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Fractional Schrödinger equation with noninteger dimensions

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ABSTRACT

The spatial and time dependent solutions of the Schrödinger equation incorporating the fractional time derivative of distributed order and extending the spatial operator to noninteger dimensions are investigated. They are obtained by using the Green function approach in two situations: the free case and in the presence of a harmonic potential. The results obtained show an anomalous spreading of the wave packet which may be related to an anomalous diffusion process.

1. Introduction

The anomalous behavior found in several phenomena such as diffusion on fractals [1,2], biological cells [3,4], animal foraging behavior [5], nanoscience [6,7], motion of colloidal particles [8], systems with long range interactions [9,10], and adsorption–desorption process [11–13] has motivated researchers of many scientific fields to investigate the non-Markovian nature of the processes related to anomalous diffusion [14–16]. One of the main characteristics of the anomalous diffusion is the time dependence of the mean square displacement which in several cases may be expressed as $\langle (r-\langle r\rangle)^2\rangle \sim t^{\alpha}$, where $\alpha < 1,\ \alpha = 1$ or $\alpha > 1$ corresponds to sub-, normal or superdiffusive cases, respectively. It is also possible to have situations in which the mean square displacement is not defined [14]. This feature may occur when Lévy distributions are involved. In order to cover these scenarios, some formalisms, such as the random walks [17], master equations [18], Langevin equations [15] and diffusion equations [19], have been used with suitable considerations. In particular, the diffusion equation has been extended by incorporating spatial and time fractional derivatives and have been systematically investigated such as the developments performed in Refs. [20–32]. Others extensions or applications involving the fractional calculus have also been performed, for example, in physics [33,34], engineering [35–37], and chemistry [38], as pointed out in Ref. [39] where some of the major documents and events in the area of fractional calculus are reported. A direct consequence of extension of the usual time derivative to a fractional one is a nonusual spreading of the system which may be related to a rich class of anomalous diffusions. In this scenario, the Schrödinger equation has been extended to incorporate spatial and time fractional derivatives. This procedure leads to the presence of a nonusual spreading of the system, i.e., the wave packet, and may be related to a rich class of anomalous diffusions. These situations have been systematically investigated in Refs. [40–42,47,43–46]. In Ref. [48], an extension of the Schrödinger equation was obtained from a random walk thus avoiding the cumbersome situations discussed in Ref. [47]; and in Refs. [49,50], nonlocal terms are considered in the usual and fractional Schrödinger equation. Nonlinear extensions of the Schrödinger equation have also been considered in Ref. [51]. In the framework of these formal developments, the solutions of the following Schrödinger equation will be considered:

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$$i\hbar\int_0^1 d\overline{\gamma}p(\overline{\gamma})\frac{\partial^{\overline{\gamma}}}{\partial t^{\overline{\gamma}}}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m_\gamma}\widetilde{\nabla}^2\psi(\mathbf{r},t) + V(\mathbf{r},t)\psi(\mathbf{r},t), \tag{1}$$

where $\mathbf{r} = (r,\theta), m_\gamma$ is an effective mass. Note that the $p(\gamma)$ is a distribution and the fractional time derivative considered is the Caputo one [52], i.e.,

$$\frac{\partial^\gamma}{\partial t^\gamma}\psi(\mathbf{r},t) = \frac{1}{\Gamma(n-\gamma)}\int_0^t \frac{\psi^{(n)}(\mathbf{r},\overline{t})}{(t-\overline{t})^{\gamma+1-n}}d\overline{t}, \tag{2}$$

with $n-1<\gamma<n,\ \psi^{(n)}(\mathbf{r},t) = d^n\psi(\mathbf{r},t)/dt^n$, and the spatial operator is given by

$$\widetilde{\nabla}^2\psi(\mathbf{r},t) \equiv \frac{1}{r^{\alpha-1}}\frac{\partial}{\partial r}\left(r^{\alpha-1}\frac{\partial}{\partial r}\psi(\mathbf{r},t)\right) + \frac{1}{r^2\sin^{\alpha-2}\theta}\frac{\partial}{\partial\theta}\left(\sin^{\alpha-2}\theta\frac{\partial}{\partial\theta}\psi(\mathbf{r},t)\right), \tag{3}$$

