there are no solutions for $C_1 \neq 0$ and the condition of equation (3*a*). For a diffusion problem with $d = 1$ and $\theta = 0$, the additional boundary condition is $\mathrm{d}R(z)/\mathrm{d}z = 0$ and hence $C_1 = 0$ by symmetry of the one-dimensional problem [3, 9, 28]. For other dimensions we can check if C_1 may be nonzero [28]. The boundary condition on the diffusion function ρ can be replaced by a boundary condition on $R(z)$. From equation (10), we see that the second term on the right-hand side will be zero at $z = 0$ since the dimension d is positive and $R(z)$ must be finite at $z = 0$. The behaviour of the first term on the right-hand side of equation (10) at boundary $z = 0$ is more complicated. We have, at $z = 0$, the boundary condition

$$K_0 z^{d-1-\theta} \left.\frac{\mathrm{d}R^{\nu}}{\mathrm{d}z}\right|_{z=0} = C_1. \tag{12}$$

This condition is equivalent to the boundary condition, equation (3*c*), for the clamped flux where there is no net time dependence on the left-hand side if $p = -s(d-2-\theta)$. Since the norm conservation requires $p = -sd$ for no net time dependence, both conditions hold only if $\theta = -2$. This condition does not hold for any cases that were studied. For example, consider linear diffusion where $\nu = 1$. Then equation (10) can be integrated by the standard integrating factor. The integration constant is determined from equation (8*b*) with the upper limit $z = b$ such that $R(b) = 0$.

$$\rho(r,t) = \frac{k_1 t^p \exp\left(-\frac{s^2 z^{\theta+2}}{K_0}\right)[M_1(0,b) - M_1(0,z)]}{\Omega_d \int_0^b M_2(0,z)\frac{\mathrm{d}M_1(0,z)}{\mathrm{d}z}\,\mathrm{d}z} \tag{13}$$

is the result for $z < b$ where C_1 has been eliminated and $\rho(r,t) = 0$ for $z \geqslant b$. The parameters and functions are defined as

$$s = \frac{1}{\theta+2}, \qquad p = -\frac{d}{\theta+2}, \qquad M_1(0,z) = \int_0^z \bar{z}^{\theta+1-d} \exp\left(\frac{s^2\bar{z}^{\theta+2}}{K_0}\right)\mathrm{d}\bar{z},$$

$$M_2(0,z) = \int_0^z \bar{z}^{d-1} \exp\left(-\frac{s^2\bar{z}^{\theta+2}}{K_0}\right)\mathrm{d}\bar{z}.$$

If $C_1 = 0$, then we find a stretched Gaussian

$$\rho(r,t) = \frac{k_1 t^p \exp\left(-\frac{s^2 z^{\theta+2}}{K_0}\right)}{\Omega_d M_2(0,\infty)}. \tag{14}$$

The constant $C_1 \neq 0$ only if $\theta > d-1$, otherwise it is zero. Also $\theta > -1$ is required if $b \to \infty$ in equation (13); $\theta > -2$ is required in equation (14) for no singularity at $z = 0$. Since the dimension d is positive, $\theta = -2$ is excluded for linear diffusion or $C_1 = 0$.

We next consider nonlinear diffusion. Let $\nu = 1/2$ in equation (10) and $T = R^{1/2}$. The resultant nonlinear ODE is a Riccati equation. The standard transformation converts the Riccati equation to a linear second-order ODE

$$z\frac{\mathrm{d}^2u}{\mathrm{d}z^2} - (q+1)\frac{\mathrm{d}u}{\mathrm{d}z} - \frac{C_1 s}{K_0^2} z^{2\theta+3-d} u = 0 \tag{15}$$

with

$$T = \frac{K_0}{s z^{\theta+1}}\frac{\mathrm{d}u}{\mathrm{d}z}.$$

The choices θ and d that will satisfy the boundary conditions on $R(z)$, equations (8*a*) and (8*b*), are not obvious. To find the class that will give acceptable solutions for $R(z)$, we perform a perturbation expansion on equation (15) with the small parameter C_1 and require that $R(z)$ be finite at $z = 0$. This leads to $\theta + 2 > 0$, $\theta + 2 - d > 0$, $2\theta + 4 - d > 0$, $3\theta + 6 - d > 0$, etc. As a result the requirement that $\theta = -2$ does not hold for this case either. There is also the possibility of choosing equation (3*b*) or equation (3*c*) rather than the norm conservation condition, equation (3*a*), for equation (1). There are no first integrals in those cases. If there is no first integral for equation (7), it still can be reduced to a first-order ODE since there is a Lie group stretching symmetry. Phase-plane analysis of the resulting first-order ODE can produce the appropriate two initial conditions for a numerical integration for $R(z)$. The numerical integration has been performed for $R(z)$ and its first derivative for $\nu = 2$, $\theta = -1$ and $d = 1/2$ with equation (3c). Further details of this procedure have been given previously [9].

5. Mean-squared displacement

The time dependence of the mean-squared displacement is an important characteristic of diffusion. The Lie symmetry solutions show the time dependence easily. The mean-squared displacement $\langle r^2 \rangle$ is

$$\langle r^2 \rangle = t^{p+s(d+2)} \Omega_d \int_0^\infty R(z) z^{d+1}\, \mathrm{d}z \propto t^\beta. \tag{16}$$

For the norm conservation set β is $2s$ with $p = -sd$ and $s = 1/[d(1-\nu) + \theta + 2]$. For the clamped diffusion set, β is $s(d+2)$ with $p = 0$ and $s = 1/(\theta + 2)$. For the clamped flux set β is $1 + 2s$ with $p = 1 - ds$ and $s = \upsilon/[\upsilon(1-d) + \theta + 2]$. We note that the time dependence can be determined without performing the integral in equation (16) for the mean-squared displacement.

6. Conclusion

The application of Lie group symmetries to the solution of an anomalous diffusion equation has been demonstrated. The nonlinear diffusion equation is more general than previous nonlinear diffusion equations treated by the classical Lie symmetry method. The equation includes fractal dimensions and power-law dependence of the diffusion coefficient on the radial variable and diffusion function. This method replaces an ansatz based on a thermostatistical argument that was used previously to find a class of analytic solutions. Essential to the method used here is the analysis of the Lie symmetries and the inclusion of appropriate boundary and initial conditions that restrict the class of stretching symmetries for each set of conditions. This report offers the first published solution by Lie symmetries with boundary and initial conditions of the anomalous diffusion equation.

The recovery of a previous diffusion solution by the symmetry method elucidates the necessary and sufficient conditions for the solution. The analytic solutions reported here result from a first integral that arises with norm conservation for a boundary condition. Other possible solutions may be computed numerically with a mixed Lie symmetry and phase-plane analysis. Finally, the mean-squared displacement varies as time t to an exponent in the solutions reported here. The exponent can be determined with the group parameters of the stretching symmetries, the fractal dimension and the power-law parameters of the diffusion coefficient. This affords an easy and quick calculation of the time dependence, where the diffusion can be classified as subdiffusion, normal or superdiffusion. This calculation replaces the necessity of finding the explicit form of the diffusion function.

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