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Numerical analysis of fractional order discrete Bloch equations

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Abstract

By defining a new kind of h-extorial function with constant coefficient, this research seeks to solve discrete fractional Bloch equations. By using an extorial function of the Mittag-Leffler type, we are able to discover the general solutions for the magnetization's B_x, B_y, and B_z components. These findings demonstrate the innovative method of fractional order Bloch equations. In addition, we offer a graphical representation of our results.

Keywords: Numerical analysis, fractional derivative, difference equation, discrete Laplace transform, Bloch equation, Caputo derivative.

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1. Introduction

For the past few decades, fractional calculus has attracted a lot of attention. The findings that some academics discovered when they used fractional operators to model some dynamic systems are the sources of this interest [7, 8, 12, 14, 15]. In recent years, the study of boundary value problems for partial differential equations is also a very strong instrument to describe the behavior of biological populations [6, 9–11].

The Bloch equation is a collection of differential equations. Nucleic acids, proteins, RNA, and DNA are some of the costly biological components that may be investigated effectively. Only a few of its practical uses include process control, liquid media, petrochemical plants, and process optimisation in oil refineries. The water content of the saturated and unsaturated zones can be estimated using surface

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magnetic resonance measurements, which are based on the NMR principle. The standard system of the Bloch equations is listed below:

$$\frac{dM_z(t)}{dt} = \frac{M_0 - M_z(t)}{T_1}, \quad \frac{dM_x(t)}{dt} = \bar{\omega}_0 M_y(t) - \frac{M_x(t)}{T_2}, \quad \frac{dM_y(t)}{dt} = -\bar{\omega}_0 M_x(t) - \frac{M_y(t)}{T_2}.$$

The discrete fractional calculus, on the other hand, has also caught the interest of many academics. Numerous applications exist in numerous domains for this kind of calculus that deals with sums and differences of non-integer numbers [1, 3–5].

2. Basic Results on Fractional Difference Operators

For the values $a, b \in \mathbb{R}$ and $h \in \mathbb{R}^+$, we define and use the sets of the following notation $\mathbb{N}_{a,h}$ and ${}_{b,h}\mathbb{N}$ by

$$\mathbb{N}_{a,h} := \{a, a+h, a+2h, \ldots\}, \quad {}_{b,h}\mathbb{N} := \{b, b-h, b-2h, \ldots\}.$$

Definition 2.1. Let $f(\xi)$, $\xi \in [0, \infty)$, be a real or complex valued function and $h > 0$ be a fixed shift value. Then, the backward nabla difference operator on the time scale $h\mathbb{Z}$ is defined by

$$\nabla_h f(\xi) = \frac{f(\xi) - f(\xi - h)}{h}$$

and the forward nabla difference operator is defined by

$$\Delta_h f(\xi) = \frac{f(\xi + h) - f(\xi)}{h}.$$

Definition 2.2. The definitions of the forward jump operator and the backward jump operator for the $h\mathbb{Z}$ are respectively $\rho_h(xi) = \xi - h$ and $\sigma_h(\xi) = \xi + h$.

Definition 2.3 ([13])**.** The (generalized) nabla h-rising function is defined by

$$\xi_h^{\bar{\mu}} = h^{\mu} \frac{\Gamma(\frac{\xi}{h} + \mu)}{\Gamma(\frac{\xi}{h})}, \tag{2.1}$$

for those values of ξ and μ so that the right-hand side of equation (2.1) is defined. We also use the convention that if $\frac{\xi}{h} \in \{0, -1, -2, \ldots\}$, but $\frac{\xi}{h} + \mu \notin \{0, -1, -2, \ldots\}$, then $\xi_h^{\bar{\mu}} := 0$. In particular, $\xi_h^{\bar{0}} = 1$, $\frac{\xi}{h} \notin \{0, -1, -2, \ldots\}$.

Remark 2.4. By using the nabla operator in equation (2.1), we arrive at

$$\nabla_h \xi_h^{\bar{\mu}} = \mu\, \xi_h^{\overline{\mu-1}} \tag{2.2}$$

for those values of ξ and μ so that the expressions in equation (2.2) are well-defined.