where α represents a noninteger dimension [53]. A particular case of Eq. (1) has been investigated in Ref. [54] in the context of the anomalous diffusion and for $p(\overline{\gamma}) = \delta(\overline{\gamma}-1)$ the usual form of the Schrödinger equation is recovered. The propagator for Eq. (1) is investigated for the free case and in the presence of a harmonic potential. In both cases, the boundary condition employed is $\lim_{|\mathbf{r}|\to\infty}\psi(\mathbf{r},t) = 0$ and the distribution $p(\gamma)$ considered is $p(\overline{\gamma}) = \mathcal{A}\delta(\overline{\gamma}-1) + \mathcal{B}\delta(\overline{\gamma}-\gamma)$ with $\mathcal{A}+\mathcal{B} = 1$. These developments are performed in Section 2 while in Section 3 the discussions and conclusions are presented.

2. Schrödinger equation

The discussion starts by considering Eq. (1) for the free case. It can be written as follows

$$i\hbar\int_0^t d\overline{\gamma}p(\overline{\gamma})\frac{\partial^{\overline{\gamma}}}{\partial t^{\overline{\gamma}}}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m_\gamma}\widetilde{\nabla}^2\psi(\mathbf{r},t). \tag{4}$$

To solve this equation and find the propagator, one may use the Laplace transform to obtain

$$\frac{\hbar}{2m_\gamma i}\widetilde{\nabla}^2\psi(\mathbf{r},s) + \Lambda(s)\psi(\mathbf{r},s) = \overline{\Lambda}(s)\psi(\mathbf{r},0), \tag{5}$$

where $\Lambda(s) = \int_0^1 d\overline{\gamma}p(\overline{\gamma})s^{\overline{\gamma}},\ \overline{\Lambda}(s) = \Lambda(s)/s$, and the last term represents an arbitrary initial condition which is normalized. The formal solution for this equation is given by

$$\psi(\mathbf{r},s) = \overline{\Lambda}(s)\int_0^\infty dr r^{\alpha-1}\int_0^\pi d\theta\sin^{\alpha-2}\theta\psi(\mathbf{r}',0)\mathcal{G}(\mathbf{r},\mathbf{r}';s), \tag{6}$$

with the propagator (or Green function) determined by the equation

$$\frac{\hbar}{2m_\gamma i}\widetilde{\nabla}^2\mathcal{G}(\mathbf{r},\mathbf{r}';s) + \Lambda(s)\mathcal{G}(\mathbf{r},\mathbf{r}';s) = \frac{1}{r^{\alpha-1}\sin^{\alpha-2}\theta}\delta(r-r')\delta(\theta-\theta'). \tag{7}$$

Since the propagator has a radial and an angular dependence, it is convenient to first investigate the situation characterized by radial symmetry and, then, to consider the angular dependence. For the case in which the system only depends on the variable r, one may use the eigenfunctions of the Sturm–Liouville problem related to the spatial operator, i.e., one solves the equation $\widetilde{\nabla}^2\varphi = -p^2\varphi$, with φ satisfying the boundary conditions of ψ. For this operator, by taking the radial symmetry into account, one finds

$$\mathcal{G}(r,r';s) = \int_0^\infty dp\, p\,\varphi(r,p)\overline{\mathcal{G}}(p,r';s), \tag{8}$$

whose inverse is given by

$$\overline{\mathcal{G}}(p,r';s) = \int_0^\infty dr\, r^{\alpha-1}\varphi(r,p)\mathcal{G}(r,r';s), \tag{9}$$

where $\varphi(r,p) = r^{1-\alpha/2}\mathrm{J}_\nu(pr),\ \nu = \alpha/2-1$, and $\mathrm{J}_\nu(x)$ is the Bessel function. It is possbile to show that

$$\overline{\mathcal{G}}(p,r';s) = \frac{\varphi(r',p)}{\Lambda(s) + i\hbar p^2/(2m_\gamma)}. \tag{10}$$

