



Application of the Fractional Calculus to the Radial Schrödinger Equation given by the Makarov Potential

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Abstract: Fractional calculus and its generalizations are used for the solutions of some classes of differential equations and fractional differential equations. In this paper, our aim is to solve the radial Schrödinger equation given by the Makarov potential by the help of fractional calculus theorems. The related equation was solved by applying a fractional calculus theorem that gives fractional solutions of the second order differential equations with singular points. In the last section, we also introduced hypergeometric form of this solution.

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1. Introduction

The fractional calculus theory enables a set of methods to generalize the derivative notions from integer k to arbitrary order ρ , $\{x^k, \partial^k/\partial x^k\} \rightarrow \{x^\rho, \partial^\rho/\partial x^\rho\}$ in a good light. Fractional differential equations are applied in a widespread manner in robot technology, Proportional-Integral-Derivative control systems, Schrödinger equation, heat transfer, relativity theory, economy, filtration, controller design, mechanics, optics, modelling and so on.

Riemann-Liouville fractional integration and fractional differentiation are, respectively,

$$\begin{aligned} {}_a D_t^{-\rho} f(t) &= \frac{1}{\Gamma(\rho)} \int_a^t f(\omega) (t-\omega)^{\rho-1} d\omega \quad (t > a, \rho > 0), \\ {}_a D_t^\rho f(t) &= \frac{1}{\Gamma(k-\rho)} \left(\frac{d}{dt}\right)^k \int_a^t f(\omega) (t-\omega)^{k-\rho-1} d\omega \quad (k-1 \leq \rho < k), \end{aligned} \quad (1)$$

where $k \in \mathbb{N}$, \mathbb{N} is the set of positive integers and, Γ is Euler's gamma function [1-5].

Explicit solutions of some differential equations with singular coefficients were obtained by using the fractional calculus theorems. An important example of Fuchsian differential equations is provided by the celebrated hypergeometric equation

$$z(1-z) \frac{d^2 f}{dz^2} + [\gamma - (\alpha + \beta + 1)z] \frac{df}{dz} - \alpha\beta f = 0,$$

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whose study can be traced back to L. Euler, C.F. Gauss and E.E. Kummer. Other classes of non-Fuchsian differential equations which we shall consider in this investigation include the so-called Fokuhara equation [6]

$$z^2 \frac{d^2 f}{dz^2} + z \frac{df}{dz} - (1 - z + z^2)f = 0,$$

the Tricomi equation [7]

$$\frac{d^2 f}{dz^2} + \left(\alpha + \frac{\beta}{z} \right) \frac{df}{dz} + \left(\gamma + \frac{\delta}{z} + \frac{\varepsilon}{z^2} \right) f = 0,$$

and the Bessel equation [8]

$$z^2 \frac{d^2 f}{dz^2} + z \frac{df}{dz} - (z^2 - \nu^2)f = 0.$$

Furthermore, Laskin [9] introduced some properties of the fractional Schrödinger equation and proved the Hermiticity of the fractional Hamilton operator and established the parity conservation law for fractional quantum mechanics and also studied on the relationships between the fractional and standard Schrödinger equations. Yasuk [10] obtained the general solutions of Schrödinger equation for non central potential by using Nikiforov-Uvarov method. The numerical methods used for the solution of the Schrödinger equation was presented [11]. An exponentially-fitted method was introduced for the numerical solution of the Schrödinger equation and, trigonometric fitting was also explained and applied [12]. Jumarie [13] studied from Lagrangian mechanics fractal in space to space fractal Schrödinger's equation via fractional Taylor's series. Higher-order difference schemes were considered [14] for the numerical solution of Schrödinger's radial equation. A spherically harmonic oscillatory ring-shaped potential was proposed [15] and its exactly complete solutions were presented by the Nikiforov-Uvarov method. Aygun et al. [16] presented the exact and iterative solutions of the radial Schrödinger equation for a class of potentials, $V(r) = A/r^2 - B/r + Cr^\kappa$, for various values of κ from -2 to 2 , for any n and l quantum states by applying the asymptotic iteration method. Fractional solutions of the radial equation of the fractional Schrödinger equation were obtained by using N-fractional calculus operator and, hypergeometric forms of these solutions were also presented [17]. Radial Schrödinger equation for some physical potentials such as pseudoharmonic and Mie-type potentials was solved by means of the nabla discrete fractional calculus operator [18]. And, we also mentioned the fractional solutions of the radial Schrödinger equation given by the Makarov potential by applying the fractional calculus theorems.

