

Continuous-time random walk as a guide to fractional Schrödinger equation

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We argue that the continuous-time random walk approach may be a useful guide to extend the Schrödinger equation in order to incorporate nonlocal effects, avoiding the inconsistencies raised by Jeng *et al.* [J. Math. Phys. **51**, 062102 (2010)]. As an application, we work out a free particle in a half space, obtaining the time dependent solution by considering an arbitrary initial condition. © 2010 American Institute of Physics. [doi:10.1063/1.3491333]

I. INTRODUCTION

Diffusion, an ubiquitous phenomena in nature, may be related to stochastic processes which depending on the characteristics can be Markovian or non-Markovian. The usual diffusion, which has the mean square displacement with linear dependence on time, i.e., $\langle(x-\langle x \rangle)^2\rangle \sim t$, is a typical Markovian process and is usually described by the differential equation $\partial_t \rho = D \partial_x^2 \rho$, which may be formally related to the Schrödinger equation. Non-Markovian processes lead to anomalous diffusion and has a different time dependence to the mean square displacement which in many situations is given by $\langle(x-\langle x \rangle)^2\rangle \sim t^\alpha$ (α less and greater than one corresponds to subdiffusion and superdiffusion, respectively). In order to investigate these nonusual processes, several formalisms have been employed such as nonlinear diffusion equations,¹ Langevin equations,² continuous-time random walk (CTRW),³ and fractional Fokker–Planck equations.^{4,5} The last one has been successfully used to investigate anomalous diffusion with the advantage of incorporating external fields and to employ analogous procedure of calculations of the boundary value problems of the corresponding standard equations.

As the Fokker–Planck equations, the Schrödinger equation has been analyzed by extending the usual differential operator to fractional ones. These extensions of the Schrödinger equation have been analyzed by considering several situations.^{6–11} However, there are some inconsistencies which were pointed out in Ref. 12. In order to avoid these inconsistencies and to get the correct solution, we argue that the CTRW approach may be used as a guide to obtain consistent extensions of the Schrödinger equation. The following analysis is focused on this direction, i.e., how it is possible to use the CTRW as guide to prescribe differential operators to the Schrödinger equation. In Sec. II, we investigate this point and in Sec. III an application is presented. Discussions and conclusions are in Sec. IV.

II. CTRW AND FRACTIONAL SCHRÖDINGER EQUATION

In order to perform the desired analysis, it is interesting to note that the usual diffusion and Schrödinger equations essentially have the same mathematical structure in the absence of potential. In fact, the solutions for Schrödinger equation may be obtained from the diffusion equation by considering $t \rightarrow t/(i\hbar)$ and $\mathcal{D} \rightarrow -\hbar^2/(2m)$. Another feature is that diffusion equations can be obtained from the CTRW by performing a suitable choice to the probability density function.^{3,4} This

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means that to describe a diffusive process subjected, for example, to an absorbent or reflecting surfaces, it is possible to use a CTRW approach or a diffusion equation. In addition, memory effects or other characteristics which are not conveniently described by usual diffusion equation may be described by the CTRW approach if an appropriated choice of the probability density function is employed. Depending on the effects considered, we are led to diffusion-like equations which may have, for example, fractional time derivatives (e.g., $\partial_t^\gamma \rho = \mathcal{D} \partial_x^2 \rho$),¹³ spatial fractional derivatives (e.g., $\partial_x^\alpha \rho = \mathcal{D} \partial_t \rho$),¹⁴ and fractional time derivatives of distributed order [e.g., $\int_0^\infty d\gamma p(\gamma) \partial_t^\gamma \rho = \mathcal{D} \partial_x^2 \rho$].¹⁵ Notice that in such cases the boundary conditions are considered when the CTRWs are formulated to investigate these phenomena. In this direction, it should be mentioned that the spatial operator may not preserve its form depending on the conditions considered as pointed out in Ref. 16. Typical examples are the cases of a system restricted to a half space with reflecting boundary conditions¹⁷ or absorbing boundary conditions.¹⁸ These situations may be related to a diffusion equations with a fractional operator which are different from that one obtained when the system is not restricted. These examples suggest that the Schrödinger equation may have different representations to the spatial operator depending on the situation considered.

In the scenario proposed here, extensions of the Schrödinger equation may be formulated by using the CTRW approach as guide to obtain a suitable form for nonlocal spatial operators which accomplishes the conditions required by the system. This procedure basically consists to obtain diffusion-like equations from the CTRW approach and based on the operators present in these equations to modify the usual form of the Schrödinger equation in order to incorporate the non-local operators. In this manner, we also avoid the cumbersome calculations which may arise in other formulations of the Schrödinger equation to find its solutions. An application is worked in Sec. III to show how the CTRW approach may be used to get a consistent extension of the Schrödinger equation.

