From non-Brownian Functionals to a Fractional Schrödinger Equation

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We derive backward and forward fractional Schrödinger type of equations for the distribution of functionals of the path of a particle undergoing anomalous diffusion. Fractional substantial derivatives introduced by Friedrich and co-workers [PRL 96, 230601 (2006)] provide the correct fractional framework for the problem at hand. In the limit of normal diffusion we recover the Feynman-Kac treatment of Brownian functionals. For applications, we calculate the distribution of occupation times in half space and show how statistics of anomalous functionals is related to weak ergodicity breaking.

PACS numbers: 02.50.Ey,05.40.-a,45.10.Hj

Brownian functionals have many applications in physics, and hence are well investigated [1, 2]. With the path of a Brownian particle \( x(t) \) in the time interval \((0, t)\), we define the functional as \( A = \int_0^t U[x(t)]\,dt \), where \( U(x) \) is some prescribed function. Since \( x(t) \) is a random path, \( A \) is a random variable. As discussed in a recent review [2], Brownian functionals model many phenomena, such as: fluctuating interfaces \( U(x) \approx x^2 \), statistics of occupation times \( U(x) \) is equal to the step function \( \theta(x) \), Obukhov’s model of advection of particles in turbulent flow \( U(x) = x \) and the velocity field is modeled with Brownian motion, and finance of stock prices \( U(x) = \exp(-\beta x) \) [2], to name only a few examples. Kac used Feynman’s path integral method to obtain the (imaginary time) Schrödinger equation for the distribution function \( \theta(x) \) of a particle undergoing anomalous diffusion [2]. The celebrated Feynman-Kac formula is based on the assumption that the diffusion is normal Brownian motion. However, we know today that in a vast number of applications in physics the underlying distribution of the path of a particle undergoing anomalous diffusion. Examples include the (imaginary time) Schrödinger equation for the differential derivative [11], and the function \( U(x) \) plays the role of a potential. A few applications are then worked out.

CTRW model. We consider a random walk on a one dimensional lattice with lattice spacing \( a \). Jumps are to nearest neighbors only and with equal probability of jumping left or right. Waiting times between jump events are independent identically distributed random variables with a probability density function (PDF) \( \psi(\tau) \). Thus, the particle waits on lattice point \( x_0 \) (the starting point) for time \( \tau \) drawn from \( \psi(\tau) \), then jumps with probability 1/2 to \( x_0 + a \) or \( x_0 - a \), and then the process is renewed. The main interest of this Letter is the case \( \psi(\tau) \sim B_0 \tau^{-(1+\alpha)/[\Gamma(-\alpha)]} \), when \( 0 < \alpha < 1 \). In this case, the waiting time is moment-less \((\tau = \infty)\) and the diffusion becomes anomalous. Values of \( \alpha \) for a large number of systems and models are given in [6, 7, 10].

CTRW Functionals. Let \( G(x, A, t) \) be the joint probability density function of finding the particle on \((x, A)\) at time \( t \). Denote the time the particle performed the last jump in the sequence as \( t - \tau \). According to the model the particle is on \((x, A)\) at time \( t \) if it was on \((x - \tau U(x), A - \tau U(x))\) at time \( t - \tau \), immediately after the last jump was made. Let \( Q_n(x, A, t)\,dxdA \) be the probability per unit time, to arrive in \([x + dx, (A, A + dA)]\) after \( n \) jumps. Then

\[
G(x, A, t) = \int_0^t \frac{W(\tau)}{\int_0^\infty W(\tau')\,d\tau'} \sum_{n=0}^{\infty} Q_n \{ x - \tau U(x), A - \tau U(x), t - \tau \} \,d\tau,
\]

where \( W(\tau) = 1 - \int_0^\tau \psi(\tau')\,d\tau' \) is the probability for \( \tau \) moving in time interval \((t - \tau, t)\). The summation over \( n \) is over the random number of jumps made. The probability of arriving in \((x, A)\) after \( n + 1 \) jumps \( Q_{n+1}(x, A, t) \), is recursively related to \( Q_n(x, A, t) \) according to

\[
Q_{n+1}(x, A, t) = \int_0^t \psi(\tau) \frac{1}{\tau} \left\{ Q_n [x - a, A - \tau U(x - a), t - \tau] + Q_n [x + a, A - \tau U(x + a), t - \tau] \right\} \,d\tau.
\]

