Proceedings of the 2nd IFAC
Workshop on Fractional Differentiation and its Applications
Porto, Portugal, July 19-21, 2006

FRACTIONAL CALCULUS AND THE SCHRÖDINGER EQUATION

Enrico Scalas[a,b] Dumitru Baleanu[c,d], Francesco Mainardi[e], Antonio Mura[e]

[a]Università del Piemonte Orientale, Dipartimento di Scienze e Tecnologie Avanzate, via Bellini 25g, 15100, Alessandria, Italy
[b]INFM Genova, via Dodecaneso 33, 16146, Genova, Italy
[c]Çankaya University, Department of Mathematics and Computer Sciences, Faculty of Arts and Sciences, 06530, Balgat, Ankara, Turkey
[d]Institute of Space Sciences, Magurele-Bucharest, PO Box, MG-23, R 76900 Romania
[e]Università di Bologna, Dipartimento di Fisica, via Irnerio 46, 40126 Bologna, Italy

Abstract: In this paper, a derivation of the fractional Schrödinger equation is presented for the simple case of a pure diffusive process with dissipation. The Gaussian white noise is replaced by more general kinds of white noise and both the Markovian both the Markovian ($\beta = 1$) and non-Markovian case ($0 < \beta < 1$) are considered.

Keywords: Fractional calculus, Quantum mechanics, Diffusion equation, Schrödinger equation.

1. INTRODUCTION, MOTIVATION AND THEORY

Recently, a fractional Schrödinger equation has been introduced (Laskin, 2000; Laskin, 2002). These papers revived early attempts by Elliott Montroll (Montroll, 1974; West, 2000) for the Markovian case. The non-Markovian case has been investigated more recently (Naber, 2004). In our opinion, a justification for the use of fractional calculus in a quantum mechanical framework can be found within the Fényes-Nelson theory (Fényes, 1952; Nelson, 1967; Davidson, 1979) that is summarized below, following the presentation in (Nelson, 1999).

1.1 Conservative case

A *conservative diffusion process* can be defined starting from the usual diffusive stochastic differential equation:

$$d\boldsymbol{x}(t) = \boldsymbol{v}_+(\boldsymbol{x},t)\,dt + \sigma d\boldsymbol{W}(t) \qquad (1)$$

where $\boldsymbol{x}$ represents the position of the particle, $\boldsymbol{W}$ is a Wiener process with standard deviation 1. The forward velocity is defined through the forward derivative:

$$\boldsymbol{v}_+(\boldsymbol{x},t) = D_+\boldsymbol{x}(t) = \lim_{\Delta t \to 0^+} E\left[\frac{\boldsymbol{x}(t+\Delta t) - \boldsymbol{x}(t)}{\Delta t}\right] \qquad (2)$$

The time-reversed version of eq. (1) is:

$$d\boldsymbol{x}(t) = \boldsymbol{v}_-(\boldsymbol{x},t)\,dt + \sigma d\boldsymbol{W}_*(t) \qquad (3)$$

where $\boldsymbol{W}_*$ is a time-reversed Wiener process and the backward velocity is:

$$\boldsymbol{v}_-(\boldsymbol{x},t) = D_-\boldsymbol{x}(t) = \lim_{\Delta t \to 0^+} E\left[\frac{\boldsymbol{x}(t) - \boldsymbol{x}(t-\Delta t)}{\Delta t}\right] \qquad (4)$$

Defining the *mean velocity* as the average of the forward and backward velocity:

$$\boldsymbol{v}(\boldsymbol{x},t) = \frac{1}{2}\left(\boldsymbol{v}_+(\boldsymbol{x},t) + \boldsymbol{v}_-(\boldsymbol{x},t)\right) \qquad (5)$$

one can write the Ito Fokker-Planck equation for the probability density $p(\boldsymbol{x},t)$ of finding the particle in position $\boldsymbol{x}$ at time t; it is the sum of the forward and the backward Ito Fokker-Planck equations corresponding to eqs. (1) and (3) and it coincides with the continuity equation:

$$\frac{\partial}{\partial t} p(\boldsymbol{x},t) + \nabla \cdot \left[v(\boldsymbol{x},t) p(\boldsymbol{x},t) \right] = 0 \tag{6}$$