Definition 2.5. The nabla h-discrete Mittag-Leffler functions for the values $\lambda \in R, |\lambda| < 1$ and $\theta, \beta, \rho, \xi \in C$ with $\mathrm{Re}(\theta) > 0$, is defined by

$${}_hE^{\rho}_{\overline{\theta,\beta}}(\lambda, \xi) = \sum_{k=0}^{\infty} \lambda^k \frac{\xi_h^{\overline{k\theta+\beta-1}} (\rho)_k}{\Gamma(\theta k + \beta) k!}. \tag{2.3}$$

For $h = \beta = \rho = 1$, we can write it as

$$E_{\overline{\theta}}(\lambda, \xi) = \sum_{k=0}^{\infty} \lambda^k \frac{\xi^{\overline{k\theta}}}{\Gamma(\theta k + 1)},$$

where, we have $(\rho)_k = \rho(\rho+1)\cdots(\rho+k-1)$ and $(1)_k = k!$.

3. Discrete h-Laplace transform and its convolution

The nabla discrete Laplace transform on $\mathbb{N}_{a,h}$ has the following definition after the time scale calculus, which is a modification of Lemma 3.7 using the closed form (inverse difference operator).

Definition 3.1. The nabla h-Laplace transform of the function $f : \mathbb{N}_{a+h,h} \to \mathbb{R}$ is defined by

$$\mathcal{N}_{a,h}\{f\}(s) = \int_a^\infty {}_h\tilde{e}_{\ominus s}(\rho(\xi), a) f(\xi) \nabla_h \xi = \int_a^\infty (1-hs)^{\frac{\xi-a-h}{h}} f(\xi)\nabla_h \xi$$

for those values of $s \neq \frac{1}{h}$ such that the improper integral converges.

When $a = 0$, we write

$$\mathcal{N}_{0,h}\{f\}(s) = \mathcal{N}_h\{f\}(s) = \int_0^\infty (1-hs)^{\frac{\xi-h}{h}} f(\xi)\nabla_h \xi.$$

Theorem 3.2. *Using the summation notation, the Laplace transform can be written as*

$$\mathcal{N}_{a,h}\{f\}(s) = h \sum_{k=\frac{a}{h}+1}^{\infty} (1-hs)^{k-\frac{a}{h}-1} f(kh)$$

for those values of s *such that this infinite series converges.*

When $a = 0$, we have

$$\mathcal{N}_h\{f\}(s) = h \sum_{k=1}^{\infty} (1-hs)^{k-1} f(kh).$$

Lemma 3.3. *For* $\mu \in \mathbb{C} \setminus \mathbb{Z}$*, we have that*

$$\mathcal{N}_h\{\xi_h^{\overline{\mu}}\}(s) = \frac{\Gamma(\mu+1)}{s^{\mu+1}}, \quad \textit{for} \quad |sh-1| < 1.$$

Definition 3.4 ([2])**.** Let $s \in R, 0 < \nu < 1$ and $f, g : \mathbb{N}_{a,h} \to R$ be two functions. The nabla h-discrete convolution of f with g is defined by

$$(f * g)(\xi) = \int_a^\xi f(s) g(\xi - \rho(s) + a)\nabla_h s = h \sum_{k=a/h+1}^{\xi/h} f(kh) g(\xi - \rho(kh) + a).$$

Theorem 3.5 ([2])**.** *(The h-convolution theorem) For any* $\nu \in R/\{\dots, -2, -1, 0\}, s \in R$ *and* f, g *defined on* $\mathbb{N}_{a,h}$*, we have*

$$\mathcal{N}_{a,h}[(f * g)(\xi)](s) = \mathcal{N}_{a,h}[f(\xi)](s) + \mathcal{N}_{a,h}[g(\xi)](s).$$

Lemma 3.6. *For* $\lambda \in R, |\lambda| < 1$ *and* $\theta, \beta, \nu, \xi \in C$ *with* $\mathrm{Re}(\theta) > 0$*, we have*

$$\mathcal{N}_h\left[{}_hE^{\nu}_{\theta,\beta}(\lambda, \xi)\right] = \frac{s^{\theta\nu-\beta}}{(s^\theta - \lambda)^\nu}. \tag{3.1}$$

Proof. Applying Laplace transform in (2.3) and using nabla transform, we get

$$\begin{aligned}\mathcal{N}_h\left[{}_hE^{\nu}_{\theta,\beta}(\lambda, \xi)\right] &= \sum_{k=0}^{\infty} \frac{\lambda^k (\nu)_k}{\Gamma(\theta k+\beta) k!} \mathcal{N}_{a,h}\left[\xi_h^{\overline{k\theta+\beta-1}}\right] \\ &= \sum_{k=0}^{\infty} \frac{\lambda^k}{s^{\theta k+\beta}} \frac{(\nu)_k}{k!} = s^{-\beta} \sum_{k=0}^{\infty} \left(\frac{\lambda}{s^\theta}\right)^k \frac{(\nu)_k}{k!} = s^{-\beta}\left(\frac{s^\theta}{s^\theta - \lambda}\right)^\nu = \frac{s^{\theta\nu-\beta}}{(s^\theta-\lambda)^\nu}.\end{aligned}$$

□

The h-discrete Laplace transform for both the integer difference operator and the Caputo fractional difference is shown in the results below.