Note that this solution was obtained for a general fractional time differential operator of distributed order leading us to a cumbersome calculations if a general $p(\overline{\gamma})$ is considered. For this reason and to face an interesting situation where different regimes can be manifested we consider $p(\overline{\gamma}) = \mathcal{A}\delta(\overline{\gamma}-1) + \mathcal{B}\delta(\overline{\gamma}-\gamma)$. This choice for $p(\overline{\gamma})$ implies the presence of different regimes one of them governed by the usual case and the other influenced by the index γ, where $0<\gamma<1$. By performing the inverse Laplace transform of Eq. (10), we obtain

$$\overline{\mathcal{G}}(p,r';t)=\varphi(r',p)\Omega_\gamma(p,t), \tag{11}$$

$$\Omega_\gamma(p,t)=\frac{1}{\mathcal{A}}\sum_{n=0}^{\infty}\frac{1}{\Gamma(1+n)}\left(-\frac{\mathcal{B}}{\mathcal{A}}t^{1-\gamma}\right)^n \mathrm{E}^{(n)}_{1,1-n\gamma}\left(\frac{\hbar p^2 t}{2m_\gamma i\mathcal{A}}\right), \tag{12}$$

where $\mathrm{E}^{(n)}_{\alpha,\beta}(x)$ is defined as the nth derivate of the generalized Mittag–Leffler function $\mathrm{E}_{\alpha,\beta}(x)$ ($\mathrm{E}_{\alpha,\beta}(x)=\sum_{n=0}^{\infty}x^n/\Gamma(\beta+\alpha n)$), i.e., $\mathrm{E}^{(n)}_{\alpha,\beta}(x)=d^n\mathrm{E}_{\alpha,\beta}(x)/dx^n$.

Let us first analyze, for simplicity, the case $\mathcal{A}=0$ with $\mathcal{B}=1$ which corresponds to a fractional case characterized by only one diffusive regime governed by the index γ. After, we extend the result for the case $\mathcal{A}\neq 1$ with $\mathcal{B}\neq 1$. For the first case, Eq. (11) yields

$$\overline{\mathcal{G}}(p,r';t)=t^{\gamma-1}\varphi(r',p)\mathrm{E}_{\gamma,\gamma}\left(\frac{\hbar p^2 t^\gamma}{2m_\gamma i}\right). \tag{13}$$

Note the presence of the generalized Mittag–Leffler function [52] in the previous equation, instead of the exponential function. This feature indicates that the relaxation of the initial wave packet is not usual because the Mittag–Leffler function is asymptotically governed by a power law. In fact, the function $\mathrm{E}_{\overline{\alpha},\beta}(x)$ has as asymptotic limit, for $x\to\infty$, $\mathrm{E}_{\overline{\alpha},\beta}(x)\sim -1/(\Gamma(\beta-\overline{\alpha})x)-1/\left(\Gamma(\beta-2\overline{\alpha})x^2\right)$ (for details see Ref. [52]). By using the previous results, one finds that the propagator is given by

$$\mathcal{G}(r,r';t)=t^{\gamma-1}\int_0^\infty dp\,p\,\varphi(r',p)\,\varphi(r,p)\mathrm{E}_{\gamma,\gamma}\left(\frac{\hbar p^2}{2m_\gamma i}t^\gamma\right). \tag{14}$$

In particular, it can be written as

$$\mathcal{G}(r,r';t)=2t^{\gamma-1}(rr')^{1-\alpha/2}\mathrm{H}^{1,0,1,1,1}_{2,[0:1],0,[0:2]}\left[\begin{matrix}(r'/r)^2\\ 2i\hbar t^\gamma/(m_\gamma r^2)\end{matrix}\left|\begin{matrix}\left(\frac{2-\nu}{2},1\right);\left(\frac{2+\nu}{2},1\right)\\ --;(0,1)\\ \left(-\frac{\nu}{2},1\right);\left(\frac{\nu}{2},1\right);(0,1),(1-\gamma,\gamma)\end{matrix}\right.\right], \tag{15}$$

where

$$\mathrm{H}^{L,M,M_1,N,N_1}_{E,[A:C],F,[B,D]}\left[\begin{matrix}x\\ y\end{matrix}\left|\begin{matrix}(\varepsilon_1,\omega_1),\ldots,(\varepsilon_E,\omega_E)\\ (a_1,\alpha_1),\cdots,(a_A,\alpha_A);(c_1,\gamma_1),\ldots,(c_C,\gamma_C)\\ (\xi_1,\varpi_1),\ldots,(\xi_F,\varpi_F)\\ (b_1,\beta_1),\ldots,(b_B,\beta_B);(d_1,\delta_1),\cdots,(d_C,\delta_D)\end{matrix}\right.\right] \tag{16}$$

is the generalized Fox H function [55,56]. For the particular case $\gamma=1$, Eq. (14) is reduced to

$$\mathcal{G}(r,r';t)=\frac{m}{i\hbar t}(rr')^{1-\alpha/2}e^{-\frac{mi}{2\hbar t}\left(r^2+r'^2\right)}\mathrm{I}_\nu\left(\frac{m}{i\hbar t}rr'\right). \tag{17}$$