The *osmotic velocity* is defined as as the half-difference of the forward and the backward velocities:

$$\boldsymbol{u}(\boldsymbol{x},t) = \frac{1}{2}\left(\boldsymbol{v}_+(\boldsymbol{x},t) - \boldsymbol{v}_-(\boldsymbol{x},t) \right) \tag{7}$$

It is related to $p(\boldsymbol{x},t)$ through the following equation, which can be derived by subtracting the forward and backward Ito Fokker-Planck equations and integrating the resulting equation:

$$\boldsymbol{u}(\boldsymbol{x},t) = \frac{\sigma^2}{2} \nabla \ln p(\boldsymbol{x},t) \tag{8}$$

The partial derivative with respect to time of eq. (8), together with eq. (6), yields the first hydrodynamic equation for the description of the Brownian motion:

$$\frac{\partial}{\partial t}\boldsymbol{u} = -\frac{\sigma^2}{2}\nabla(\nabla \cdot \boldsymbol{v}) - \nabla(\boldsymbol{v} \cdot \boldsymbol{u}) \tag{9}$$

For the second equation, one has to define the *mean acceleration*:

$$\boldsymbol{a}(\boldsymbol{x},t) = \frac{1}{2}(D_+D_- + D_-D_+)\boldsymbol{x}(t) \tag{10}$$

The application of Ito's formula to the definition of backward and forward derivative gives:

$$\frac{\partial}{\partial t}\boldsymbol{v} = \boldsymbol{a} - \boldsymbol{v} \cdot \nabla \boldsymbol{v} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \frac{\sigma^2}{2}\Delta \boldsymbol{u} \tag{11}$$

Eqs. (9) and (11) fully describe the hydrodynamics of the diffusion process. If the Brownian particle of mass m moves in an external potential $U(\boldsymbol{x})$, we assume that:

$$\boldsymbol{a}(\boldsymbol{x},t) = -\frac{1}{m}\nabla U(\boldsymbol{x}) \tag{12}$$

and the two hydrodynamic equations become:

$$\begin{aligned} \frac{\partial}{\partial t}\boldsymbol{u} &= -\frac{\sigma^2}{2}\nabla(\nabla \cdot \boldsymbol{v}) - \nabla(\boldsymbol{v} \cdot \boldsymbol{u}) \\ \frac{\partial}{\partial t}\boldsymbol{v} &= -\frac{1}{m}\nabla U - \boldsymbol{v} \cdot \nabla \boldsymbol{v} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \frac{\sigma^2}{2}\Delta \boldsymbol{u} \end{aligned} \tag{13}$$

thus describing a conservative process. For the sake of convenience, define a scalar field $R(\boldsymbol{x}, t)$ related to the probability density:

$$p(\boldsymbol{x},t) = \exp\left[2R(\boldsymbol{x},t)\right]$$

The osmotic velocity can be expressed in terms of this scalar field:

$$\boldsymbol{u}(\boldsymbol{x},t) = \sigma^2 \nabla R(\boldsymbol{x},t) \tag{14}$$

On the other side, requiring that $\boldsymbol{v}$ does not contain closed flow lines, one can define another scalar field (the action $S(\boldsymbol{x}, t)$) and write:

$$\boldsymbol{v}(\boldsymbol{x},t) = \frac{1}{m}\nabla S(\boldsymbol{x},t) \tag{15}$$