To derive this equation, we notice that to reach point \( x \) after \( n + 1 \) steps one has to be after \( n \) steps, in one of the nearest neighbors \((x - a \text{ or } x + a)\) with probability 1/2 for each event. Hence to reach \( A \), one has to jump from \( A - \tau U(x \pm a) \), where here \( \tau \), the time interval between jumps, is randomly distributed with the PDF \( \psi(\tau) \).

In what follows we consider \( U(x) \geq 0 \), namely functionals with positive support, where it is natural to in-
roduce the Laplace transform $A \rightarrow p$\cite{12}. It is easy to see that
\[ \int_0^\infty Q_n(x, A-U(x)\tau, t-\tau)e^{-pA}dA = e^{-pU(x)\tau}Q_n(x, p, t-\tau), \]  
where along this work we use the convention that the variables in the parenthesis define the space we are working in, and thus $Q_n(x, p, t)$ is the Laplace $A \rightarrow p$ transform of $Q_n(x, A, t)$. We now Laplace transform Eq. (1) with respect to time, $t \rightarrow s$, using the convolution theorem and Eq. (3) to find
\[ G(x, p, s) = \sum_{n=0}^\infty \frac{1 - \hat{\psi}[s + pU(x)]}{s + pU(x)} Q_n(x, p, s), \]  
where $\hat{\psi}(s) = \int_0^\infty \psi(t) \exp(-st)dt$ is the Laplace transform of the waiting time PDF. Fourier transform, $x \rightarrow k$, of Eq. (4) yields
\[ G(k, p, s) = \sum_{n=0}^\infty \frac{1 - \hat{\psi}[s + pU(-i\frac{\partial}{\partial k})]}{s + pU(-i\frac{\partial}{\partial k})} Q_n(k, p, s), \]  
where the well known Fourier transformation $x \rightarrow -i\frac{\partial}{\partial k}$ was used. To complete this part of the derivation we calculate $Q_n(k, p, s)$ using Eq. (2) and find the iteration rule
\[ Q_{n+1}(k, p, s) = \cos(ka)\hat{\psi}\left[s + pU\left(-\frac{\partial}{\partial k}\right)\right] Q_n(k, p, s). \]  
The initial input for $n = 0$ is $Q_0(k, p, s) = 1$, since $Q_0(x, A, t) = \delta(x)\delta(A)\delta(t)$, namely the particle is on $x = 0$ and $A = 0$ at time $t = 0$, when the process begins. The iteration rule gives $Q_1(k, p, s) = \cos(ka)\hat{\psi}(s + pU(0))$. This makes perfect sense since, just after the first jump we have $A = U(0)\tau$ and $x$ is either on $+a$ or $-a$ (which comes from the inverse Fourier transform of $\cos(ka)$). Notice that the order of the operators in Eq. (6) is important, since $\cos(ka)$ does not commute with $\hat{\psi}[s + pU(-i\frac{\partial}{\partial k})]$. This order of operators is natural, since in CTRW we first wait and then make a jump. Summing Eq. (5) over the number of jumps $n$, and using Eq. (6), we find the formal solution
\[ G(k, p, s) = \frac{1 - \hat{\psi}[s + pU(-i\frac{\partial}{\partial k})]}{s + pU(-i\frac{\partial}{\partial k}) - 1 - \cos(ka)\hat{\psi}[s + pU(-i\frac{\partial}{\partial k})]}. \]  
When $p = 0$, we find the well known Montroll-Weiss equation $\cit{7, 13}$
\[ G(k, p = 0, s) = \frac{1 - \hat{\psi}(s)}{s} \frac{1}{1 - \cos(ka)\hat{\psi}(s)}, \]  
since $G(k, p = 0, s)$ is the Fourier-Laplace transform of the PDF of finding the particle on $x$ at time $t$.