2. Preliminaries

Definition 2.1. If the function $f(z)$ is analytic (*regular*) and has no branch point inside and on C , where $C = \{C^-, C^+\}$, C^- is an integral curve along to cut joining the points z and $-\infty + i\text{Im}(z)$ and, C^+ is an integral curve along to cut joining the points z and $+\infty + i\text{Im}(z)$

$$f_\rho(z) = (f(z))_\rho = \frac{\Gamma(\rho + 1)}{2\pi i} \int_C \frac{f(t)dt}{(t-z)^{\rho+1}} \quad (\rho \in \mathbb{R} \setminus \mathbb{Z}^-),$$

$$f_{-k}(z) = \lim_{\rho \rightarrow -k} f_\rho(z) \quad (k \in \mathbb{Z}^+),$$

where $t \neq z$,

$$\begin{aligned} -\pi &\leq \arg(t-z) \leq \pi && \text{for } C^-, \\ 0 &\leq \arg(t-z) \leq 2\pi && \text{for } C^+. \end{aligned} \quad (3)$$

Then, $f_\rho(z)$ ($\rho > 0$) is the fractional derivative of $f(z)$ of order ρ and, $f_\rho(z)$ ($\rho < 0$) is the fractional integral of $f(z)$ of order $-\rho$, provided that

$$|f_\rho(z)| < \infty \quad (\rho \in \mathbb{R}), \quad (4)$$

[19,20].

Lemma 2.1 (Linearity). Let $f(z)$ and $g(z)$ be single-valued and analytic functions in some domain $\Omega \subseteq \mathbb{C}$. If f_ρ and g_ρ exist, then

$$(Kf + Lg)_\rho = Kf_\rho + Lg_\rho, \tag{5}$$

hold where K and L are constants and, $\rho \in \mathbb{R}, z \in \Omega$ [5].

Lemma 2.2 (Index law). Let $f(z)$ be single-valued and analytic function in some domain $\Omega \subseteq \mathbb{C}$. If $(f_\sigma)_\rho$ and $(f_\rho)_\sigma$ exist, then

$$(f_\sigma)_\rho = f_{\sigma+\rho} = (f_\rho)_\sigma, \tag{6}$$

where $\sigma, \rho \in \mathbb{R}, z \in \Omega$ and, $\left| \frac{\Gamma(\sigma+\rho+1)}{\Gamma(\sigma+1)\Gamma(\rho+1)} \right| < \infty$ [5].

Lemma 2.3 (Generalized Leibniz rule). Let $f(z)$ and $g(z)$ be single-valued and analytic functions in some domain $\Omega \subseteq \mathbb{C}$. If f_ρ and g_ρ exist, then

$$(fg)_\rho = \sum_{k=0}^{\infty} \frac{\Gamma(\rho+1)}{\Gamma(\rho-k+1)\Gamma(k+1)} f_{\rho-k} g_k, \tag{7}$$

where $\rho \in \mathbb{R}, z \in \Omega$ and, $\left| \frac{\Gamma(\rho+1)}{\Gamma(\rho-k+1)\Gamma(k+1)} \right| < \infty$ [5].

Property 2.1. For any $\vartheta \neq 0, \rho \in \mathbb{R}$ and $z \in \mathbb{C}$, we have

$$(e^{\vartheta z})_\rho = \vartheta^\rho e^{\vartheta z}, \tag{8}$$

$$(e^{-\vartheta z})_\rho = e^{-i\pi\rho} \vartheta^\rho e^{-\vartheta z}, \tag{9}$$

$$(z^\vartheta)_\rho = e^{-i\pi\rho} \frac{\Gamma(\rho-\vartheta)}{\Gamma(-\vartheta)} z^{\vartheta-\rho}, \tag{10}$$

where ϑ is a constant and, $\left| \frac{\Gamma(\rho-\vartheta)}{\Gamma(-\vartheta)} \right| < \infty$ [5].