Lemma 3.7. *For the function* $f(\xi)$ *defined on* $\mathbb{N}_{a,h}$ *and* $n-1<\nu\leqslant n$*, we have*

$$\mathcal{N}_{a,h}[{}^{C}_{a}\nabla^{\nu}_{h}f(\xi)](s)=s^{\nu}\mathcal{N}_{a,h}[f(\xi)](s)-\sum_{k=0}^{n-1}s^{\nu-1-k}\nabla^{k}_{h}f(a). \tag{3.2}$$

For integer n*, we arrive at the result as*

$$\mathcal{N}_{a,h}[{}_{a}\nabla^{n}_{h}f(\xi)](s)=s^{n}\mathcal{N}_{a,h}[f(\xi)](s)-\sum_{k=0}^{n-1}s^{n-1-k}\nabla^{k}_{h}f(a).$$

4. Numerical solution of discrete fractional Bloch equation

We look at the discrete fractional Bloch equation in this section.

$$^{C}\nabla^{\nu}_{h}B_z(\xi)=\frac{B_0-B_z(\xi)}{R_1'}, \tag{4.1}$$

$$^{C}\nabla^{\nu}_{h}B_x(\xi)=\bar{\omega}_0B_y(\xi)-\frac{B_x(\xi)}{R_2'}, \tag{4.2}$$

$$^{C}\nabla^{\nu}_{h}B_y(\xi)=-\bar{\omega}_0B_x(\xi)-\frac{B_y(\xi)}{R_2'}, \tag{4.3}$$

where $0<\nu<1, \bar{\omega}_0=\frac{\omega_0}{\sigma_2^{\nu-1}}, \frac{1}{R_1'}=\frac{\sigma_1^{1-\nu}}{R_1}$, and $\frac{1}{R_2'}=\frac{\sigma_2^{1-\nu}}{R_2}$. By employing the nabla h-Laplace transform in equation (4.1) and applying (3.2), we conclude that

$$\mathcal{N}_h\{^{C}\nabla^{\nu}_{h}B_z\}(s)=\frac{B_0}{R_1'}\mathcal{N}_h\{1\}(s)-\frac{1}{R_1'}\mathcal{N}_h\{B_z\}(s),$$

$$s^{\nu}\mathcal{N}_h\{B_z\}(s)-s^{\nu-1}B_z(0)=\frac{B_0}{R_1's}-\frac{1}{R_1'}\mathcal{N}_h\{B_z\}(s),$$

$$\mathcal{N}_h\{B_z\}(s)=\frac{B_0}{R_1'}\frac{s^{-1}}{\left(s^{\nu}+\frac{1}{R_1'}\right)}+B_z(0)\frac{s^{\nu-1}}{\left(s^{\nu}+\frac{1}{R_1'}\right)}.$$

Now, by applying the inverse nabla h-Laplace transform and using (3.1), we have

$$\mathcal{B}_z(\xi)=\frac{B_0}{R_1'}{}_hE^{1}_{\overline{\nu,\nu+1}}\left(-\frac{1}{R_1'},\xi\right)+B_z(0){}_hE^{1}_{\overline{\nu,1}}\left(-\frac{1}{R_1'},\xi\right).$$

The solutions for $B_x(\xi)$ and $B_y(\xi)$ can be found by solving the corresponding fractional order difference equation

$$B_+(\xi)=B_x(\xi)+iB_y(\xi) \tag{4.4}$$

with $B_+(0)=B_x(0)+iB_y(0)$ and applying fractional nabla operator for the above equation, we have

$$\begin{aligned}^{C}\nabla^{\nu}_{h}B_+(\xi)&={}^{C}\nabla^{\nu}_{h}B_x(\xi)+i{}^{C}\nabla^{\nu}_{h}B_y(\xi)\\&=\bar{\omega}_0B_y(\xi)-\frac{B_x(\xi)}{R_2'}-i\bar{\omega}_0B_x(\xi)-i\frac{B_y(\xi)}{R_2'}\\&=-i\bar{\omega}_0[B_x(\xi)+iB_y(\xi)]-\frac{1}{R_2'}[B_x(\xi)+iB_y(\xi)]=-i\bar{\omega}_0B_+(\xi)-\frac{1}{R_2'}B_+(\xi).\end{aligned}$$