III. APPLICATION

Let us consider as an application, of our propose, a particle in a half space in absence of potential which has as initial condition an arbitrary wave function $\bar{\Psi}(x)$ satisfying the boundary conditions $\Psi(0, t) = \Psi(\infty, 0) = 0$. In order to obtain a Schrödinger-like equation in terms of the fractional operators, we first investigate the corresponding diffusion equation. More precisely, by using the CTRW approach, the mathematical structure of this diffusion equation based on a long tailed distribution for the jumping probability density is considered. In order to perform this analysis, we use the developments presented in Ref. 17 to get a diffusion-like equation to a system in half space with absorbing boundary conditions, i.e., $\rho(0, t) = \rho(\infty, t) = 0$. The spatial operator obtained from this analysis will be used to formulate the Schrödinger equation and, consequently, to avoid the inconsistencies discussed in Ref. 12.

Following the development performed in Ref. 17, the probability $\rho(x, t) dx$ of finding a particle in $[x, x+dx]$ at instant t satisfies the generalized master equation,

$$\rho(x, t) = \delta(x) \int_t^\infty dt' \psi(t') + \int_0^\infty dx' \int_0^t dt' \rho(x', t') \Lambda(x, x') \psi(t-t'), \quad (1)$$

where $\psi(t)$ represents the waiting time distribution and $\Lambda(x, x')$ is the probability density for the particle jumping from x' arrives in $[x, x+dx]$. Note that the second term of Eq. (1) involves a spatial integration over the interval $[0, \infty)$ since the particles are constrained to stay in the half space. Suitable choices to Eq. (1) have to be done in order to accomplish the conditions required in previous paragraph. One of them concerns to a short tailed waiting time distribution such as $\psi(t) = e^{-t/\tau} / \tau$ which lead us to a first-order time derivative, as in the case of the usual diffusion equation. The other choice to be done is about the jumping probability which needs to incorporate a long tailed behavior and to satisfy the boundary condition imposed on $x=0$. A typical choice to the probability jumping in order $\rho(x, t)$ to satisfy these conditions required by the system is $\Lambda(x, x') \propto (1/|x-x'|^{1+\alpha} - 1/|x+x'|^{1+\alpha})$ (for the reflective case, see Ref. 17). Note that this choice naturally accomplishes the symmetries of the sine Fourier transform. Similar situation was worked

out in Ref. 18 to investigate Riesz fractional derivative in the presence of an absorbing boundary conditions. By substituting these assumptions in Eq. (1) and performing some calculations, it is possible to show that the diffusion equation which emerges in this scenario can be written as

$$\partial_t \rho(x, t) = \mathcal{D}_\alpha \tilde{\partial}_x^\alpha \rho(x, t), \quad (2)$$

with

$$\tilde{\partial}_x^\alpha \rho(x, t) = \mathcal{A}_\alpha \frac{\partial^2}{\partial x^2} \int_0^\infty dx' \rho(x', t) (|x - x'|^{1-\alpha} - |x + x'|^{1-\alpha}), \quad (3)$$

where $\mathcal{A}_\alpha = \sqrt{\pi/2} / (\Gamma(2-\alpha) \sin(\pi\alpha/2))$. Based on these results, a possible extension to the Schrödinger equation which accomplishes the conditions required for a particle in a half space is

$$i\hbar \partial_t \Psi(x, t) = -\mathcal{K}_\alpha \tilde{\partial}_x^\alpha \Psi(x, t), \quad (4)$$

where \mathcal{K}_α is a constant which for $\alpha=2$ recovers the usual form, i.e., $\mathcal{K}_{\alpha=2} = \hbar^2 / (2m)$. Thus, Eq. (4) also recovers the usual form of the Schrödinger equation to $\alpha=2$, however, restricted to the interval $[0, \infty)$. Note that the spatial fractional operator present in Eq. (4) is different from that one worked out in Refs. 6–12 since the conditions required by the system restrict the movement to a half space. It is also important to mention that the spatial operator may change its formal aspect when other conditions are imposed to the system.