Theorem 2.1. Let $\mathcal{P}(z; \wp)$ and $\mathcal{Q}(z; \mathcal{q})$ be polynomials in z of degrees \wp and \mathcal{q} , respectively, defined by

$$\mathcal{P}(z; \wp) = \sum_{k=0}^{\wp} a_k z^{\wp-k} = a_0 \prod_{j=1}^{\wp} (z - z_j) \quad (a_0 \neq 0, \wp \in \mathbb{N}), \tag{11}$$

and,

$$\mathcal{Q}(z; \mathcal{q}) = \sum_{k=0}^{\mathcal{q}} b_k z^{\mathcal{q}-k} \quad (b_0 \neq 0, \mathcal{q} \in \mathbb{N}). \tag{12}$$

Suppose also that $f_{-\nu} \neq 0$ exists for a given function f .

Then the nonhomogeneous linear ordinary fractional differintegral equation

$$\begin{aligned} \mathcal{P}(z; \wp) \varphi_\rho(z) + \left[\sum_{k=1}^{\wp} \binom{\nu}{k} \mathcal{P}_k(z; \wp) + \sum_{k=1}^{\mathcal{q}} \binom{\nu}{k-1} \mathcal{Q}_{k-1}(z; \mathcal{q}) \right] \varphi_{\rho-k}(z) \\ + \binom{\nu}{\mathcal{q}} \mathcal{q}! b_0 \varphi_{\rho-\mathcal{q}-1}(z) = f(z) \quad (\wp, \mathcal{q} \in \mathbb{N}, \rho, \nu \in \mathbb{R}), \end{aligned} \tag{13}$$

has a particular solution of the form

$$\varphi(z) = \left[\left(\frac{f_{-v}(z)}{\mathcal{P}(z; \mathcal{p})} e^{\mathcal{H}(z; \mathcal{p}, \mathcal{q})} \right)_{-1} e^{-\mathcal{H}(z; \mathcal{p}, \mathcal{q})} \right]_{v-\rho+1} \quad (z \in \mathbb{C} \setminus \{z_1, \dots, z_p\}), \quad (14)$$

where, for convenience,

$$\mathcal{H}(z; \mathcal{p}, \mathcal{q}) = \int^z \frac{\mathcal{Q}(\zeta; \mathcal{q})}{\mathcal{P}(\zeta; \mathcal{p})} d\zeta \quad (z \in \mathbb{C} \setminus \{z_1, \dots, z_p\}), \quad (15)$$

provided that the second component of (14) exists. Moreover, the homogeneous linear ordinary fractional differintegral equation

$$\begin{aligned} \mathcal{P}(z; \mathcal{p}) \varphi_\rho(z) + \left[\sum_{k=1}^{\mathcal{p}} \binom{v}{k} \mathcal{P}_k(z; \mathcal{p}) + \sum_{k=1}^{\mathcal{q}} \binom{v}{k-1} \mathcal{Q}_{k-1}(z; \mathcal{q}) \right] \varphi_{\rho-k}(z) \\ + \binom{v}{\mathcal{q}} \mathcal{q}! b_0 \varphi_{\rho-\mathcal{q}-1}(z) = 0 \quad (\rho, v \in \mathbb{R}, \mathcal{p}, \mathcal{q} \in \mathbb{N}), \end{aligned} \quad (16)$$

has solutions of the form

$$\varphi(z) = K \left(e^{-\mathcal{H}(z; \mathcal{p}, \mathcal{q})} \right)_{v-\rho+1}, \quad (17)$$

where $\mathcal{H}(z; \mathcal{p}, \mathcal{q})$ is given by (15) and, K is an arbitrary constant [21].

3. The Radial Schrödinger Equation given by the Makarov Potential

The radial Schrödinger equation given by the Makarov potential is an analytically solvable problem in physics and can be used to describe ring-shaped molecules such as benzene and interactions between deformed pairs of nuclei. In spherical coordinates (r, θ, φ) , the Makarov potential is given by

$$V(r, \theta) = -\frac{\alpha}{r} + \frac{\beta}{r^2 \sin^2 \theta} + \frac{\gamma \cos \theta}{r^2 \sin^2 \theta} \quad (\alpha > 0), \quad (18)$$

where the first term of Equ. (18) is the Coulomb potential, the second and the third are the short range ring-shape terms. Different methods were applied to obtain exact solutions of Schrödinger equation for the Makarov potential such as supersymmetric approach, path integral representation, Nikiforov-Uvarov method, and Asymptotic Iteration Method. For relativistic cases, Yasuk et al. [22] and Zhang et al. [23,24] derived exact solutions of bound states of the Klein–Gordon equation and the Dirac equation with equal scalar and vector Makarov potentials, respectively.

