Journal of King Saud University - Science 36 (2024) 103263

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Journal of King Saud University - Science

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Full Length Article

Numerical computation of fractional Bloch equation by using Jacobi operational matrix

Jagdev Singh [a,b,*], Jitendra Kumar [a], Dumitru Baleanu [c,d]

[a] Department of Mathematics, JECRC University, Jaipur 303905, Rajasthan, India
[b] Department of Mathematics, Kyung Hee University, 26 Kyungheedae-ro, Dongdaemun-gu, Seoul, 02447, Korea
[c] Department of Computer Science and Mathematics, Lebanese American University, Beirut, Lebanon
[d] Institute of Space Sciences, Magurele-Bucharest, Romania

ARTICLE INFO

Keywords:
Fractional Bloch model
NMR
Operational matrix
Caputo-Fabrizio fractional derivative
Caputo-Fabrizio fractional integral
Jacobi polynomial

ABSTRACT

In this work, we present a numerical scheme based on the operational matrix of fractional Caputo-Fabrizio (CF) integration for handling fractional Bloch equation (FBE) in nuclear magnetic resonance (NMR). The understanding of Bloch equation provides us a fundamental framework for describing magnetic resonance phenomena, facilitating breakthrough in diverse fields such as medical diagnostics, quantum computing and materials characterization. The non-integer order derivative and integration are presented in the Caputo-Fabrizio sense. To construct the operational matrix, Jacobi polynomial is used as a basis. The fractional Bloch equation is transformed into a set of algebraic equations by using the operational matrix. In order to examine the fractional order problem, we obtain an approximate solution for FBE and present the numerical results in graphical and tabular forms.

1. Introduction

Bloch model is a system of differential equations. It is most useful for studying costly biological materials like nucleic acids, proteins, DNA and RNA. Petrochemical plants, liquid media, process control and process optimization in oil refineries are just a few of the real-world applications of the Bloch equation. Based on the NMR concept, surface magnetic resonance allows for measurements that can be used to infer the saturated and unsaturated zone's water content. The classical system of Bloch equations can be written as

$$\begin{aligned}\frac{dP_x(\xi)}{d\xi} &= \mu_0 P_y(\xi) - \frac{P_x(\xi)}{T_2}\\ \frac{dP_y(\xi)}{d\xi} &= -\mu_0 P_x(\xi) - \frac{P_y(\xi)}{T_2}\\ \frac{dP_z(\xi)}{d\xi} &= \frac{P_0 - P_z(\xi)}{T_1}\end{aligned} \tag{1}$$

with the initial conditions $P_x(0) = b_1, P_y(0) = b_2$ and $P_z(0) = b_3$.

Here $P_x(\xi), P_y(\xi)$ and $P_z(\xi)$ are indicting system magnetization in x, y in addition z components respectively, μ_0 indicates the resonant frequency provided by the relation $\mu_0 = \gamma M_0$, where M_0 represents static magnetic field in z-component, P_0 stands for equilibrium magnetization, T_2 and T_1 are the spin–spin relaxation and spin–lattice time respectively, b_1 , b_2 and b_3 are real constants.

For the mathematical model given in Eq. (1), the exact solution is expressed as

$$\begin{aligned}P_x(\xi) &= e^{-\frac{\xi}{T_2}}\left(P_x(0)\cos\mu_0\xi + P_y(0)\sin\mu_0\xi\right)\\ P_y(\xi) &= e^{-\frac{\xi}{T_2}}\left(P_y(0)\cos\mu_0\xi - P_y(0)\sin\mu_0\xi\right)\\ P_z(\xi) &= P_z(0)e^{-\frac{\xi}{T_2}} + P_0\left(1 - e^{-\frac{\xi}{T_2}}\right)\end{aligned} \tag{2}$$

* Corresponding author at: Department of Mathematics, JECRC University, Jaipur 303905, Rajasthan, India.
E-mail addresses: jagdevsinghrathore@gmail.com (J. Singh), jrao562@gmail.com (J. Kumar), dumitru.baleanu@gmail.com (D. Baleanu).

https://doi.org/10.1016/j.jksus.2024.103263
Received 28 January 2024; Received in revised form 8 May 2024; Accepted 15 May 2024
Available online 16 May 2024
1018-3647/