Now, we solve Eq. (4) for an arbitrary initial condition that accomplishes the conditions $\Psi(0, t) = \Psi(\infty, 0) = 0$. Applying the sine Fourier transform $[\mathcal{F}_S\{\dots\} = \sqrt{2/\pi} \int_0^\infty dx \sin(kx) \dots]$ and $\mathcal{F}_S^{-1}\{\dots\} = \sqrt{2/\pi} \int_0^\infty dk \sin(kx) \dots]$, Eq. (4) can be simplified to

$$i\hbar \frac{d}{dt} \Psi(k, t) = \mathcal{K}_\alpha k^\alpha \Psi(k, t) \quad (5)$$

since $\mathcal{F}_S\{\tilde{\partial}_x^\alpha \Psi(x, t)\} = -k^\alpha \Psi(k, t)$ with k non-negative. The solution of Eq. (5) is given by

$$\Psi(k, t) = \Psi(k, 0) e^{-i(\mathcal{K}_\alpha/\hbar)k^\alpha t}. \quad (6)$$

By performing the inverse Fourier transform, we obtain that

$$\Psi(x, t) = \int_0^\infty dx' \bar{\Psi}(x') \mathcal{G}(x, x', t), \quad (7)$$

with

$$\mathcal{G}(x, x', t) = \frac{1}{\alpha |x - x'|} \mathbf{H}_{2,2}^{1,1} \left[\frac{|x - x'|}{(\bar{\mathcal{K}}_\alpha t)^{1/\alpha}} \left| \begin{matrix} (1, 1/\alpha)(1, 1/2) \\ (1, 1)(1, 1/2) \end{matrix} \right. \right] - \frac{1}{\alpha |x + x'|} \mathbf{H}_{2,2}^{1,1} \left[\frac{|x + x'|}{(\bar{\mathcal{K}}_\alpha t)^{1/\alpha}} \left| \begin{matrix} (1, 1/\alpha)(1, 1/2) \\ (1, 1)(1, 1/2) \end{matrix} \right. \right], \quad (8)$$

where $\bar{\mathcal{K}}_\alpha = i\mathcal{K}_\alpha/\hbar$ and $\mathbf{H}_{p,q}^{m,n} [x^{(a_1, A_1), \dots, (a_p, A_p)} / (b_1, B_1), \dots, (b_q, B_q)]$ is the Fox H function¹⁹ (see Appendix for some properties). Note that this solution satisfies Eq. (4) and the boundary conditions required by the system, in contrast to the situations discussed in Ref. 12. For $|x| \rightarrow \infty$ the asymptotic limit of Eq. (8) for $\alpha < 2$ is given by

$$\mathcal{G}(x, x', t) \sim \frac{\mathcal{N}_\alpha}{(\bar{\mathcal{K}}_\alpha t)^{1/\alpha}} \left(\frac{1}{|z_-|^{1+\alpha}} - \frac{1}{|z_+|^{1+\alpha}} \right), \quad (9)$$

where $z_\pm = (x \pm x') / (\bar{\mathcal{K}}_\alpha t)^{1/\alpha}$ and $\mathcal{N}_\alpha = \sin(\pi\alpha/2) \Gamma(1+\alpha) / \pi$.

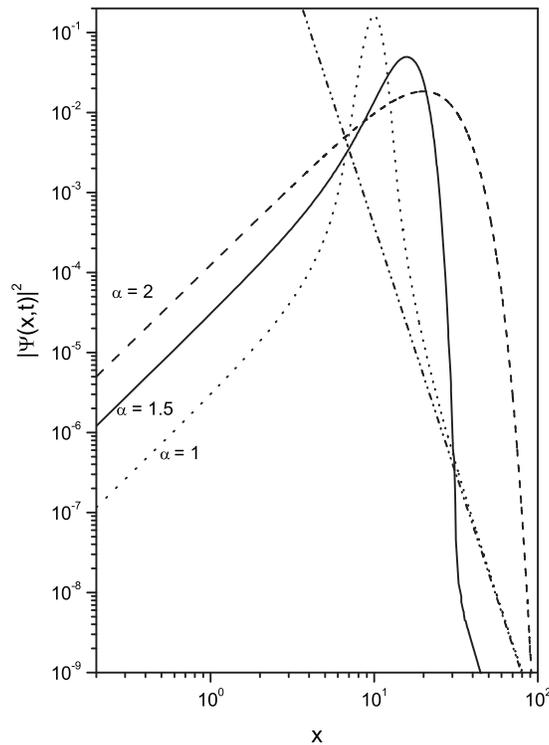


FIG. 1. Behavior of $|\Psi(x,t)|^2$ vs x is illustrated for different values of α by considering, for simplicity, $\mathcal{K}_\alpha=1$ and $t=10$. A dashed-dotted line was incorporated to evidence the power-law behavior presented by the solution in the asymptotic limit, i.e., $x \rightarrow \infty$, when $\alpha \neq 2$.

