

ON DISCRETE FRACTIONAL SOLUTIONS OF THE HYDROGEN ATOM TYPE EQUATIONS

by

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Discrete fractional calculus deals with sums and differences of arbitrary orders. In this study, we acquire new discrete fractional solutions of hydrogen atom type equations by using discrete fractional nabla operator ∇^α ($0 < \alpha < 1$). This operator is applied homogeneous and non-homogeneous hydrogen atom type equations. So, we obtain many particular solutions of these equations.

Key words: discrete fractional analysis, hydrogen atom equation, Schrodinger equation

Introduction

Fractional analysis has many applications in diverse fields of science and engineering such as Schrodinger equation, diffusion, control theory, and statistics [1-3]. The similar theory for discrete fractional analysis was initiated and properties of the theory of fractional differences and sums were established. Recently, many books and articles related to discrete fractional analysis have been published [4-12].

In 1956 [4], differences of fractional order were introduced by Kuttner. Diaz and Osler [5], define the concept of fractional difference:

$$\Delta^\rho f(\tau) = \sum_{k=0}^{\infty} (-1)^k \binom{\rho}{k} f(\tau + \rho - k)$$

where ρ is any real number. Granger, Joyeux, and Hosking [13, 14] defined the concept of fractional difference:

$$\nabla^\rho f(\tau) = \sum_{k=0}^{\infty} (-1)^k \binom{\rho}{k} f(\tau - k), \quad \binom{\rho}{k} = \frac{\Gamma(\rho+1)}{\Gamma(k+1)\Gamma(\rho-k+1)}$$

where ρ is any real number and $q^k f(\tau) = f(\tau - k)$ – the shift operator. Gray and Zhang [15] studied on a new definition of the fractional difference through summation.

In this article, we will consider the equation:

$$\frac{d^2\Psi}{dr^2} + \frac{n}{r} \frac{d\Psi}{dr} - \frac{\ell(\ell+1)}{r^2} \Psi + \left(\kappa + \frac{n}{r}\right) \Psi = 0, \quad 0 < r < \infty \quad (1)$$

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where Ψ is the distance of the mass center to the origin, n – the real number, ℓ – the positive integer, κ – the energy constant, and r – the distance among the nucleus and electron [16]. If we take $\Psi = u/r$ in eq. (1), then we have the hydrogen atom type equations (HAE):

$$\frac{u}{r^2} + \left[+\frac{n}{r} - \frac{\ell(\ell+1)}{r^2} \right] = \quad (2)$$

In many works:

$$q(r) = \frac{n}{r} - \frac{\ell(\ell+1)}{r^2} \quad (3)$$

this part takes a centripetal and Colomb part, the usual singularities of the nuclear problem [17]. Yilmazer [18] acquired fractional solutions of eq. (2) by using the Nishimoto operator. Panakhov and Yilmazer [19] investigated the Hochstadt-Lieberman theorem for eq. (2). Bas *et al.* [20] researched the uniqueness for the HAE eq. (2).

The aim of this article is to obtain new discrete fractional solutions (DFS) of the HAE by means of fractional calculus operator.

Preliminary and properties

Let $\rho \in \mathbb{R}^+$ such that $k-1 \leq \rho < k$ where k is an integer. The ρ^{th} order fractional sum of g :

$$\nabla_b^{-\rho} g(\tau) = \frac{1}{\Gamma(\rho)} \sum_{s=b}^{\tau} (\tau - \delta(s))^{\overline{\rho-1}} g(s) \quad (4)$$

where $\tau \in \mathbb{N}_b = \{b\} + \mathbb{N}_0 = \{b, b+1, b+2, \dots\}$, $b \in \mathbb{R}$, $\delta(\tau) = \tau - 1$ is jump operator.

The ascending factorial:

$$\tau^{\overline{k}} = \prod_{n=0}^{k-1} (\tau + n) = \tau(\tau+1)(\tau+2)\dots(\tau+k-1), \quad k \in \mathbb{N}, \quad \tau^{\overline{0}} = 1$$

Let $\rho \in \mathbb{R}$. Then τ to the ρ rising:

$$\tau^{\overline{\rho}} = \frac{\Gamma(\tau + \rho)}{\Gamma(\tau)}, \quad \tau \in \mathbb{R} - \{\dots, -2, -1, 0\}, \quad 0^{\overline{\rho}} = 0 \quad (5)$$

Let us note:

$$\nabla(\tau^{\overline{\rho}}) = \rho \tau^{\overline{\rho-1}} \quad (6)$$

where $\nabla u(\tau) = u(\tau) - u[\delta(\tau)] = u(\tau) - u(\tau-1)$.