In this paper, we obtain solutions of the radial Schrödinger equation. Therefore, we take advantage of the fractional calculus theorems. Thus, we find fractional forms of the solutions of the radial Schrödinger equation. And, we also obtain hypergeometric forms of the solutions.

The Schrödinger equation for the Makarov potential is defined as

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r, \theta) - \mathcal{E} \right] \psi(r, \theta, \varphi) = 0. \quad (19)$$

where m is the mass of the electron, \hbar is the Planck constant, ∇ is the Laplacian operator, r is the distance from a fixed center, θ is the polar angle, φ is the azimuthal one, V is the potential energy, \mathcal{E} is the total energy, and ψ is the wave function.

In analogy to the practice for usual spherical potential, we can write

$$\psi(r, \theta, \varphi) = \frac{R(r)}{r} Y(\theta) \phi(\varphi), \quad (20)$$

and then separate variables of the Schrödinger equation

$$\left[\frac{d^2}{dr^2} + \frac{2m}{\hbar^2} \left(\mathcal{E} + \frac{\alpha}{r} \right) - \frac{\ell(\ell + 1)}{r^2} \right] R(r) = 0, \tag{21}$$

$$\left[\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d}{d\theta} \right) + \ell(\ell + 1) - \frac{\epsilon^2}{\sin^2 \theta} - \frac{2m(\beta + \gamma \cos \theta)}{\hbar^2 \sin^2 \theta} \right] Y(\theta) = 0, \tag{22}$$

$$\left[\frac{d^2}{d\varphi^2} + \epsilon^2 \right] \phi(\varphi) = 0, \tag{23}$$

where ϵ^2 is separation constant which is real and dimensionless [25].

For continuous states $\mathcal{E} > 0$, we take $\kappa = \sqrt{2m\mathcal{E}/\hbar^2} > 0$, $\sigma = m\alpha/\hbar^2$ and $\tau = \ell(\ell + 1)$ in Equ. (21). Thus, we can write Equ. (21) as

$$r^2 \frac{d^2 R(r)}{dr^2} + [\kappa^2 r^2 + 2\sigma r - \tau] R(r) = 0. \tag{24}$$

4. Main Results

In order to apply Theorem 2.1 to a class of ordinary homogeneous differential equations as:

$$Az^2 \frac{d^2 \varphi}{dz^2} + (Bz + C) \frac{d\varphi}{dz} + (Dz^2 + Ez + F)\varphi(z) = 0 \quad (z \in \mathbb{C} \setminus \{0\}), \tag{25}$$

which obviously corresponds to (24) when the coefficients $A \neq 0, B, C, D \neq 0, E$ and F are privately stated as follows:

$$A = 1, \quad B = C = 0, \quad D = \kappa^2, \quad E = 2\sigma, \quad F = -\tau.$$

Theorem 4.1. If $|f_\rho(z)| < \infty$ ($\rho \in \mathbb{R}$) and $f_{-\rho} \neq 0$, then

$$Az^2 \frac{d^2 \varphi}{dz^2} + Bz \frac{d\varphi}{dz} + (Dz^2 + Ez + F)\varphi(z) = f(z) \quad (A \neq 0, D \neq 0), \tag{26}$$

has a particular solution such as:

$$\varphi(z) = z^\lambda e^{\vartheta z} \left[\left(A^{-1} z^{-\rho-1+(2A\lambda+B)/A} e^{2\vartheta z} \left(z^{-\lambda-1} e^{-\vartheta z} f(z) \right)_{-\rho} \right)_{-1} \times z^{\rho-(2A\lambda+B)/A} e^{-2\vartheta z} \right]_{\rho-1} \quad (A \neq 0; D \neq 0, z \in \mathbb{C} \setminus \{0\}), \tag{27}$$

where λ and ϑ are in the form

$$\lambda = \frac{A - B \pm \sqrt{(A - B)^2 - 4AF}}{2A}, \quad \vartheta = \pm i \sqrt{\frac{D}{A}} \tag{28}$$

and,

$$\rho = \frac{(2A\lambda + B)\vartheta + E}{2A\vartheta}. \tag{29}$$

Moreover,

$$Az^2 \frac{d^2 \varphi}{dz^2} + Bz \frac{d\varphi}{dz} + (Dz^2 + Ez + F)\varphi(z) = 0, \tag{30}$$

has solutions of the form

$$\varphi(z) = Kz^\lambda e^{\vartheta z} (z^{\rho - (2\lambda + B)/A} e^{-2\vartheta z})_{\rho-1} \quad (A, D \neq 0, z \in \mathbb{C} \setminus \{0\}), \quad (31)$$

where λ and ϑ are given by (28) and, ρ is given by (29) and, K is an arbitrary constant [21].