Figure 1 illustrates the behavior of solution (7) by considering, for simplicity, the initial condition $\bar{\Psi}(x) = \sqrt{4/\sqrt{\pi x}} e^{-x^2/2}$ and typical values of α . The asymptotic behavior manifested by the solution is a power-law when long times are considered, as illustrated by Fig. 1. Figure 2 illustrates the time evolution of the solution for $\alpha=1$ by considering, for simplicity, the initial condition used in Fig. 1. In addition, it shows that of the solution is initially dominated by the behavior of the wave function used here (short tailed) as initial condition and for long times it is governed by the Green function which contains the dynamic aspects of the system (see also Ref. 20). It is also interesting to mention that this result can be extended to situations with different spreading regimes. In these cases, the spatial fractional operators of distributed order to the Schrödinger equation will be obtained from the prescription used here.

IV. DISCUSSIONS AND CONCLUSIONS

We have discussed how the continuous-time random walks may be used as a guide to prescribe Schrödinger equations to processes where nonlocal effects may be present, accomplishing the boundary conditions of the system. This procedure is essentially motivated by the formal relation between the diffusion and Schrödinger equations. For this reason, we first investigate what is the form of the corresponding diffusion equation (e.g., incorporating nonlocal effects and boundary conditions) by using the CTRW and, after, we propose the form of the differential operators to the Schrödinger equation. In this manner, the equation which emerges from this prescription satisfies the conditions imposed to the system (e.g., boundary conditions) and incorporates the nonlocal effects manifested by the presence of unusual differential operators. In fact, for the usual Schrödinger equation, we have $\partial_x^2 \psi \sim \psi_{n+1} - 2\psi_n + \psi_{n-1}$ in a lattice which essentially contains first neighbor terms. Situations where we effectively have to consider that many additional neighbors terms go in the direction of fractional derivatives. In a phenomenological point of

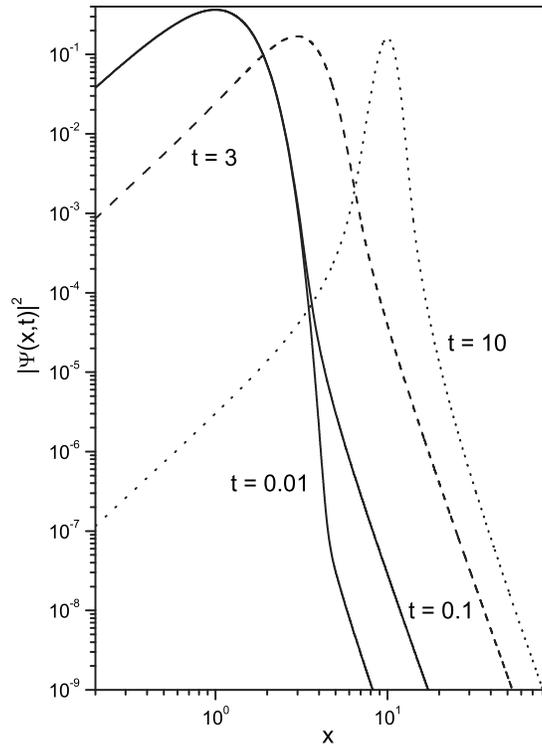


FIG. 2. Behavior of $|\Psi(x,t)|^2$ vs x is illustrated for different times by considering, for simplicity, $\mathcal{K}_\alpha=1$ and $\alpha=1$.

view, the specific heat for noncrystalline solids by taking very low temperature into account has been investigated by considering a fractional Schrödinger equation.²¹ In addition, scenarios containing self-similarity, memory, non-Gaussian fluctuations are possible situations where the fractional extensions of the Schrödinger may be useful⁷ as occurs when we consider anomalous diffusion. Finally, we hope that the analysis presented here be useful to discuss situations involving extensions of the Schrödinger equation with nonlocal effects.

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APPENDIX: THE FOX H FUNCTION

The Fox H function (or H-function) may be defined in terms of the Mellin-Branes-type integral,¹⁹

$$H_{pq}^{mn} [x | \begin{smallmatrix} (a_p, A_p) \\ (b_q, B_q) \end{smallmatrix}] = H_{pq}^{mn} [x | \begin{smallmatrix} (a_1, A_1), \dots, (a_p, A_p) \\ (b_1, B_1), \dots, (b_q, B_q) \end{smallmatrix}] = \frac{1}{2\pi i} \int_L \chi(\xi) x^{-\xi} d\xi,$$

$$\chi(\xi) = \frac{\prod_{j=1}^m \Gamma(b_j - B_j \xi) \prod_{j=1}^n \Gamma(1 - a_j + A_j \xi)}{\prod_{j=m+1}^q \Gamma(1 - b_j + B_j \xi) \prod_{j=n+1}^p \Gamma(a_j - A_j \xi)}, \tag{A1}$$

where $m, n, p,$ and q are integers satisfying $0 \leq n \leq p$ and $1 \leq m \leq q$. It may also be defined by its Mellin transform,

$$\int_0^\infty \mathbf{H}_{pq}^{mn} [ax^{(a_p, A_p)}_{(b_q, B_q)}] x^{\xi-1} dx = a^{-\xi} \chi(\xi). \quad (\text{A2})$$