**Derivation of forward fractional Schrödinger equation.** As mentioned in the introduction we assume that the underlying process is described by power law waiting times with diverging first moment. For that case we have the small $s$ expansion
\[ \hat{\psi}(s) = 1 - B_\alpha s^\alpha + \cdots. \]  
As well known in this case, the diffusion is anomalous with $(x^2(t)) = 2K_\alpha t^\alpha/\Gamma(1+\alpha)$, and $K_\alpha = a^2/2B_\alpha$ (units $\text{m}^2/\text{sec}^\alpha$)\cite{13}. Substituting Eq. (9) in Eq. (8) we find the long wavelength $k \rightarrow 0$ and long time $s \rightarrow 0$ limit
\[ G(k, p, s) \sim \left[ s + pU(-i\frac{\partial}{\partial k}) \right]^{\alpha-1} \left( 1 \right)^{\alpha-1} K_\alpha k^2 + \left[ s + pU(-i\frac{\partial}{\partial k}) \right]^{1-\alpha} G(k, p, s) - 1 = -K_\alpha k^2 \left[ s + pU(-i\frac{\partial}{\partial k}) \right]^{1-\alpha} G(k, p, s). \]  
Rearranging the expression in the last equation we find
\[ \frac{\partial G(x, p, t)}{\partial t} = K_\alpha \frac{\partial^2}{\partial x^2} \alpha D_t^{1-\alpha} G(x, p, t) - pU(x)G(x, p, t). \]  
\[ \cit{12} \]

The operator $\alpha D_t^{1-\alpha}$ is a fractional Riemann-Liouville substantial derivative, introduced by Friedrich and coworkers\cite{11}. In Laplace space, $\alpha D_t^{1-\alpha} \rightarrow (s + pU(x))^{1-\alpha}$. When $\alpha = 1$, Eq. (12) is the Schrödinger type of equation for Brownian functionals, originally derived from Feynman-Kac formula $\cit{2}$. Also note that if $p = 0$, Eq. (12) reduces to the expected fractional diffusion equation $\cit{5}$. Using Eq. (12), it is easy to show that $\frac{\partial(A)}{\partial t} = \langle U(x) \rangle$, where $\langle U(x) \rangle = \int U(x)P(x,t)dx$, and $P(x,t)$ is the PDF of finding the particle on $x$, i.e. the solution of the fractional diffusion equation. Of course this is the expected behavior since $\partial A/\partial t = U[x(t)]$.

**Backward Schrödinger equation.** We now derive a backward equation which turns out to be very useful $\cit{13}$. Let $G_{x_0}(A, t)$ be the PDF of the functional $A$, when the process starts on $x_0$. According to the CTRW model, the particle, after its first jump at time $\tau$, goes through either $x_0 + a$ or $x_0 - a$. Alternatively, the particle does not move at all during the measurement time $(0, t)$. Translating this observation to an equation, we have
\[ G_{x_0}(A,t) = \int_0^t d\tau \psi(\tau) \frac{1}{2} \left( G_{x_0+\tau} \left[ A - \tau U(x_0), t - \tau \right] + G_{x_0-\tau} \left[ A - \tau U(x_0), t - \tau \right] \right) + W(t) \delta \left[ A - U(x_0)t \right], \]  

where \( \tau U(x_0) \) is the contribution to \( A \) from the pausing time on \( x_0 \) in the time interval \( (0, \tau) \). The last term on the right hand side of Eq. (13) describes motionless particles, hence the Dirac delta function. Using Laplace transform technique similar to that used in the derivation of the forward equation, we find in the continuum limit, the backward fractional Schrödinger equation

\[ \frac{\partial G_{x_0}(p,t)}{\partial t} = K_\alpha \partial^\alpha_1 t G_{x_0}(p,t) - pU(x_0)G_{x_0}(p,t). \]  

