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Partial differential equations for collective behaviors of path integrals of sub-diffusive processes

Marie-Christine Néel, Catherine Choquet[1],

SUMMARY

Various models represent the spreading of dissolved chemicals by assuming individual molecule positions described by some stochastic process, whose probability density function (p.d.f) satisfies a partial differential equation (p.d.e). Though the classical paradigm of Brownian motion and diffusion equation clearly describes solute spreading in a fluid at rest, data recorded in some complex media suggest immobile stays of random duration: experiments are needed to discuss such assumption. While many experiments document solute concentration (i.e. the density of a stochastic process representing molecule position $x(t)$ at each time instant t), recent techniques measure ensemble functionals of quantities noted $a(t)$, and deduced from each molecule trajectory by integrating some function u of space and time:

$$a(t) = \int_0^t u(x(t'), t')dt'.$$

If $x(t)$ represents Brownian motion super-imposed to some average velocity field v, the density $\mathcal{P}$ of $x(t)$ satisfies the Advection-Diffusion Equation (i.e. diffusion equation with a convective term). The joint density $P(x, a, t)$ of the position $x(t)$ and of the path integral $a(t)$ of an ensemble of molecules then satisfies the classical Feynmann-Kac Equation (FKE), deduced from the ADE by a adding the derivative of uP w.r.t. a. We investigate the p.d.e. satisfied by P when $x(t)$ represents a stochastic process deduced from the above Brownian motion with bias, by inserting immobile stays whose random duration has a p.d.f. falling off as $t^{-\alpha-1}$ with $0 < \alpha < 1$ at large t. In this case, the density $\mathcal{P}$ of $x(t)$ satisfies

$$\partial\mathcal{P} = (\mathrm{Id} + \Lambda I_{0,+}^{1-\alpha})^{-1}\partial_x[\partial_x D\mathcal{P} - v\mathcal{P}]. \tag{1}$$

It is the fractal Mobile-Immobile Model (f-MIM), similar to the ADE, except for the non-local operator $(\mathrm{Id}+\Lambda I_{0,+}^{1-\alpha})^{-1}$ deduced from the fractional integral $I_{0,+}^{1-\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{f(t')}{(t-t')^\alpha} dt'$. We show that the joint density $P(x, a, t)$ of x and a satisfies a generalized FKE, is deduced from (1) by adding the derivative $\partial_a(uP)$ (w.r.t. the path integral value a) and transposing $(\mathrm{Id} + I_{0,+}^{1-\alpha})^{-1}$ with translations of the a variable. After a rapid outline of the proof, we demonstrate practical applications related with the interpretation of Nuclear Magnetic Resonance (NMR) signals.

Keywords: fractional equations, anomalous dispersion, path integrals

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[1]Department: UMR 1114 EMMAH
University: Université d'Avignon et des Pays de Vaucluse
Postal address: 84018 Avignon Cedex, France
mcneel@avignon.inra.fr

[2]Department: Laboratoire MIA, EA 3165
University: Université de La Rochelle
Postal address: F-17000 La Rochelle, France
cchoquet@univ-lr.fr