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Fractional Schrödinger Wave Equation and Fractional Uncertainty Principle

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Abstract

Free particle wavefunction of the fractional Schrödinger wave equation is obtained. The wavefunction of the equation is represented in terms of generalized three-dimensional Green's function that involves fractional powers of time as variable t^{α}. It is shown that the wavefunction corresponding to the integral order Schrödinger wave equation follows as special case of that of the corresponding Schrödinger equation with fractional derivatives with respect to time. The wavefunction is obtained using Laplace and Fourier transforms methods and eventually the wavefunction is expressed in terms of Mittag-Leffler function. Heisenberg Uncertainty principle is deduced from the wavefunction of the fractional Schrödinger equation using the integral value of fractional parameter α=1.

1 Introduction

Recent applications of fractional equations to number of systems such as those exhibiting enormously slow diffusion or sub-diffusion have given opportunity for physicists to study even more complicated systems. Those systems include charge transport in amorphous semiconductors, the relaxation in polymer systems, fluid mechanics and viscoelasticity and Hall Effect. The generalized diffusion equation allows describing complex systems with anomalous behavior in much the same way as simpler systems. Anyway, fractional calculus is now considered as a practical technique in many branches of science including physics [1]. Several authors including [1-9] have discussed many examples of homogeneous fractional ordinary differential equations, homogenous fractional diffusion equation and homogenous wave equations. Debnath [7-9] considered solutions of fractional order homogeneous and nonhomogenous partial differential equations and integral equations in fluid mechanics.

The practical use of fractional calculus is underlined by the fact that Laplace transform of the operator ${}_0D_t^{-\alpha}f(t)$ has the simple form, $\mathcal{L}\left\{{}_0D_t^{-\alpha}f(t)\right\} = s^{-\alpha}\mathcal{L}\left\{f(t)\right\}$, where $\mathcal{L}$ represents Laplace transform.

In this paper, we are concerned with fractional time derivatives with 0< $\alpha < 1$ representing as the fractional parameter. The physical significance of the parameter α is unknown. The fractional Schrödinger wave equation may represent wave equation for quasi-particles when the parameter takes fractional values between $0 < \alpha < 1$, otherwise it will represent particle wave equation for α =1. We set $\beta = 0$ in the α-th fractional derivative ${}_\beta D_t^{-\alpha} = \frac{d^n}{dx^n}{}_\beta D_t^{\alpha-n}$, specifies $t = 0$ as the starting of the system's time evolution with $0 \leq \alpha \leq 1$ [3]. If this definition is applied to the diffusion equation for a particle at the origin of coordinates in n-dimensional space, it's mean squared displacement is proportional to time t. In a variety of physical systems, however, the simple scaling law is violated [10, 11]. The fractional diffusion equation provided the scaling law as t^α for the mean square distance [12].

In the the following, we use the fractional calculus to solve the Schrödinger wave equation for a free moving particle. The solution to this equation is presented in a closed form and the uncertainty principle is deduced for the special case α=1 for a free particle.

2 The Fractional Schrödinger Wave Equation

We will consider the solution of the fractional Schrödinger equation in the form given by

$$\frac{\partial^\alpha \psi(\mathbf{x},\mathrm{t})}{\partial t^\alpha} = \frac{i\hbar}{2m}\nabla^2\psi(\mathbf{x},\mathrm{t}), \tag{2.1}$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$, $\hbar$ is the Planck's constant divided by 2 π , m is the mass and $\psi(\mathbf{x},\mathrm{t})$ is a wave function of the particle. Also we set $a = \frac{i\hbar}{2m}$ as a complex constant and solve this equation (2.1) with the following initial and boundary conditions

$$\begin{aligned} &\psi(\mathbf{x},0) = \psi_0(\mathbf{x}) \\ &\psi(\mathbf{x},\mathrm{t}) \to 0 \quad \text{as } |\mathbf{x}| \to \infty,\ t > 0. \end{aligned} \tag{2.2}$$

We apply the joint Laplace transform with respect to t and the Fourier transform with respect to $\mathbf{x}$ (see reference [13]) defined by

$$\tilde{\bar{\psi}}(\mathrm{k},\mathrm{s}) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\,\mathrm{k}\bullet\mathrm{x}}\,d^3\mathrm{x}\int_0^{\infty} e^{-s\,t}\psi(\mathrm{x},\mathrm{t})\,dt. \tag{2.3}$$