Here, the fractional substantial derivative \( \partial^\alpha_1 t \) is in Laplace space \( t \rightarrow s \) space \( (s + pU(x_0)) \). Notice that this operator appears to the left of the Laplacian \( \partial^2 / \partial(x_0)^2 \) in Eq. (14), in contrast to the forward equation (12). Since in Eq. (13) the operators depend on \( x_0 \) and not on \( x \), Eq. (14) is called a backward equation. Eqs. (12,14) are the main equations of this manuscript since they provide a general framework for treating functionals of anomalous processes. When \( \alpha = 1 \) both equations reduce to the usual Schrödinger equations found in the Feynman-Kac treatment of Brownian functionals [2].

First Illustration: Lamperti’s law for distribution of occupation times. We consider the occupation time in half space: \( A = \int_0^t \theta(x(\tau)) d\tau \), usually denoted with \( t^+ \). This distribution was first computed by Lamperti using probabilistic methods [14] (see also [3]). Substituting \( U(x_0) = \theta(x_0) \) in Eq. (14), we solve the backward equation separately for \( x_0 > 0 \) and \( x_0 < 0 \), demanding the continuity of the solution and its derivative. In addition we have \( \lim_{x_0 \rightarrow -\infty} G_{x_0}(p,s) = (s + p)^{-1} \) since if \( x_0 \rightarrow \infty \), the particle is always in \( x > 0 \) and thus \( A = t \). Similarly \( \lim_{x_0 \rightarrow -\infty} G_{x_0}(p,s) = s^{-1} \) since then \( A = 0 \). At least in Laplace space, the solution of the fractional equation is easily obtained. For initial condition \( x_0 = 0 \), we find, after inversion of the solution to the time domain, the PDF of the scaled functional \( p^+ = t^+ / t \) i.e. the fraction of time spent in half of the space

\[ f(p^+) = \frac{\sin \pi p^+}{\pi} \left( p^+ \right)^{\alpha/2-1} \left( 1-p^+ \right)^{\alpha/2-1}. \]  

Naively, one expects that the particle spends half of the time in \( x > 0 \). In contrast, the Lamperti PDF Eq. (15) has two peaks at \( p^+ = 1 \) and \( p^+ = 0 \), while its minimum on \( p^+ = 1/2 \) coincides with its average \( \langle p^+ \rangle = 1/2 \). In the limit \( \alpha \rightarrow 0 \) we get two delta functions on \( p^+ = 1 \) and \( p^+ = 0 \), indicating that the particle is localized in either \( x > 0 \) or \( x < 0 \) for the whole observation time. For \( \alpha \rightarrow 1 \) we recover the well known arcsine law of P. Lévy [2].

Second Illustration: Weak Ergodicity breaking. The technique used so far is valid for free sub-diffusion. Our approach can be easily extended to study functionals in an external binding field, to give new insights on the problem of ergodicity. We consider CTRW in the harmonic potential \( V(x) = m\omega^2 x^2 / 2 \) as modeled by the fractional Fokker-Planck equation [7, 14, 17] (see [18] for normal diffusion). Algorithms that generate the stochastic continuous trajectories were recently proposed [19, 20]. Consider the time average \( x = \int_0^t x(\tau) d\tau / t \), hence \( A = \int_0^t x(\tau) d\tau \) and \( U(x_0) = x_0^2 / 2T \). If the process is ergodic, then, due to the symmetry of the harmonic field, the time average \( x = \int_0^t x(\tau) d\tau / t \), in the long time limit, is statistically equal to zero. For anomalous sub-diffusion \( \alpha < 1 \) it is well known that ergodicity is broken [21, 22]. With our tool box for anomalous functionals, we now treat the problem of fluctuations of the time average \( x \).