If eqs. (14) and (15) are inserted in (13), one gets the following two equations for the scalar fields:

$$\begin{aligned} &\frac{\partial}{\partial t}R + \frac{1}{2m}\Delta S + \frac{1}{m}\nabla R \cdot \nabla S = 0 \\ &\frac{\partial}{\partial t}S + U + \frac{1}{2m}(\nabla S)^2 - \frac{m\sigma^4}{2}\left[(\nabla R)^2 + \Delta R\right] = 0 \end{aligned} \tag{16}$$

which coincide with the *Hamilton-Jacobi* equations for $\sigma = 0$. The first equation is another form of the continuity equation. In quantum mechanics, eqs. (16) are also known as the equations of the Madelung fluid, in which case σ^2 is replaced by $\hbar / m$. In this framework, the time-dependent Schrödinger equation becomes an auxiliary equation, with the wave function given by:

$$\psi(\boldsymbol{x},t) = \exp\left[R(\boldsymbol{x},t) + \frac{i}{\sigma^2 m} S(\boldsymbol{x},t) \right] \tag{17}$$

and satisfying:

$$i\sigma^2 m \frac{\partial}{\partial t}\psi = \left(-\frac{\sigma^4 m^2}{2m}\Delta + U \right)\psi \tag{18}$$

For a non–vanishing wave function, the real part of (18) coincides with the second of eqs. (16), whereas the imaginary part gives the continuity equation. The square modulus of the wave function is the probability density of finding the particle in position x at time t.

1.2 Non-conservative case

The theory outlined above can be used also for the non-conservative purely diffusive case. Suppose that the one-dimensional stochastic process $x(t)$ obeys the following Langevin equation:

$$dx = \sigma\, dW \tag{19}$$

then, the Fokker Planck equation (6) simplifies to:

$$\frac{\partial p(x,t)}{\partial t} = \frac{\sigma^2}{2}\frac{\partial^2 p(x,t)}{\partial x^2} \tag{20}$$

As shown by Fényes and recalled above, for a Fokker-Planck equation there is a corresponding Schrödinger equation and it can be derived from (20) by means of the substitution (17). For the sake of simplicity, let us call $r(x,t) = \exp[R(x,t)]$. As $v = 0$, the action $S(x,t)$ is constant and it is sufficient to study the evolution equation for the amplitude, $r(x,t)$. This turns out to be:

$$\frac{\partial r^2(x,t)}{\partial t} = \frac{\partial^2 r^2(x,t)}{\partial x^2} \quad (21)$$

The next part of this paper is organized as follows. In section 2, we present a fractional generalization of equation (21) in the simplified case of a pure diffusive process in one dimension ($v = 0$). Section 3 is devoted to discussion and conclusions.

2. FRACTIONAL SCHRÖDINGER EQUATION

The basic idea is that the fractional diffusion equation discussed in refs. (Scalas, *et al.*, 2000; Mainardi, *et al.*, 2000; Raberto, *et al.*, 2002; Scalas, *et al.*, 2003; Scalas, *et al.*, 2004; Scalas, 2005; Scalas, 2006) is equivalent to the *Fokker-Planck* equation for a *Langevin* equation where Gaussian white noise is replaced by more general white noise types. In this case, eq (19) becomes:

$$dx = dW \quad (22)$$

where $W(t)$ is a generalization of the Wiener process (Scalas, 2006). The process $W(t)$ can be characterized by means of the continuous-time random walk (CTRW) method. For uncoupled continuous-time random walks with exponentially distributed waiting times, the limiting process is a Markovian Lévy flight with an α-stable one-point unconditional probability distribution ($0 < \alpha \leq 2$). If the waiting-time distribution is not exponential, the limiting process is non-Markovian. It differs from fractional Brownian motion and its probability distribution has another parameter β with values in the interval (0,1), the case $\beta = 1$ being Markovian (Mainardi, *et al.*, 2000; Scalas, 2006; Meerschaert and Scheffler, 2004; Meerschaert, *et al.*, 2002). In its turn, eq. (20) becomes:

$$\frac{\partial^\beta p(x,t)}{\partial t^\beta} = \frac{\partial^\alpha p(x,t)}{\partial |x|^\alpha} \quad (23)$$