By incorporating the angular variable in previous calculations, the propagator becomes

$$\mathcal{G}(\mathbf{r},\mathbf{r}';t)=t^{\gamma-1}\sum_{l=0}^{\infty}\int_0^\infty dp\,p\,\Theta_l(\theta)\Theta_l(\theta')\varphi_l(r',p)\varphi_l(r,p)\mathrm{E}_{\gamma,\gamma}\left(\frac{\hbar p^2}{2m_\gamma i}t^\gamma\right), \tag{18}$$

with

$$\Theta_l(\theta)=\mathcal{N}_l C_l^{\alpha/2-1}(\cos\theta), \tag{19}$$

where $C_l^{\widetilde{\alpha}}(\cos\theta)$ are the Gegenbauer polynomials [57], and

$$\mathcal{N}_l^2=\frac{l!\left(l+\frac{\alpha}{2}-1\right)}{2^{3-\alpha}\pi\Gamma(l+\alpha-2)}\left[\Gamma\left(\frac{\alpha}{2}-1\right)\right]^2. \tag{20}$$

The eigenfunctions $\varphi_l(r,p)$ are defined as before, with $\nu=\alpha/2+l-1$. The general form for the Green function with $\mathcal{A}\neq 1$ and $\mathcal{B}\neq 1$ is given by

$$\mathcal{G}(\mathbf{r},\mathbf{r}';t)=\sum_{l=0}^{\infty}\int_0^\infty dp\,p\,\Theta_l(\theta)\Theta_l(\theta')\varphi_l(r',p)\varphi_l(r,p)\Omega_\gamma(p,t). \tag{21}$$

The solution of Eq. (6), after inverting the Laplace transform, can be written in terms of Green's function as follows:

$$\psi(\mathbf{r},t)=\int_0^t d\bar{t}\,\overline{\Lambda}(t-\bar{t})\int_0^\infty dr'\,r'^{\alpha-1}\int_0^\pi d\theta'\sin^{\alpha-2}\theta'\psi(\mathbf{r}',0)\mathcal{G}(\mathbf{r},\mathbf{r}';\bar{t}), \tag{22}$$

with $\overline{\Lambda}(t)=\mathcal{A}+\mathcal{B}/[\Gamma(1-\gamma)t^\gamma]$. By using Eq. (22), one may investigate the spreading of the wave packet characterized by the initial condition $\psi(\mathbf{r},0)\propto e^{-\xi\mathbf{r}^2}$ with $\mathcal{A}=0$ and $\mathcal{B}=1$. Fig. 1 illustrates Eq. (22) for the previous initial condition in order to show the influence of the fractional time derivative on the time evolution of the wave function. It is remarkable that this

