FRACTIONAL DIFFUSION EQUATIONS AND ANOMALOUS DIFFUSION

Anomalous diffusion has been detected in a wide variety of scenarios, from fractal media, systems with memory, transport processes in porous media to fluctuations of financial markets, tumour growth, and complex fluids. Providing a contemporary treatment of this process, this book examines the recent literature on anomalous diffusion and covers a rich class of problems in which surface effects are important, offering detailed mathematical tools of usual and fractional calculus for a wide audience of scientists and graduate students in physics, mathematics, chemistry, and engineering. Including the basic mathematical tools needed to understand the rules for operating with the fractional derivatives and fractional differential equations, this self-contained text presents the possibility of using fractional diffusion equations with anomalous diffusion phenomena to propose powerful mathematical models for a large variety of fundamental and practical problems in a fast-growing field of research.

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To Lucas Evangelista Gomes,
who has just arrived among us
L. R. E.

To Alice and Pedro, with love
E. K. L.

Se tu se' or, lettore, a creder lento
ciò ch'io dirò, non sarà maraviglia,
ché io che 'l vidi, a pena il mi consento.

[If thou art, Reader, slow now to believe
What I shall say, it will no marvel be,
For I who saw it hardly can admit it.]

(Dante, Inferno XXV, 46–48)

Contents

Preface

The very irregular state of motion observed by Robert Brown for small pollen grains suspended in water initiated one of the the most fascinating fields of science. The importance of such discovery – the so-called diffusion process – is immeasurable; it has been found in many contexts and is widespread in nature. A characteristic feature of this random motion is the linear growth with time exhibited by the mean square displacement, which is typical of a Markovian process. In contrast with this situation, a large class of systems and processes present a diffusion behaviour characterised by a nonlinear time dependence of the same quantity, thus constituting what is called anomalous diffusion behaviour.

The last decades have witnessed an increased interest in the anomalous diffusion processes that seem to be indeed present in a variety of experimental scenarios in physics, chemistry, biology, and several other branches of engineering; it is a rapidly growing field of research, attracting the attention of the scientific community. This happens from the theoretical side – due to the new mathematical problems evoked – but also from the point of view of experimental or practical applications. It is noteworthy that the number of studies reporting experimental problems dealing with anomalous diffusion has strongly increased – this attests to the ubiquity of a phenomenon initially considered a rare event.

The power of the mathematical tools based on fractional calculus, on the other hand, has also attracted the attention of the community working with pure and applied mathematics. The association of these techniques with the diffusional problem represents in practice a new field of research. It was shown in several ways that fractional calculus, if it is not unique, is nevertheless a suitable or even the natural mathematical framework to use to face the high complexity represented by anomalous diffusion phenomena. One powerful way of using these mathematical tools to analyse diffusion processes leads naturally to the necessity to search for solutions of fractional linear and nonlinear diffusion equations.

The purpose of this book is to provide an updated literature on anomalous diffusion, covering also a rich class of problems in which surface effects in diffusion problems are important. Our motivations to write it come from the necessity to communicate recent consolidated advances of our research field to a wide audience of scientists and students in physics, mathematics, chemistry, engineering, and other, interdisciplinary areas. This is done by showing the possibility of using fractional diffusion equations in connection with anomalous diffusion phenomena to propose useful mathematical models for a large variety of fundamental and practical problems.

As a result, this book offers detailed mathematical tools of usual and fractional calculus to explore the deep significance of anomalous diffusion phenomena. Likewise, it also presents a discussion about the significance and meaning of fractional calculus. Some of the basic mathematical tools needed to understand the rules for operating with fractional derivatives and fractional differential equations are discussed in detail, in order to convey to the reader the essential techniques employed. It is hoped that it may be used by the reader to navigate the complex literature represented by these challenging problems, offering a comprehensive approach that combines, in a systematic and well-organised way, the study of contemporary anomalous diffusion problems with advanced techniques of calculus, emphasising the recent developments of fractional calculus.

The first part of the book is dedicated to presenting and discussing essential physical and mathematical concepts, forming the background material for the reading of the rest of the work.