Where – and ˜ are used to denote the Laplace and the Fourier transforms respectively, k and s are the Fourier and the Laplace transform variables respectively. Application of the joint transform to equations (2.1) and (2.2) give

$$s^{\alpha}\tilde{\bar{\psi}}(\mathrm{k},\mathrm{s}) - s^{\alpha-1}\,\tilde{\psi}(\mathrm{k},0) = a\,(i\,\mathrm{k})^2\,\tilde{\bar{\psi}}(\mathrm{k},\mathrm{s}). \tag{2.4}$$

We combine the terms and take the inverse Laplace transform of equation (2.4) to yield

$$\tilde{\psi}(\mathrm{k},\mathrm{s}) = \mathcal{L}^{-1}\left\{\frac{s^{\alpha-1}}{s^{\alpha}+a\,\mathrm{k}^2}\right\}\tilde{\psi}(\mathrm{k},0) = \mathrm{G}_{\alpha}(k,s)\,\tilde{\psi}(\mathrm{k},0). \tag{2.5}$$

Next, we use the formula for the inverse Laplace transform to express the solution in Mittag-Leffler function

$$\mathcal{L}^{-1}\left\{\frac{m!s^{\alpha-\beta}}{(s^{\alpha}+a)^{m+1}}\right\} = t^{m\,\alpha+\beta-1}E^{(m)}_{\alpha,\beta}(-a\,t^{\alpha}), \tag{2.6}$$

where $E_{\alpha,\beta}(z)$ is the Mittag-Leffler function (see Erdèlyi, 1955) defined by the series

$$E_{\alpha,\beta}(z) = \sum_{m=0}^{\infty}\frac{z^m}{\Gamma(m\,\alpha+\beta)}\,,\ \ \alpha>0,\ \ \beta>0 \tag{2.7}$$

where $\Gamma(x)$ is the Gamma function and

$$E^{(m)}_{\alpha,\beta}(z) = \frac{d^m}{dx^m}E_{\alpha,\beta}(z) \tag{2.8}$$

Application of the inverse Laplace transform combined with the formula in equation (2.5) and using equation (2.6) yields solution

$$\tilde{\psi}(\mathrm{k},t) = \tilde{\psi}(\mathrm{k},0)\,E_{\alpha,1}(-a\,\mathrm{k}^2t^{\alpha}) = G_{\alpha}(k,t)\tilde{\psi}(\mathrm{k},0), \tag{2.9}$$

where $\mathrm{k}^2 = \mathrm{k}_{\mathrm{x}}^2 + \mathrm{k}_{\mathrm{y}}^2 + \mathrm{k}_{\mathrm{z}}^2$ and the Green function is defined as $G_{\alpha}(k,t) = E_{\alpha,1}(-a\,k^2t^{\alpha}) = \sum_{m=0}^{\infty}\frac{(-a\,k^2t^{\alpha})^m}{\Gamma(m\,\alpha+1)}$. Alternatively, the Green function in Eq. (2.5) in momentum space may be simplified and the complex integration in variable s can be carried out to obtain

$$G_{\alpha}(\mathrm{k},\mathrm{t}) = \int_0^{\infty}\frac{\mathrm{s}^{\alpha-1}\mathrm{e}^{\mathrm{s}\,\mathrm{t}}}{\mathrm{s}^{\alpha}+\mathrm{a}\,\mathrm{k}^2}\,ds = \begin{cases} e^{-a\,k^2\,t} & \text{for } \alpha=1 \\ \frac{\sin(\pi\alpha)}{\pi\alpha}\int_0^{\infty}\frac{\mathrm{e}^{-(\mathrm{a}\,\mathrm{k}^2\,x)^{1/\alpha}\,t}}{\mathrm{x}^2+2x\cos(\pi\alpha)+1}\,dx & \text{for } 0<\alpha<1 \end{cases} \tag{2.10}$$

Both forms of the Green function in Eqs. (2.9) and (2.10) agree for $\alpha = \frac{1}{2}$ and α=1. For $\alpha = \frac{1}{2}$, the expression for Green function is $G_{1/2}(k,t) = E_{1/2,1}(-a\,\mathrm{k}^2 t^{1/2}) = e^{a^2\,k^4\,t} erfc(a\,k^2 t^{1/2})$.