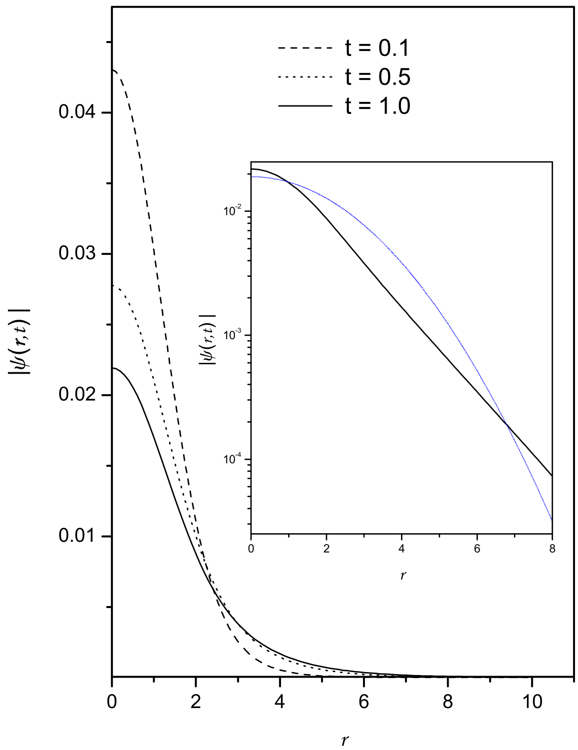

Fig. 1. Behavior of $|\psi(\mathbf{r},t)|$ versus r is illustrated in different times by considering, for simplicity, $\gamma = 1/2,\ \xi = 2,\ \hbar/(2m_\gamma) = 1$, and $\alpha = 3$. The inset graph compares the solution obtained from Eq. (22) with the usual one, i.e., $\gamma = 1$, in order to illustrate the differences in the asymptotic limit.

anomalous spreading of the wave packet is essentially governed by the fractional derivative: it adds non-Markovian characteristics, such as memory effects, to the system. In fact, the inset of Fig. 1 evidences the differences of the usual Gaussian behavior (see the blue dotted line)[1] and the exponential asymptotic behavior manifested by the solution (see the black solid line). In Fig. 2, we show the behavior of Eq. (22) for different values of γ. The blue and the red dotted lines correspond to the case $\gamma = 1/2$ and $\gamma = 1/4$, respectively. The black line is the usual case. Now, Eq. (1) subjected to the harmonic potential is considered. In this case, one is faced with the problem:

$$i\hbar\int_0^t d\overline{\gamma}p(\overline{\gamma})\frac{\partial^{\overline{\gamma}}}{\partial t^{\overline{\gamma}}}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m_\gamma}\widetilde{\nabla}^2\psi(\mathbf{r},t) + \frac{1}{2}m_\gamma\omega_\gamma^2\mathbf{r}^2\psi(\mathbf{r},t), \tag{23}$$

being subjected to the boundary condition discussed in Section 1. In order to find the solution for this case, the same procedure of the free case can be employed. One arrives at Eq. (22), with the propagator now given by

$$\mathcal{G}(\mathbf{r},\mathbf{r}';t) = e^{-\frac{m_\gamma\omega_\gamma}{2\hbar}(r^2-r'^2)}\sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\Theta_l(\theta')\Theta_l(\theta)\varphi_{n,l}(r')\varphi_{n,l}(r)\Upsilon_\gamma(\lambda_{n,l},t), \tag{24}$$

where

$$\Upsilon_\gamma(\lambda_{n,l},t) = \frac{1}{\mathcal{A}}\sum_{n=0}^{\infty}\frac{1}{\Gamma(1+n)}\left(-\frac{\mathcal{B}}{\mathcal{A}}t^{1-\gamma}\right)^n \mathrm{E}_{1,1-n\gamma}^{(n)}\left(\frac{\lambda_{n,l}}{i\hbar}t\right), \tag{25}$$

$$\varphi_{n,l}(r) = \overline{\mathcal{N}}_{n,l}r^l\mathrm{L}_n^{(\overline{\alpha})}\left(\frac{m_\gamma\omega_\gamma}{\hbar}r^2\right), \tag{26}$$

$$\overline{\mathcal{N}}_{n,l}^2 = \frac{2\Gamma(1+n)}{\Gamma(n+\alpha/2+l)}\left(\frac{m_\gamma\omega_\gamma}{\hbar}\right)^{\frac{1}{2}(\alpha+2l)} \tag{27}$$

and $\lambda_{n,l} = \omega_\gamma\hbar(2n+l+\alpha/2)$. In Eq. (26), $\overline{\alpha} = \alpha/2 + l - 1$ and $\mathrm{L}_n^{(\overline{\alpha})}(x)$ are the associated Laguerre polynomials. In Fig. 3, we illustrate for $\mathcal{A} = 0$ with $\mathcal{B} = 1$ the behavior of the solution when the harmonic potential is considered.

[1] For interpretation of color in Figs. 1 and 2, the reader is referred to the web version of this article.