Here, the parameters have to be defined, such that $A_j > 0$ and $B_j > 0$ and $a_j(b_h + \nu) \neq B_h(a_j - \lambda - 1)$, where $\nu, \lambda = 0, 1, 2, \dots$, $h = 1, 2, \dots, m$, and $j = 1, 2, \dots, m$. The contour L separates the poles of $\Gamma(b_j - B_j \xi)$ for $j = 1, 2, \dots, m$ from those of $\Gamma(1 - a_j + A_j \xi)$ for $j = 1, 2, \dots, n$.¹⁹ The H-function is analytic in x if either (i) $x \neq 0$ and $M > 0$ or (ii) $0 < |x| < 1/B$ and $M = 0$, where $M = \sum_{j=1}^q B_j - \sum_{j=1}^p A_j$ and $B = \prod_{j=1}^p A_j \prod_{j=1}^q B_j^{-B_j}$.

Some useful properties of the Fox H function found in Refs. 19 are listed below.

- (i) The H-function is symmetric in the pairs $(a_1, A_1), \dots, (a_p, A_p)$, likewise $(a_{n+1}, A_{n+1}), \dots, (a_p, A_p)$; in $(b_1, B_1), \dots, (b_q, B_q)$ and in $(b_{n+1}, B_{n+1}), \dots, (b_q, B_q)$.
- (ii) For $k > 0$

$$\mathbf{H}_{pq}^{mn} [x^{(a_p, A_p)}_{(b_q, B_q)}] = k \mathbf{H}_{pq}^{mn} [x^{k(a_p, A_p)}_{(b_q, kB_q)}]. \quad (\text{A3})$$

- (iii) The multiplication rule is

$$x^k \mathbf{H}_{pq}^{mn} [x^{(a_p, A_p)}_{(b_q, B_q)}] = \mathbf{H}_{pq}^{mn} [x^{(a_p + kA_p, A_p)}_{(b_q + kB_q, B_q)}]. \quad (\text{A4})$$

- (iv) For $n \geq 1$ and $q > m$,

$$\mathbf{H}_{pq}^{mn} [x^{(a_1, A_1)(a_2, A_2) \dots (a_p, A_p)}_{(b_1, B_1) \dots (b_{q-1}, B_{q-1})(a_1, A_1)}] = \mathbf{H}_{p-1, q-1}^{mn-1} [x^{(a_2, A_2) \dots (a_p, A_p)}_{(b_1, B_1) \dots (b_{q-1}, B_{q-1})}]. \quad (\text{A5})$$

- (v) For $m \geq 2$ and $p > n$,

$$\mathbf{H}_{pq}^{mn} [x^{(a_1, A_1) \dots (a_{p-1}, A_{p-1})(b_1, B_1)}_{(b_1, B_1)(b_2, B_2) \dots (b_q, B_q)}] = \mathbf{H}_{p-1, q-1}^{m-1n} [x^{(a_2, A_2) \dots (a_{p-1}, A_{p-1})}_{(b_2, B_2) \dots (b_q, B_q)}]. \quad (\text{A6})$$

- (vi) If the poles of $\prod_{j=1}^m \Gamma(b_j - B_j \xi)$ are simple, the following series expansion is valid:

$$\begin{aligned} \mathbf{H}_{pq}^{mn} [x^{(a_p, A_p)}_{(b_q, B_q)}] &= \sum_{h=1}^m \sum_{\nu=0}^{\infty} \frac{(-1)^\nu x^{(b_h + \nu)/B_h}}{\nu! B_h} \frac{\prod_{j=1, j \neq h}^m \Gamma\left(b_j - \frac{B_j}{B_h}(b_h + \nu)\right)}{\prod_{j=m+1}^q \Gamma\left(1 - b_j + \frac{B_j}{B_h}(b_h + \nu)\right)} \\ &\quad \times \frac{\prod_{j=1}^n \Gamma\left(1 - a_j + \frac{A_j}{B_h}(b_h + \nu)\right)}{\prod_{j=n+1}^p \Gamma\left(a_j - \frac{A_j}{B_h}(b_h + \nu)\right)}. \end{aligned} \quad (\text{A7})$$

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