Finally, we take the Fourier transform of equation (2.9) to obtain the solution of the wave equation (2.1).

$$\psi(\mathrm{x},t) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} e^{-i\,\mathrm{k}\bullet\mathrm{x}}\, \tilde{\psi}_0(\mathrm{k})\, \mathrm{E}_{\alpha,1}(-a\,\mathrm{k}^2 t^{\alpha}) d^3\mathrm{k}\,. \tag{2.11}$$

We assume that the Fourier transform of the initial wave function at t=0 to be as

$$\psi(\mathrm{k}) = \frac{1}{(2\pi)^{3/2}} \int_{-\infty}^{\infty} e^{-i\,\mathrm{k}\bullet\xi}\, \psi_0(\xi)\, d^3\xi\,. \tag{2.12}$$

By the convolution theorem of the Fourier transform (see Debnath [13]), the solution in equation (2.11) may be expressed in the form

$$\psi(\mathbf{x},t) = \int_{-\infty}^{\infty} G_{\alpha}(x-\xi,t)\, \psi_0(\xi)\, d^3\xi, \tag{2.13}$$

where the Green function is given by

$$G_{\alpha}(\mathrm{x},\mathrm{t}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} e^{i\,\mathrm{k}\bullet\mathrm{x}}\, \mathrm{E}_{\alpha,1}(-a\,\mathrm{k}^2 t^{\alpha}) d^3\mathrm{k}\,. \tag{2.14}$$

For the case $\alpha = 1$, the fractional wave equation (2.1) reduces to the Schrödinger wave equation. In this special case, the solution (2.13) after integration over k reduces to the familiar form

$$\psi(x,t) = \frac{1}{\sqrt{(4\pi\,at)^3}} \int_{-\infty}^{\infty} e^{-\frac{(x-\xi)^2}{4\,a\,t}} \psi_0(\xi) d^3\xi, \tag{2.15}$$

where the 3-D Green function for α =1 in spatial coordinates is given by

$$G(x,t) = \frac{1}{(4\pi\,at)^{3/2}} e^{-\frac{x^2}{4\,a\,t}}. \tag{2.16}$$

In equation (2.15), the result $E_{1,1}(z) = e^z$ is used. The solution is in perfect agreement with the standard solution of the integer order $\alpha = 1$ of the wave equation (2.1).

We also calculated [12] the mean square distance $< r^2 >$ in spherical coordinates using the Green function given in equation (2.13). The Green function is expressed in spherical coordinates given by

$$G_\alpha(r,t) = \frac{4\pi}{(2\pi)^3}\int_0^\infty \sqrt{\frac{\pi}{2\,k\,r}}\,J_{1/2}(k\,r)\,E_{\alpha,1}(-a\,k^2 t^\alpha)\,k^2 dk. \tag{2.17}$$

By taking the Laplace transform of equation (2.17) and integrating over k, we get

$$\bar{G}_\alpha(r,s) = \frac{1}{4\pi}\,\frac{1}{a\,r} s^{\alpha-1}\,e^{-\frac{r}{\sqrt{a}}\,s^{\alpha/2}}. \tag{2.18}$$

Taking the inverse Laplace transform of the above equation (2.18) we get

$$G_\alpha(r,t) = \frac{1}{4\pi}\,\frac{1}{(a\,t^\alpha)^{\frac{3}{2}}}\,\frac{1}{z} W(-z,-\frac{\alpha}{2},1-\alpha). \tag{2.19}$$

Where $W(z,\alpha,\beta) = \sum_{n=0}^{\infty} \frac{z^n}{n!\,\Gamma(\alpha\,n+\beta)}$ is called Wright Function [see Erdèlyi, 1955] and $z = \frac{r}{\sqrt{a}t^{\alpha/2}}$. We define a new function for odd values of n = 2m + 1 for $\beta = 0$ as:

$$B(z,\alpha) = \sum_{m=0}^{\infty} \frac{z^{2m+1}}{(2m+1)!\Gamma(\alpha(2m+1))}. \tag{2.20}$$