In Chapter 1, we review some basic mathematical results, focusing on the essential properties of integral transforms of Fourier, Laplace, Hankel, and Mellin and their applications to simple problems. This presentation is followed by an account of special functions, emphasising the ones that arise more naturally in the framework of fractional calculus, such as the Mittag-Leffler, Wright, and the H-function of Fox, as well as their integral transforms. In Chapter 2, we propose a survey of fractional calculus, starting with a brief historical account of the evolution of the concepts of differentiation and integration of arbitrary order, and finishing with a concise discussion of the main properties of the fractional operators to be used in subsequent chapters. To complete this part of the book dedicated to fundamentals, in Chapter 3, we also present a brief history of the approaches to the diffusion phenomena, emphasising the first investigations of Brownian motion, the random walk problem, and its connection with the diffusion process, until the appearance of the concept of anomalous diffusion.

The second part of the book is devoted to presenting, in successive steps – each one incorporating a further degree of generalisation with respect to the previous one – a large number of solutions of the fractional diffusion equations in different applications.

Our presentation starts in Chapter 4 with the one-dimensional diffusion equation, written in terms of fractional operators in time and space variables, and focusing on some simple problems and applications. We discuss the concept of Lévy flights and the use of the continuous-time random walk formalism to understand the physical implications of the presence of fractional derivatives in the theoretical description of these systems. In Chapter 5, we consider the influence of the surfaces or membranes on diffusive processes. The problems we treat are intended to explore how the surface may modify the diffusive process of a system governed by a fractional diffusion equation. In the cases we analyse, the system may exhibit an anomalous diffusive behaviour for which surface effects play a nonnegligible role. In Chapter 6, we investigate situations in which nonlinear terms intervene in the diffusion equation as well as d-dimensional problems. These linear and nonlinear fractional diffusion equations take into account a diffusion coefficient with spatial dependences and external forces. Of particular importance in this regard is analysis of intermittent motion – the transition between diffusion and rest – to understand how it can can be described in the framework of the random walk approach, because this permits us to explore the manifestation of different diffusive regimes in the system. In Chapter 7, the phenomenon of anisotropic diffusion is explored by means of both usual and fractional diffusion equations. The analytical solutions of the two-dimensional comb-model with integer and fractional derivatives, and also with a drift term, are obtained. This opens different perspectives on the phenomenon, because it is shown that anomalous diffusion may be well described even in the framework of usual diffusion equations for some constrained systems. We show also that it can be investigated by means of some simplified picture of highly disordered systems. In Chapter 8, we investigate the time-dependent solutions of the fractional Schrödinger equation in presence of nonlocal terms. Extensions of the Schrödinger equation encompassing fractional derivatives in the spatial and temporal variables are an elegant way to tackle nonlocal and non-Markovian effects. For this reason, the continuous-time random walk approach is used to obtain consistent formulations of the fractional Schrödinger equation. A series of formal solutions is obtained for problems involving the presence of memory kernels, distributed order memory kernels, and nonlocal terms.

The third part of the book is formed by two chapters dedicated to a deep exploration of the role of the anomalous diffusion phenomena in the impedance spectroscopy response of liquid samples.

In Chapter 9, we present some analytical results obtained by means of a pioneering application of the fractional diffusion equations to the electrochemical impedance technique. After reviewing the fundamental equations of the continuum Poisson–Nernst–Planck (PNP) model, these main equations are rewritten in terms of time-fractional and distributed order derivatives, and the predictions of the model are analysed, emphasising the low frequency behaviour of the impedance by means of analytical solutions. This is the first step towards an extension of the PNP model to encompass anomalous diffusion. Some experimental data are invoked to test the robustness of the model in treating interfacial effects on the impedance in the low frequency region. Finally, in Chapter 10, the pathways towards the construction of PNP anomalous (PNPA) models are presented. It is analytically demonstrated that the effect of a constant-phase element in an equivalent electrical circuit may be represented by an appropriated term added to the boundary conditions of PNP or PNPA models. Thus, it is shown that the impedance spectroscopy models based on the fractional diffusion equations may be used to build an entire framework of continuum models general enough to analyse impedance data of high complexity.

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It is time to invite the reader to explore with us the new class of problems and scenarios treated in this book. We are sure it can be used as a textbook in scientific and technological areas as well as an advanced monograph in frontier physics and applied mathematics, helping the reader to discover or to deepen their knowledge of fractional calculus and anomalous diffusion phenomena. The warning represented by Dante's quotation at the beginning of the enterprise may be slightly modified just to remember that, if the reader is slow now to believe what we shall tell, that should be no cause for wonder, for we, who saw it slightly before, remain enlightened – as we hope the reader becomes, after reading it!