where $\partial^\beta / \partial t^\beta$ is the Caputo derivative (Caputo, 1967; Caputo and Mainardi, 1971), and $\partial^\alpha / \partial |x|^\alpha$ is the (symmetric) Riesz derivative (Saichev and Zaslavsky, 1997; Zaslavsky, 2005) for $0 < \beta \leq 1$ and $0 < \alpha \leq 2$. Again, it is possible to write an auxiliary function:

$$\psi(x,t) = r(x,t)\exp(iS(x,t)) \quad (24)$$

($\hbar = 1$) so that:

$$p(x,t) = |\psi(x,t)|^2 = r^2(x,t) \quad (25)$$

As in Section 1.2, $v = 0$ and the action $S(x,t)$ is constant. It is sufficient to study the evolution equation for the amplitude, $r(x,t)$. This turns out to be (Mainardi, *et al.*, 2000; Raberto, *et al.*, 2002; Scalas, *et al.*, 2001; Scalas, *et al.*, 2004; Scalas, 2005; Scalas, 2006; Meerschaert and Scheffler, 2004; Meerschaert, *et al.*, 2002):

$$\frac{\partial^\beta r^2(x,t)}{\partial t^\beta} = \frac{\partial^\alpha r^2(x,t)}{\partial |x|^\alpha} \quad (26)$$

The solution of the Cauchy problem ($r^2(x,0) = \delta(x)$) for eqs. (23) or (26) is known as (Scalas, *et al.*, 2004; Podlubny, 1999; Samko, *et al.*, 1993):

$$r^2(x,t) = p(x,t) = \frac{1}{2\pi}\frac{1}{t^{\beta/\alpha}}\int_{-\infty}^{+\infty}\exp\left(-i\kappa\frac{x}{t^{\beta/\alpha}}\right)E_\beta\left(-|\kappa|^\alpha\right)d\kappa \quad (27)$$

where E_β denotes the one-parameter Mittag-Leffler function of order β. An exhaustive study of the solution in the space-time domain is found in (Podlubny, 1999), and therefore also the amplitude $r(x,t)$, the square root of the above solution, is to be considered as known.

The equation for the amplitude $r(x,t)$ can be considered (or defined) as the Schrödinger equation for our problem. In this simple case, imaginary terms do not appear as the action is constant. Moreover, the dissipative case is considered and no stationary solution is present, in contrast with eq. (16), where a constant action, S, yields a stationary amplitude R.

3. DISCUSSION AND CONCLUSIONS

It is very important to find a physical justification for the use of fractional operators in Physics and, in particular, in Quantum Mechanics. Indeed, the origin of the Laplacian spatial operator in the Schrödinger equation is the presence of a quadratic linear-momentum term in the classical Hamiltonian. A mere replacement of this term with a different exponent cannot be easily explained (Montroll, 1974; West, 2000).

In this paper, a derivation of a fractional Schrödinger equation (26) has been presented for the simple case of a pure diffusive process with dissipation. The Gaussian white noise has been replaced by more general kinds of white noise and both the Markovian ($\beta = 1$) and non-Markovian ($0 < \beta < 1$) cases have been considered. This derivation is based on Fényes-Nelson theory.

Extensions of this approach to conservative diffusive processes will face a main difficulty: using appropriate chain and Leibniz rules for the fractional operators involved (Podlubny, 1999). This problem is already present in the simple case considered above, where these rules are necessary to formally write down a fractional differential equation for the amplitude, r(x,t).

ACKNOWLEDGEMENTS

D. Baleanu acknowledges support from Dipartimento di Scienze e Tecnologie Avanzate, Università del Piemonte Orientale, Alessandria, Italy for a short visit.

REFERENCES

Caputo, M. (1967). Linear models of dissipation whose Q is almost frequency independent. *Geophysical Journal of the Royal Astronomical Society*, **13**, 529-539.

Caputo, M. and F. Mainardi (1971). Linear models of dissipation in anelastic solids. *Rivista del Nuovo Cimento (Ser. II)*, **1**, 161-198.