The ρ^{th} order fractional difference of g :

$$\nabla_b^{\rho} g(\tau) = \nabla^k \left[\nabla^{-(k-\rho)} g(\tau) \right] = \nabla^k \left[\frac{1}{\Gamma(k-\rho)} \sum_{s=b}^{\tau} (\tau - \delta(s))^{\overline{k-\rho-1}} g(s) \right] \quad (7)$$

where $g : \mathbb{N}_b^+ \rightarrow \mathbb{R}$ [8].

Theorem 1 [11]. Let $f(\tau)$ and $g(\tau) : \mathbb{N}_0^+ \rightarrow \mathbb{R}$, $\rho, \eta > 0$, h, v are scalars. The following equality holds:

$$\nabla^{-\rho} \nabla^{-\eta} f(\tau) = \nabla^{-(\rho+\eta)} f(\tau) = \nabla^{-\eta} \nabla^{-\rho} f(\tau) \quad (8)$$

$$\nabla^{\rho} [hf(\tau) + vg(\tau)] = h\nabla^{\rho} f(\tau) + v\nabla^{\rho} g(\tau) \quad (9)$$

Lemma 2 (Power Rule) [6]. Let $\rho > 0$. Then the following holds:

$$\nabla_b^{-\rho} (\tau - b + 1)^{\overline{\eta}} = \frac{\Gamma(\eta + 1)}{\Gamma(\eta + \rho + 1)} (\tau - b + 1)^{\overline{\eta + \rho}}$$

for every $\tau \in \mathbb{N}_b$.

Lemma 3 [7]. For any $\rho > 0$, the following equality holds:

$$\nabla_{b+1}^{-\rho} \nabla f(\tau) = \nabla \nabla_b^{-\rho} f(\tau) - \frac{(\tau - b + 1)^{\overline{\rho-1}}}{\Gamma(\rho)} f(b) \quad (10)$$

Lemma 4 (Leibniz Rule) [8]. For any $\rho > 0$, ρ^{th} order, the fractional difference of the product fg :

$$\nabla_0^{\rho} (fg)(\tau) = \sum_{k=0}^{\tau} \binom{\rho}{k} \left[\nabla_0^{\rho-k} f(\tau - k) \right] \left[\nabla^k g(\tau) \right] \quad (11)$$

where

$$\binom{\rho}{k} = \frac{\Gamma(\rho + 1)}{\Gamma(k + 1)\Gamma(\rho - k + 1)}$$

and $qf(\tau) = f(\tau - 1)$ is shift operator.

Lemma 5 (Index law) [18]. Let f is analytic and single-valued. The following equality holds:

$$\left[f_{\rho}(\tau) \right]_{\eta} = f_{\rho+\eta}(\tau) = \left[f_{\eta}(\tau) \right]_{\rho} \quad \left[f_{\rho}(\tau) \neq 0; f_{\eta}(\tau) \neq 0 \right] \quad (12)$$

for every $\rho, \eta \in \mathbb{R}$.

Main results

The DFS of non-homogeneous HAE

Theorem 6. Let $\Phi \in \{\Phi : 0 \neq |\Phi_{\alpha}| < \infty; \alpha \in \mathbb{R}\}$ and $\phi \in \{\phi : 0 \neq |\phi_{\alpha}| < \infty; \alpha \in \mathbb{R}\}$. Then the non-homogeneous HAE, $\tau = \ell + (1/2)$ in (2):

$$\Phi_2 + \left[\lambda + \frac{\gamma}{z} + \frac{\frac{1}{4} - \tau^2}{z^2} \right] \Phi = \phi, \quad (z \neq 0) \quad (13)$$

has particular solutions:

$$\Phi^I = z^{\tau+\frac{1}{2}} e^{-\sqrt{\lambda}iz} \left\{ \left[\left(\phi z^{\frac{1}{2}-\tau} e^{\sqrt{\lambda}iz} \right)_{\alpha} e^{-2\sqrt{\lambda}iz} z^{\tau-\frac{1}{2}-\frac{i\gamma}{2\sqrt{\lambda}}} \right]_{-1} e^{2\sqrt{\lambda}iz} z^{-\tau-\frac{1}{2}+\frac{i\gamma}{2\sqrt{\lambda}}} \right\}_{-(1+\alpha)} \quad (14)$$

$$\Phi^{II} = z^{\tau+\frac{1}{2}} e^{\sqrt{\lambda}iz} \left\{ \left[\left(\phi z^{\frac{1}{2}-\tau} e^{-\sqrt{\lambda}iz} \right)_{\beta} e^{2\sqrt{\lambda}iz} z^{\tau-\frac{1}{2}+\frac{i\gamma}{2\sqrt{\lambda}}} \right]_{-1} e^{-2\sqrt{\lambda}iz} z^{-\tau-\frac{1}{2}-\frac{i\gamma}{2\sqrt{\lambda}}} \right\}_{-(1+\beta)} \quad (15)$$

$$\Phi^{III} = z^{-\tau+\frac{1}{2}} e^{-\sqrt{\lambda}iz} \left\{ \left[\left(\phi z^{\frac{1}{2}+\tau} e^{\sqrt{\lambda}iz} \right)_{\alpha} e^{-2\sqrt{\lambda}iz} z^{-\tau-\frac{1}{2}-\frac{i\gamma}{2\sqrt{\lambda}}} \right]_{-1} e^{2\sqrt{\lambda}iz} z^{\tau-\frac{1}{2}+\frac{i\gamma}{2\sqrt{\lambda}}} \right\}_{-(1+\alpha)} \quad (16)$$

$$\Phi^{IV} = z^{-\tau+\frac{1}{2}} e^{\sqrt{\lambda}iz} \left\{ \left[\left(\phi z^{\frac{1}{2}+\tau} e^{-\sqrt{\lambda}iz} \right)_{\beta} e^{2\sqrt{\lambda}iz} z^{-\tau-\frac{1}{2}+\frac{i\gamma}{2\sqrt{\lambda}}} \right]_{-1} e^{-2\sqrt{\lambda}iz} z^{\tau-\frac{1}{2}-\frac{i\gamma}{2\sqrt{\lambda}}} \right\}_{-(1+\beta)} \quad (17)$$

where $\Phi_2 = d^2\Phi/dz^2$, $\Phi_0 = \Phi = \Phi(z)$ ($z \neq 0, z \in \mathbb{R}$), $\phi = \phi(z)$ (an arbitrary given function), τ, γ are given constants, Q is a shift operator and α, β :

$$\alpha = -Q^{-1}\left(\frac{i\gamma}{2\sqrt{\lambda}} + \tau + \frac{1}{2}\right), \quad \alpha = -Q^{-1}\left(-\frac{i\gamma}{2\sqrt{\lambda}} + \tau + \frac{1}{2}\right) \equiv \beta$$

Proof. Set:

$$\Phi = z^\sigma \psi, \quad \psi = \psi(z) \quad (18)$$

we have then:

$$z\psi_2 + 2\sigma\psi_1 + \left[\left(\sigma^2 - \sigma + \frac{1}{4} - \tau^2\right)z^{-1} + \sqrt{\lambda}z + \gamma\right]\psi = \phi z^{1-\sigma} \quad (19)$$

from eq. (13). Choose σ such that:

$$\sigma = \frac{1}{2} \pm \tau \quad (20)$$

Case of

$$\sigma = \tau + \frac{1}{2}$$

From eqs. (18) and (19):

$$\Phi = z^{\tau+\frac{1}{2}}\psi \quad (21)$$

and

$$z\psi_2 + (2\tau+1)\psi_1 + (\lambda z + \gamma)\psi = \phi z^{\frac{1}{2}-\tau} \quad (22)$$

respectively.