For the special case $\alpha = 1$, the B-function $B(-z,-\frac{\alpha}{2})$ reduces to simple exponential form of type

$$B(-z,-\frac{1}{2}) = \frac{1}{2\sqrt{\pi}} z\,e^{-\frac{z^2}{4}} \tag{2.21}$$

and the 3-D Green function in equation (2.19) which reduces to simple form given by

$$G_1(r,t) = \frac{1}{(4\pi\,a\,t)^{\frac{3}{2}}}\,e^{-\frac{r^2}{4\,a\,t}}. \tag{2.22}$$

It is also convenient to express the Green function in equation (2.18) after taking inverse Laplace transform and carrying out complex integration, we obtain

$$G_\alpha(r,t) = \frac{(-1)^{\alpha+1}}{2\pi^2\,a\,r}\int_0^\infty e^{-t\,x^2 - \frac{r}{\sqrt{a}}\,x\,\cos(\pi\alpha/2)} x^{2\alpha-1}\sin[\frac{r}{\sqrt{a}}\,x\;\sin(\pi\alpha/2)]\,dx. \tag{2.23}$$

For $\alpha = 1$, the above equation also gives the same answer as in equation (2.22).

3 Uncertainty Principle

The Green function in Eq. (2.22) $G_1(x,t) = \frac{1}{(4\pi\, a\, t)^{1/2}}\, e^{-\frac{x^2}{4\, a\, t}}$ for α =1 is used to verify the uncertainty principle in one dimension (1-D). The solution of the Schrödinger equation is then written in the form

$$\psi(r,t) = \int_{-\infty}^{\infty} G_1(\xi, t)\, \psi_0(r-\xi)\, d\xi. \tag{3.1}$$

We choose normalized initial Gaussian wave function $\psi_0(r) = \frac{1}{(\pi\, b^2)^{\frac{1}{4}}}\, e^{-\frac{r^2}{2\, b^2}}$, where constant b represents an initial Gaussian width of the initial wave function. Substituting the expression for Green function in Eq. (3.1) and performing the integration, we obtain wave function

$$\psi(r,t) = \frac{1}{(\pi\, b^2)^{\frac{1}{4}}}\, \frac{1}{\sqrt{(1 + i\, \hbar\, t/b^2)}} e^{-\frac{r^2}{2\, b^2 (1 + i\, \hbar\, t/b^2)}}. \tag{3.2}$$

Using this wave function in Eq.(3.2), we can obtain the quantum mechanical probability density by taking the complex conjugate and multiplying with the wave function itself given as

$$P(r,t) = |\psi(r,t)|^2 = \frac{1}{\sqrt{\pi}}\, \frac{1}{b\, c} e^{-\frac{r^2}{b^2\, c^2}}, \tag{3.3}$$

where the constant $c = \sqrt{(1 + \frac{\hbar^2\, t^2}{m^2\, b^4})}$. Mean square distance is calculated using the quantum mechanical probability given by

$$\langle r^2 \rangle = \frac{1}{\sqrt{\pi}} \int_0^{\infty} r^2\, \frac{e^{-\frac{x^2}{b^2 c^2}}}{b\, c} dx = \frac{1}{2}(b\, c)^2. \tag{3.4}$$

This expression Eq. (3.4) provides uncertainty in the position which is given by

$$\Delta r = \frac{1}{\sqrt{2}} b \sqrt{(1 + \frac{\hbar^2\, t^2}{m^2\, b^4})}. \tag{3.5}$$

It is straightforward to calculate expectation value of the momentum square with integral value of α=1 [14].

$$\Delta p = \langle \hbar\, k^2 \rangle = \frac{\hbar}{\sqrt{2}} \frac{1}{b}. \tag{3.6}$$

The uncertainty principle is just the product of both expressions given in equations (3.5 and 3.6)

$$\Delta r\,\Delta p = \frac{\hbar}{2}\sqrt{(1+\ \frac{\hbar^2\,t^2}{m^2\,b^4})} \tag{3.7}$$

The above expression with t=0 reduces to the known uncertainty principle given by

$$\Delta r\,\Delta p = \frac{\hbar}{2}. \tag{3.8}$$

These calculations show that fractional calculus is a powerful tool that may be used to solve the problems in general and the reduction leads to the known results when integral values of α are used.

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