We use the forward Eq. (12) for \( A = \int_0^t x(\tau) d\tau \), with the modification that the Laplacian of free diffusion, is replaced by the Fokker-Planck operator \( L_{fp} = K_\alpha (\partial^2 / \partial x^2 + m\omega^2 x^2/k_BT + \partial^2 / \partial x^2) \), which will be further justified in a longer publication and \( T \) is the temperature. Thus, the modified forward equation of motion is

\[ \frac{\partial G(x,A,t)}{\partial t} = L_{fp} G(x,A,t) - x \frac{\partial}{\partial A} G(x,A,t). \]  

Here in Laplace space \( \rightarrow s \) space we have \( \partial^\alpha_1 t \rightarrow (s + x^2 \partial^2 / \partial x^2)^{1-\alpha} \). The same equation, after renaming of variables, describes a weakly damped kinetic model of super-diffusive Lévy walks [11, 23]. We investigate the fluctuations of the time average, namely, \( \langle \tau^2 \rangle = \langle A^2 \rangle / t^2 \). Using Eq. (16), we derive equations of motion for the low order moments \( \langle x \rangle, \langle A \rangle, \langle xA \rangle, \langle A^2 \rangle \) and \( \langle x^2 \rangle \). These equations are closed in the sense that they are not coupled to any higher order moments, due to the harmonic potential under investigation and the choice of the functional. Using the relaxation time \( \tau^\alpha \equiv k_BT/(K_\alpha m\omega^2) \), we find in Laplace space
\[ \langle A^2 \rangle = \frac{2}{s^3} \left[ (1 - \alpha) + (s\tau)^{\alpha} \right] \frac{\left[ 2(x^2)_{th} + (s\tau)^{\alpha} \langle x_0 \rangle^2 \right]}{2 + (s\tau)^{\alpha}}, \]  

(17)

where \( \langle x^2 \rangle_{th} = k_0 T/m\omega^2 \) and \( x_0 \) is the initial condition. Inverting to the time domain, using \( \langle x^2 \rangle = \langle A^2 \rangle / t^2 \), we find

\[ \langle \tau^2 \rangle = (1 - \alpha) \langle x^2 \rangle_{th} + 2\alpha \left( 2 \langle x^2 \rangle_{th} - \langle x_0 \rangle^2 \right) E_{\alpha,3} \left[ - (t/\tau)^\alpha \right] + 2 \left( 1 + \alpha \right) \left( \langle x_0 \rangle^2 - \langle x^2 \rangle_{th} \right) E_{\alpha,3} \left[ - (t/\tau)^\alpha \right], \]  

(18)

where \( E_{\alpha,3}(z) = \sum_{n=0}^{\infty} z^n / \Gamma(\alpha n + 3) \) is the Mittag-Leffler function \( [24] \). To derive Eq. (18) we used [24]. For long times we have

\[ \langle \tau^2 \rangle \sim (1 - \alpha) \langle x^2 \rangle_{th} + [(3\alpha - 1) \langle x^2 \rangle_{th} + (1 - \alpha) \langle x_0 \rangle^2] \Gamma(3 - \alpha)^{-1} \left( \frac{t}{\tau} \right)^\alpha + O \left( \left( \frac{t}{\tau} \right)^{2\alpha} \right), \]  

(19)

To conclude we have found both forward and backward fractional Schrödinger equations describing distributions of functionals of widely observed sub-diffusive processes. When a binding force is included, the analysis of these functionals leads to a new kinetic approach to weak ergodicity breaking, in contrast to the equilibrium framework provided in [21, 22]. While previous work considered specific functionals, our work provides a very general toolbox for this new field.

**Acknowledgment** This work was supported by the Israel Science Foundation. S.C. is supported by the Adams Fellowship Program of the Israel Academy of Sciences and Humanities.

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[23] Sub-diffusive motion in a harmonic potential is sometimes called the fractional Ornstein-Uhlenbeck process [17]. As we show in the text, it yields the scaling $\langle A^2 \rangle \sim t^2$ which leads to ergodicity breaking. For the kinetic model of ballistic Lévy walks in [11], the velocity undergoes a fractional Ornstein-Uhlenbeck process and there $\langle x^2 \rangle \sim t^2$.

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