Next, by writing:

$$\psi = e^{\nu z} \varphi \quad [\varphi = \varphi(z)] \quad (23)$$

we have then:

$$z\varphi_2 + (2\nu z + 2\tau + 1)\varphi_1 + \left[(\nu^2 + \lambda)z + (2\tau + 1)\nu + \gamma\right]\varphi = \phi z^{\frac{1}{2}-\tau} e^{-\nu z} \quad (24)$$

From eq. (22), applying eq. (23). Choose ν such that:

$$\nu = \pm\sqrt{\lambda}i, \quad \lambda > 0 \quad (25)$$

– when $\nu = -\sqrt{\lambda}i$:

$$\psi = e^{-\sqrt{\lambda}iz} \varphi \quad (26)$$

and

$$z\varphi_2 + (-2\sqrt{\lambda}iz + 2\tau + 1)\varphi_1 + [-i\sqrt{\lambda}(2\tau + 1) + \gamma]\varphi = \phi z^{\frac{1}{2}-\tau} e^{\sqrt{\lambda}iz} \quad (27)$$

from eqs. (23) and (24).

Applying the discrete operator ∇^α to both sides of (27), we obtain:

$$z\varphi_{2+\alpha} + (-2\sqrt{\lambda}iz + 2\tau + 1 + \alpha Q)\varphi_{1+\alpha} + [\gamma - i\sqrt{\lambda}(2\tau + 1 + 2\alpha Q)]\varphi_\alpha = \left(\phi z^{\frac{1}{2}-\tau} e^{\sqrt{\lambda}iz}\right)_\alpha \quad (28)$$

from eqs. (9), (11), and (12).

Choose α :

$$\alpha = -Q^{-1}\left(\frac{i\gamma}{2\sqrt{\lambda}} + \tau + \frac{1}{2}\right) \quad (29)$$

then:

$$z\varphi_{2-Q^{-1}\left(\frac{i\gamma}{2\sqrt{\lambda}}+\tau+\frac{1}{2}\right)} + \left(-2\sqrt{\lambda}iz + \tau + \frac{1}{2} - \frac{i\gamma}{2\sqrt{\lambda}}\right)\varphi_{1-Q^{-1}\left(\frac{i\gamma}{2\sqrt{\lambda}}+\tau+\frac{1}{2}\right)} = \left(\phi z^{\frac{1}{2}-\tau} e^{\sqrt{\lambda}iz}\right)_{-Q^{-1}\left(\frac{i\gamma}{2\sqrt{\lambda}}+\tau+\frac{1}{2}\right)} \quad (30)$$

from eq. (28).

Next, by writing:

$$\varphi_{1-Q^{-1}\left(\frac{i\gamma}{2\sqrt{\lambda}}+\tau+\frac{1}{2}\right)} = w = w(z) \quad (31)$$

we obtain:

$$w_1 + \left[-2\sqrt{\lambda}i + \frac{\tau + \frac{1}{2} - \frac{i\gamma}{2\sqrt{\lambda}}}{z}\right]w = \frac{1}{z}\left(\phi z^{\frac{1}{2}-\tau} e^{\sqrt{\lambda}iz}\right)_{-Q^{-1}\left(\frac{i\gamma}{2\sqrt{\lambda}}+\tau+\frac{1}{2}\right)} \quad (32)$$

from eq. (30). A solution this differential equation:

$$w = \left[\left(\phi z^{\frac{1}{2}-\tau} e^{\sqrt{\lambda}iz}\right)_{-Q^{-1}\left(\frac{i\gamma}{2\sqrt{\lambda}}+\tau+\frac{1}{2}\right)} e^{-2i\sqrt{\lambda}z} z^{-\frac{i\gamma}{2\sqrt{\lambda}}+\tau-\frac{1}{2}} \right]_{-1} e^{2i\sqrt{\lambda}z} z^{\frac{i\gamma}{2\sqrt{\lambda}}-\tau-\frac{1}{2}} \quad (33)$$

Making use of the reverse process to obtain Φ^I , we finally obtain the solution (14) from eqs. (21), (26), (31), and (33).

– when $\nu = \sqrt{\lambda}i$:

$$\psi = e^{\sqrt{\lambda}iz} \varphi, \quad \varphi = \varphi(z) \quad (34)$$

and

$$z\varphi_2 + (2\sqrt{\lambda}iz + 2\tau + 1)\varphi_1 + [i\sqrt{\lambda}(2\tau + 1) + \gamma]\varphi = \phi z^{\frac{1}{2}-\tau} e^{-\sqrt{\lambda}iz} \quad (35)$$

from eqs. (23) and (24), respectively.