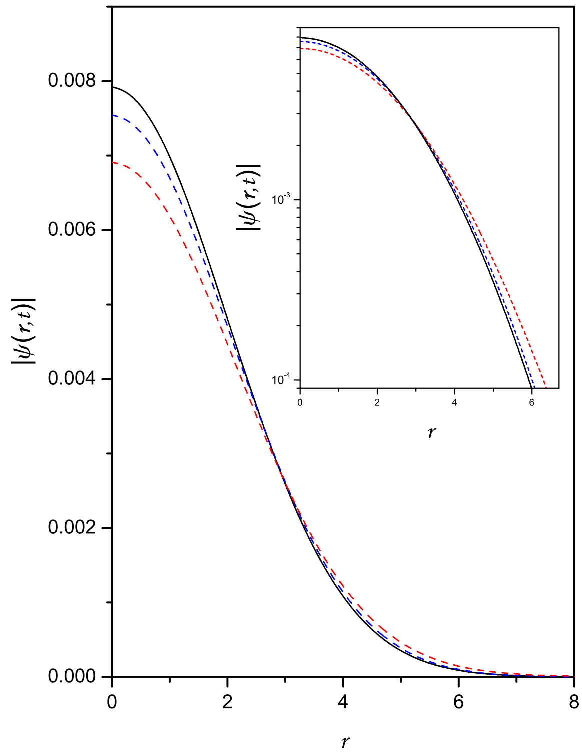

Fig. 2. Behavior of $|\psi(\mathbf{r},t)|$ versus r is illustrated for different values of γ by considering, for simplicity, $\xi = 1/2,\ \hbar/(2m_\gamma) = 1,\ t = 0.1$, and $\alpha = 3$.

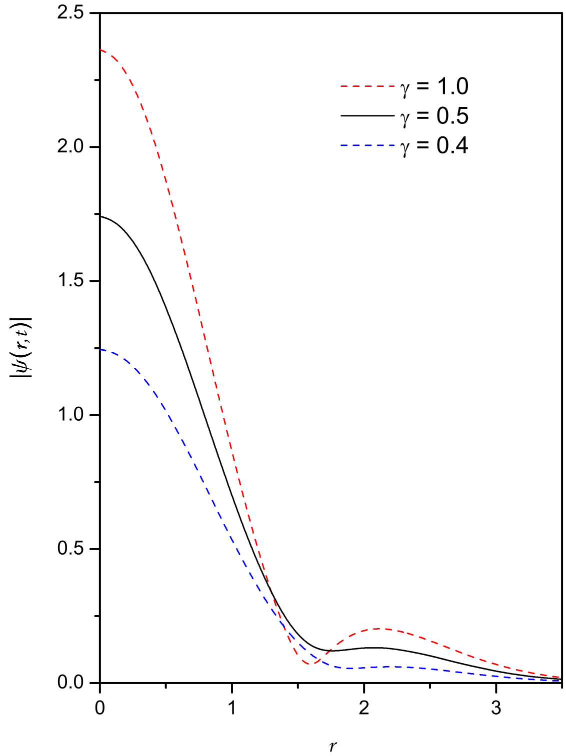

Fig. 3. Behavior of $|\psi(\mathbf{r},t)|$ versus r is illustrated for different values of γ by considering, for simplicity, $\xi = 1/2,\ m_\gamma\omega_\gamma/\hbar = 1,\ t = 0.1$, and $\alpha = 3$. The initial condition considered was $\psi(\mathbf{r},0) = \sqrt{8/(5\sqrt{\pi})}e^{-r^2/2}(5/2 - r^2)$.

3. Discussions and conclusions

Solutions for the Schrödinger equation incorporating noninteger dimensions on the spatial operator and extending the time derivative to a fractional one of distributed order by using the Caputo operator have been investigated. For the free case, the shape of the wave function is influenced by both aspects, even if the spreading of the packet is essentially governed by the fractional time derivative which produces an anomalous behavior. In particular, the presence of the fractional time derivative of distributed order may be connected to the presence of different diffusive regimes depending on the choice of $p(\gamma)$. For the choice performed here, we have the presence of two different regimes, one of them governed by the usual case and the other depending on γ. Similar features are verified when the harmonic potential is present. From the formal point of view, the results presented here can be useful to discuss situations characterized by an anomalous spreading of wave packets or probability distributions in connection to the phenomenon of anomalous diffusion.

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