Theorem 4.2. Under the hypotheses of Theorem 4.1, a homogeneous linear ordinary differential equation (radial Schrödinger equation in Equ. (24)) such as:

$$r^2 \frac{d^2 R(r)}{dr^2} + [\kappa^2 r^2 + 2\sigma r - \tau] R(r) = 0,$$

has a particular solution in the form

$$R(r) = Kr^{(1 \pm \sqrt{1+4\tau})/2} e^{\vartheta r} [r^{\rho - (1 \pm \sqrt{1+4\tau})} e^{-2\vartheta r}]_{\rho-1}, \quad (32)$$

where λ and ϑ are given by

$$\lambda = \frac{1 \pm \sqrt{1+4\tau}}{2}, \quad \vartheta = \pm i\kappa,$$

and,

$$\rho = \frac{(2\lambda + 1)\vartheta + 2\sigma}{2\vartheta},$$

it being confirmed that the second component of (32) exists and, K is an arbitrary constant. We can write (32) as follows

$$R(r) = Kr^\lambda e^{\vartheta r} [r^{\rho-2\lambda} e^{-2\vartheta r}]_{\rho-1}, \quad (33)$$

where analytical solutions of the wave function $R(r)$ can be obtained by means of the fractional calculus definitions and, the hypergeometric solution of $R(r)$ is obtained by the following theorem which is proved with Lemma 2.3 and Property 2.1.

Theorem 4.3. The Equ. (33) can be written equivalently as

$$R(r) = r^{\rho-\lambda} e^{-\vartheta r} {}_2F_0 \left[1 - \rho, 2\lambda - \rho; -\frac{1}{2\vartheta r} \right] \left(r \neq 0, \left| -\frac{1}{2\vartheta r} \right| < 1 \right), \quad (34)$$

where $\left| (r^{\rho-2\lambda})_n \right| < \infty$ ($n \in \mathbb{Z}^+ \cup \{0\}$) and, ${}_2F_0$ is the Gauss hypergeometric function.

Proof. By means of (7), we have

$$R(r) = Kr^\lambda e^{\vartheta r} \sum_{n=0}^{\infty} \frac{\Gamma(\rho)}{\Gamma(\rho-n)\Gamma(n+1)} (r^{\rho-2\lambda})_n (e^{-2\vartheta r})_{(\rho-1-n)}. \quad (35)$$

By using (9) and (10), we rewrite the Equ. (35) as follows

$$R(r) = Kr^{\rho-\lambda} e^{-\vartheta r} (2\vartheta e^{-i\pi})^{\rho-1} \sum_{n=0}^{\infty} \frac{\Gamma(n+1-\rho)}{\Gamma(1-\rho)} \frac{\Gamma(n+2\lambda-\rho)}{\Gamma(2\lambda-\rho)} \frac{1}{n!} \left(-\frac{1}{2\vartheta r} \right)^n. \quad (36)$$

Then, we obtain

$$R(r) = Kr^{\rho-\lambda} e^{-\vartheta r} \sum_{n=0}^{\infty} (1-\rho)_n (2\lambda-\rho)_n \frac{1}{n!} \left(-\frac{1}{2\vartheta r} \right)^n, \quad (37)$$

where $1/K = (2\vartheta e^{-i\pi})^{\rho-1}$.
Finally, we have

$$R(r) = r^{\rho-\lambda} e^{-\vartheta r} {}_2F_0 \left[1 - \rho, 2\lambda - \rho; -\frac{1}{2\vartheta r} \right]. \quad (38)$$

5. Conclusion

In this paper, we used fractional calculus theorems for the radial Schrödinger equation given by the Makarov potential. And, we obtained the hypergeometric form of the solution. The most important advantage of this method is that it can be applied for singular equations.

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