Applying the discrete operator ∇^α to both members of eq. (35):

$$z\varphi_{2+\alpha} + (2\sqrt{\lambda}iz + 2\tau + 1 + \alpha Q)\varphi_{1+\alpha} + [\gamma + i\sqrt{\lambda}(2\tau + 1 + 2\alpha Q)]\varphi_\alpha = \left(\phi z^{\frac{1}{2}-\tau} e^{-\sqrt{\lambda}iz}\right)_\alpha \quad (36)$$

Choosing α :

$$\alpha = -Q^{-1}\left(-\frac{i\gamma}{2\sqrt{\lambda}} + \tau + \frac{1}{2}\right) \equiv \beta \quad (37)$$

and replacing:

$$\varphi_{1-Q^{-1}\left(-\frac{i\gamma}{2\sqrt{\lambda}}+\tau+\frac{1}{2}\right)} = \mathcal{G} = \mathcal{G}(z) \quad (38)$$

we have:

$$\mathcal{G}_1 + \left[2\sqrt{\lambda}i + \frac{\tau + \frac{1}{2} + \frac{i\gamma}{2\sqrt{\lambda}}}{z}\right]\mathcal{G} = \frac{1}{z}\left(\phi z^{\frac{1}{2}-\tau} e^{-\sqrt{\lambda}iz}\right)_{-Q^{-1}\left(-\frac{i\gamma}{2\sqrt{\lambda}}+\tau+\frac{1}{2}\right)} \quad (39)$$

from eq. (36). A solution this differential equation:

$$\mathcal{G} = \left[\left(\phi z^{\frac{1}{2}-\tau} e^{-\sqrt{\lambda}iz}\right)_{-Q^{-1}\left(-\frac{i\gamma}{2\sqrt{\lambda}}+\tau+\frac{1}{2}\right)} e^{2i\sqrt{\lambda}z} z^{\frac{i\gamma}{2\sqrt{\lambda}}+\tau-\frac{1}{2}} \right]_{-1} e^{-2i\sqrt{\lambda}z} z^{-\frac{i\gamma}{2\sqrt{\lambda}}-\tau-\frac{1}{2}} \quad (40)$$

Therefore, we have eq. (15) from eqs. (21), (34), (38), and (40).

Remark 1. In the same way as the procedure in subsections we use $\sigma = -\tau + (1/2)$ and replacing τ by $-\tau$, then we have other solutions eqs. (16) and (17) different from eqs. (14) and (15), respectively, if $\tau \neq 0$.

The DFS of the homogeneous HAE

Theorem 7. Let $\Phi \in \{\Phi : 0 \neq |\Phi_\alpha| < \infty; \alpha \in \mathbb{R}\}$. Then the homogeneous HAE:

$$\Phi_2 + \left[\lambda + \frac{\gamma}{z} + \frac{\frac{1}{4} - \tau^2}{z^2} \right] \Phi = 0 \quad (41)$$

has particular solutions of the equations:

$$\Phi^{(I)} \equiv kz^{\tau+\frac{1}{2}} e^{-\sqrt{\lambda}iz} \left(e^{2\sqrt{\lambda}iz} z^{-\tau-\frac{1}{2}+\frac{i\gamma}{2\sqrt{\lambda}}} \right)_{-1+Q^{-1}\left(\tau+\frac{1}{2}+\frac{i\gamma}{2\sqrt{\lambda}}\right)} \quad (42)$$

$$\Phi^{(II)} \equiv kz^{\tau+\frac{1}{2}} e^{\sqrt{\lambda}iz} \left(e^{-2\sqrt{\lambda}iz} z^{-\tau-\frac{1}{2}-\frac{i\gamma}{2\sqrt{\lambda}}} \right)_{-1+Q^{-1}\left(\tau+\frac{1}{2}-\frac{i\gamma}{2\sqrt{\lambda}}\right)} \quad (43)$$

$$\Phi^{(III)} \equiv kz^{-\tau+\frac{1}{2}} e^{-\sqrt{\lambda}iz} \left(e^{2\sqrt{\lambda}iz} z^{\tau-\frac{1}{2}+\frac{i\gamma}{2\sqrt{\lambda}}} \right)_{-1+Q^{-1}\left(-\tau+\frac{1}{2}+\frac{i\gamma}{2\sqrt{\lambda}}\right)} \quad (44)$$

$$\Phi^{(IV)} \equiv kz^{-\tau+\frac{1}{2}} e^{\sqrt{\lambda}iz} \left(e^{-2\sqrt{\lambda}iz} z^{\tau-\frac{1}{2}-\frac{i\gamma}{2\sqrt{\lambda}}} \right)_{-1+Q^{-1}\left(-\tau+\frac{1}{2}-\frac{i\gamma}{2\sqrt{\lambda}}\right)} \quad (45)$$