Applying nabla transform on both sides, we get

$$\begin{aligned}
\mathcal{N}_h[{}^C\nabla_h^\nu B_+(\xi)] &= \mathcal{N}_h[-i\bar{\omega}_0 B_+(\xi) - \frac{1}{R_2'}B_+(\xi)],\\
s^\nu \mathcal{N}_h[B_+(\xi)] - s^{\nu-1}B_+(0) &= -i\bar{\omega}_0\mathcal{N}_h[B_+(\xi)] - \frac{1}{R_2'}\mathcal{N}_h[B_+(\xi)],\\
\left[s^\nu + i\bar{\omega}_0 + \frac{1}{R_2'}\right]\mathcal{N}_h[B_+(\xi)] &= s^{\nu-1}B_+(0),\\
\mathcal{N}_h[B_+(\xi)] &= \frac{s^{\nu-1}B_+(0)}{s^\nu + i\bar{\omega}_0 + \frac{1}{R_2'}}.
\end{aligned}$$

Now applying inverse nabla transform on both sides and using (3.1) for the particular values $\beta = 1, \lambda = -i\bar{\omega}_0 - \frac{1}{R_2'}$, we have

$$B_+(\xi) = B_+(0)_h E_{\overline{\nu,1}}^{\underline{1}}(-i\bar{\omega}_0 - \frac{1}{R_2'}, \xi). \tag{4.5}$$

Now, $\lambda = -i\bar{\omega}_0 - \frac{1}{R_2'} = -i\frac{\omega_0}{\sigma_2^{\nu-1}} - \frac{\sigma_2^{1-\nu}}{R_2} = -i\omega_0\sigma_2^{1-\nu} - \frac{\sigma_2^{1-\nu}}{R_2}$. To find the solutions of (4.5), we define a new type of h-extorial function with constant coefficient as follows.

Definition 4.1. Let $\xi \in (-\infty, \infty)$ and $h, \lambda > 0$. Then we have the h-extorial function with constant coefficient

$$e^{\lambda \xi_h^{\overline{k}}} = 1 + \frac{\lambda \xi_h^{\overline{1}}}{1!} + \frac{\lambda^2 \xi_h^{\overline{2}}}{2!} + \frac{\lambda^3 \xi_h^{\overline{3}}}{3!} + \cdots = \sum_{k=0}^{\infty} \frac{\lambda^k \xi_h^{\overline{k}}}{k!}. \tag{4.6}$$

For the particular values of $h = 1, k = 1$, and $\lambda = 1$, we have $e^{i\xi} = \cos t + i \sin t$,

$$_1E_{\overline{1,1}}^{\underline{1}}(1, \xi) = \sum_{k=0}^{\infty} \frac{\xi_1}{1!} = e^{\xi}. \tag{4.7}$$

It follows from (4.5) that

$$\begin{aligned}
B_+(\xi) = B_+(0)_h E_{\overline{\nu,1}}^{\underline{1}}(\lambda, \xi) &= B_+(0) e^{(i\omega_0 + \frac{1}{R_2})\xi_h^{\overline{k}}}\\
&= B_+(0) e^{\frac{1}{R_2}\xi_h^{\overline{k}}} e^{i\omega_0 \xi_h^{\overline{k}}} = B_+(0) e^{\frac{1}{R_2}\xi_h^{\overline{k}}}\left[\cos(\omega_0(\xi)_h^{\overline{k}}) + i\sin(\omega_0(\xi)_h^{\overline{k}})\right].
\end{aligned}$$

Now using (4.4), we arrive at $B_x(\xi) + iB_y(\xi) = [B_x(0) + iB_y(0)]e^{\frac{\xi_h^{\overline{k}}}{R_2}}\left[\cos(\omega_0(\xi)_h^{\overline{k}}) + i\sin(\omega_0(\xi)_h^{\overline{k}})\right]$. Equating the real and imaginary part, gives

$$\begin{aligned}
B_x(\xi) &= e^{\frac{\xi_h^{\overline{k}}}{R_2}}\left[B_x(0)\cos(\omega_0(\xi)_h^{\overline{k}}) - B_y(0)\sin(\omega_0(\xi)_h^{\overline{k}})\right],\\
B_y(\xi) &= e^{\frac{\xi_h^{\overline{k}}}{R_2}}\left[B_y(0)\cos(\omega_0(\xi)_h^{\overline{k}}) + B_x(0)\sin(\omega_0(\xi)_h^{\overline{k}})\right].
\end{aligned}$$