Davidson, M. (1979). A Generalization of the Fenyes-Nelson Stochastic Model of Quantum Mechanics. *Letters in Mathematical Physics*, **3**, 271-277.

Fényes, I. (1952). Probability Theoretical Foundation and Interpretation of Quantum Mechanics. *Zeitschrift für Physik*, **132**, 81-106.

Gorenflo, R., F. Mainardi, E. Scalas and M. Raberto (2001). Fractional calculus and continuous-time finance III: the diffusion limit. In: M. Kohlmann and S. Tang (Editors): *Trends in Mathematics - Mathematical Finance*, 171-180, Birkhäuser, Basel.

Laskin, N. (2000). Fractional quantum mechanics. *Physical Review E*, **62**, 3135-3145.

Laskin, N. (2002). Fractional Schrödinger equation. *Physical Review E*, **66**, 056108 -056115.

Mainardi, F., M. Raberto, R. Gorenflo and E. Scalas (2000). Fractional calculus and continuous-time finance II: the waiting-time distribution. *Physica A*, **287**, 468-481.

Mainardi, F., Yu. Luchko and G. Pagnini, (2001). The fundamental solution of the space-time fractional diffusion equation. *Fractional Calculus and Applied Analysis*, **4**, 153-192.

Meerschaert, M. M. and H.P. Scheffler (2004). Limit theorems for continuous-time random walks with infinite mean waiting times. *J. Appl. Prob.*, **41**, 623-638.

Meerschaert, M. M., D.A. Benson, H.P. Scheffler and B. Baeumer (2002). Stochastic solution of space-time fractional diffusion equations. *Physical Review E*, **65**, 041103.

Montroll, E.W. (1974). In: *Physical Reality and Mathematical Description* edited by C. Enz and M. Mehra (Reidel, Dordrecht, The Netherlands), pp. 501-598.

Naber, M. (2004). Time fractional Schrödinger equation. *Journal of Mathematical Physics*, **45**, 3339-3352.

Nelson, E. (1966). Derivation of the Schrödinger equation from Newtonian mechanics. *Physical Review E*, **150**, 1079-1085.

Nelson, E. (1967). *Dynamical Theory of Brownian Motion*. Princeton University Press. See also Paul, W. and J. Baschnagel (1999), *Stochastic processes: from physics to finance*. Springer Verlag, Berlin.

Podlubny, I. (1999). *Fractional Differential Equations*. Academic Press.

Raberto, M., E. Scalas and F. Mainardi (2002). Waiting times and returns in high-frequency financial data: an empirical study. *Physica A*, **314**, 749-755.

Saichev, A. I. and G.M. Zaslavsky (1997). Fractional kinetic equations: solutions and applications. *Chaos*, **7**, 753-764.

Samko, S.G., A.A. Kilbas, O.I. Marichev (1993). *Fractional integrals and derivatives: Theory and applications*. Gordon and Breach Science Publishers.

Scalas, E., R. Gorenflo, F. Mainardi and M. Raberto (2003). Revisiting the derivation of the fractional diffusion equation. *Fractals*, **11**, 281-289.

Scalas, E., R. Gorenflo and F. Mainardi (2004a). Uncoupled continuous-time random walks: Solution and limiting behavior of the master equation. *Physical Review E*, **69**, 011107-1/8.

Scalas, E. (2004b). Five years of continuous-time random walks in Econophysics. In: *Proceedings of WEHIA* (A. Namatame (editor)). Kyoto.

Scalas, E. (2006). Applications of continuous-time random walks in Finance and Economics. *Physica A*, **362** (2), 225-239.

West, B. (2000). Quantum Lévy propagators. *Journal of Physical Chemistry B*, **104**, 3830-3832.

Scalas, E., R. Gorenflo and F. Mainardi (2000). Fractional calculus and continuous-time finance. *Physica A*, **284**, 376-384.

Zaslavsky, G.M. (2005). *Hamiltonian Chaos and Fractional Dynamics*. Oxford University Press, Oxford UK.