Proof. Taking $\phi = 0$ in *Theorem 6*:

$$w_1 + \left[-2\sqrt{\lambda}i + \frac{\tau + \frac{1}{2} - \frac{i\gamma}{2\sqrt{\lambda}}}{z} \right] w = 0 \quad (46)$$

and

$$g_1 + \left[2\sqrt{\lambda}i + \frac{\tau + \frac{1}{2} + \frac{i\gamma}{2\sqrt{\lambda}}}{z} \right] g = 0 \quad (47)$$

for $\nu = -i(\lambda)^{1/2}$ and $\nu = i(\lambda)^{1/2}$ instead of eqs. (32) and (39), respectively. Therefore, we obtain eq. (42) for eq. (46) and eq. (43) for eq. (47).

Remark 2. In the same way, we use $\sigma = -\tau + (1/2)$ and replacing τ by $-\tau$, then we have other solutions eqs. (44) and (45) different from eqs. (42) and (43), if $\tau \neq 0$.

Example. In the case $\gamma = 0$, and $\tau = -1/2$, and $\phi(z) = z$, we have:

$$\Phi + \lambda\Phi = z \quad (48)$$

from eq. (13) the solution of equation (48):

$$\begin{aligned} \Phi(z) &= e^{-\sqrt{\lambda}iz} \left\{ \left[(z \cdot z e^{\sqrt{\lambda}iz})_0 e^{-2\sqrt{\lambda}iz} z^{-1} \right]_{-1} e^{2\sqrt{\lambda}iz} \right\} = e^{-\sqrt{\lambda}iz} \left\{ [z e^{-\sqrt{\lambda}iz}]_{-1} e^{2\sqrt{\lambda}iz} \right\}_{-1} = \\ &= e^{-\sqrt{\lambda}iz} \left\{ \left(\frac{z\sqrt{\lambda}}{\lambda} i + \frac{1}{\lambda} \right) e^{\sqrt{\lambda}iz} \right\}_{-1} = h_1 e^{-\sqrt{\lambda}iz} + h_2 e^{\sqrt{\lambda}iz} + \frac{z}{\lambda}, \quad \lambda > 0 \end{aligned} \quad (49)$$

by using eq. (14). The function obtained in eq. (49) provides the equation eq. (48).

We plotted 2-D graphs of eq. (49), as shown in fig. 1.

Conclusion

In this article, we first considered the HAE obtained from the radial part of the reduced equation by applying the method of separating variables in the spherical co-ordinates of the Schrodinger equation. We use the nabla discrete fractional operator for hydrogen atom type equations. We consider homogeneous and non-homogeneous HAE. We have obtained many different DFS for these equations. In previous time, no one achieved these solutions of HAE.

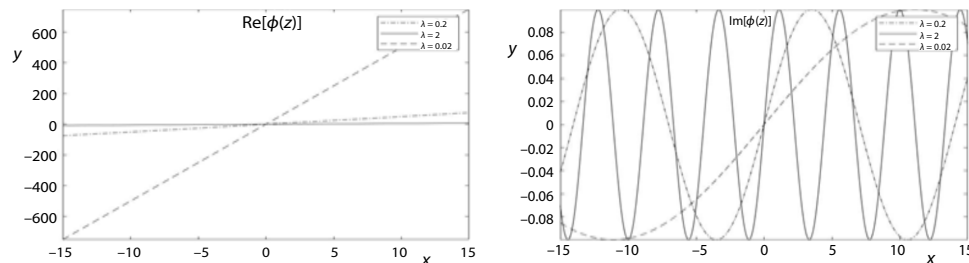


Figure 1. The 2-D dimension solutions of eq. (49), using $h_1 = 0.2$ and $h_2 = 0.3$

We will obtain particular solutions of the same type singular ordinary and partial differential equations by using the discrete fractional nabla operator in future works.

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