5. Graphical illustrations

In this part, we analyse our findings for the suggested Bloch equation using graphical examples. For the particular values of $h = 1, k = 1$, we deduce that the solutions of discrete fractional Bloch equations (4.1)-(4.3) are

$$\begin{aligned}
\mathcal{B}_z(\xi) &= \frac{B_0}{R_1'}{}_1E^{\nu}_{\overline{\nu,1+\nu}}\left(-\frac{1}{R_1'},\xi\right) + B_z(0)_1E^{\nu}_{\overline{\nu,1}}\left(-\frac{1}{R_1'},\xi\right),\\
B_x(\xi) &= e^{\frac{\xi}{R_2}}\left[B_x(0)\cos(\omega_0\xi) - B_y(0)\sin(\omega_0\xi)\right],\\
B_y(\xi) &= e^{\frac{\xi}{R_2}}\left[B_y(0)\cos(\omega_0\xi) + B_x(0)\sin(\omega_0\xi)\right].
\end{aligned}$$

For the case of numerical analysis and graphical behavior of the above solutions of Bloch equations, Figures 1, 2, and 3 are presented for various values of initial conditions like $B_x(0), B_y(0), \omega_0$ and T_2.

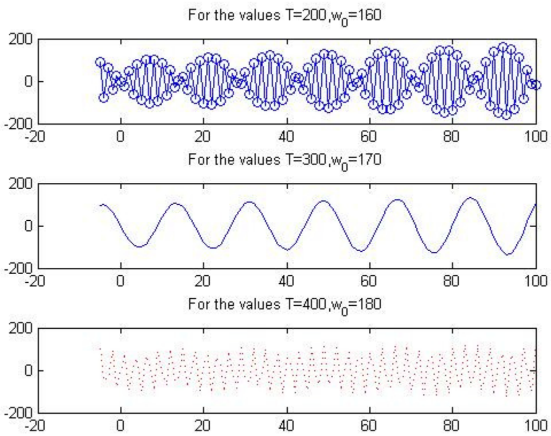

Figure 1

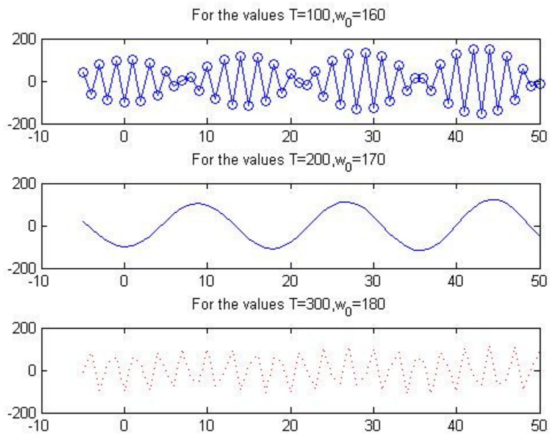

Figure 2

From the above graphical behavior one can easily change the initial parameters to get numerical cases.

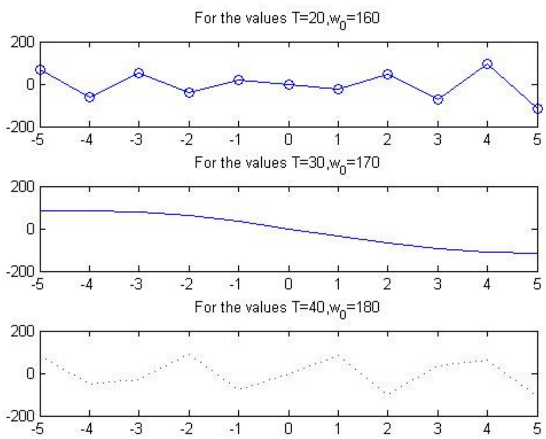

Figure 3

6. Conclusion

We examined a particular variant of the discrete Bloch equation in this study that involves a nabla h-fractional Caputo difference. The discrete Laplace transform and the discrete Mittag-Leffler functions were used as the basis for our analytical solutions. For particular settings of the beginning values, parameters, and the right side of the equation, we offered the numerical solutions. The delta difference operator can take the place of the nabla difference that is being considered. We don't believe that finding the analytical solutions in this situation will be simple. On the other hand, researchers may also substitute newly defined fractional differences involving non-singular kernels for the h-fractional Caputo difference.

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