Fractional calculus has a vast variety of practical applications including physics (Singh et al., 2020), computer security (Singh et al., 2018), viscoelasticity (Bagley and Torvik, 1983; Bagley and Torvik, 1985; Srivastava et al., 2019), fluid dynamics (Kumar et al., 2015), medical and health science (Kumar and Singh, 2020; Singh et al., 2021a, b; Robinson, 1981). For additional details, the reader should refer (Miller and Ross, 1993; Kilbas et al., 2006). The fractional Bloch equation may simulate a variety of magnetic resonance systems. Due to non-local nature, fractional operators impart past memory of the system. Therefore, to examine the resulting magnetic resonance system, we will substitute the classical derivative in the Bloch equation with CF derivative. The resulting FBE is expressed as

$$\begin{aligned} {}_0^{CF}D_\xi^\alpha P_x(\xi) &= \mu_0 P_y(\xi) - \frac{P_x(\xi)}{T_2} \\ {}_0^{CF}D_\xi^\beta P_y(\xi) &= -\mu_0 P_x(\xi) - \frac{P_y(\xi)}{T_2} \\ {}_0^{CF}D_\xi^\gamma P_z(\xi) &= \frac{P_0 - P_z(\xi)}{T_1} \end{aligned} \tag{3}$$

where $0 < \alpha, \beta, \gamma < 1$.Jajarmi et al. (2022) provided a study on the description of the immune system. Singh (2020) investigated the effect of alcohol on ingested quality and quantity by a human being. Singh and Gupta (2023) provided a computational scheme with Caputo Katugampola to solve non-linear PDE. Kumar et al. (2023) simulated fractional partial differential equation analytically. A childhood diseases SIR model was studied by Veeresha et al. (2022). A detailed investigation on gemini virus examined by Nisar et al. (2022). Kumar et al. (2022), Kumar and Kumar (2022) discussed different models for paste side effects and ecological model. Dubey et al., 2022a, b investigated a fractional LWR model on heavy traffic flow.

Researchers, such as Mahariq et al. (2014), Mahariq and Kurt (2015), Mahariq et al. (2016), have explored various models using the spectral element method due to its efficacy in accurately and efficiently solving differential equations. Dubey et al., 2022a, b studied an analytic computational scheme for solving the fractional Bloch equation appearing in NMR flows. Singh et al., 2021a, b solved the system of the Bloch equation using Sumudu transform. Kumar et al. (2014) analyzed fractional Bloch equation analytically. Bharwy et al. (2014) provided a Jacobi operational matrix of Riemann-Liouville integration. Singh (2016) solved fractional Bloch equation numerically by using an operational matrix with Legendre polynomial. Some recent work on fractional calculus can be seen (Hashmi et al., 2022; Dubey et al., 2022a, b; Singh et al., 2022).

In the present article, we describe a numerical technique for the approximate solution of FBE based on an operational matrix of Caputo-Fabrizio fractional order integration. The unique aspect of our research is centred on developing an operational matrix that harnesses the power of Jacobi polynomials specifically for Caputo-Fabrizio fractional integration. This pioneer method significantly demonstrates the effectiveness of the operational matrix technique. This method is a more resilient and adaptable solution for tackling fractional differential equations. Introducing Jacobi polynomials into the operational matrix broadens its utility across various applications and elevates the precision of approximations. Consequently, our work contributes to the progression of fractional calculus and facilitates its real-world applications by providing enhanced computational tools. By applying this method, we find some different unknown coefficients for approximate parameters. With the aid of the determined coefficient, we attain an approximate solution of the given system of arbitrary order Bloch model pertaining to Caputo-Fabrizio non-integer order derivatives.

2. Preliminaries

In this paper, fractional order differentiation and integration is Caputo-Fabrizio (CF) sense derivative.

Let $a, b, \beta \in \mathbb{R}$ s.t $0 < \beta \le 1$.

The CF non-integer derivative of order β (Nchama, 2020) of a function $u \in H'[a, b]$ is given as

$${}_0^{CF}D_\xi^\beta u(\xi) = \frac{1}{1-\beta}\int_a^\xi e^{-\left(\frac{\beta}{1-\beta}\right)(\xi - s)} u'(s)ds \tag{4}$$

The CF integration of order β (Nchama, 2020) of a function $u \in H'[a, b]$ is a linear operator represented as

$${}_0^{CF}I_\xi^\beta u(\xi) = (1-\beta)u(\xi) + \beta\int_a^\xi u(x)dx \tag{5}$$

The Jacobi polynomial of degree r (Singh and Srivastava, 2020) is given by

$$\nu_r(\xi) = \sum_{k=0}^{r}(-1)^{r-k}\frac{\Gamma(r+d+1)\Gamma(r+k+c+d+1)}{\Gamma(k+d+1)\Gamma(r+c+d+1)(r-k)!k!}\xi^k \tag{6}$$

The orthonormal property of Jacobi polynomial with weight function $w^{(c,d)}(\xi) = (1-\xi)^c\xi^d$ is expressed as

$$\int_0^1 \nu_n(\xi)\nu_m(\xi)w^{(c,d)}(\xi)d\xi = \sigma_n^{c,d}\delta_{mn} \tag{7}$$

where δ_{mn} represents the Kronecker delta function and

$$\sigma_n^{c,d} = \frac{\Gamma(n+c+1)\Gamma(n+d+1)}{(2n+c+d+1)n!\Gamma(n+c+d+1)} \tag{8}$$

A function $f \in L^2[0, 1]$, having $|f''(\xi)| \le Q$, can be extended as

$$f(\xi) = \lim_{n\to\infty}\sum_{r=0}^{n} c_r\nu_r(\xi) \tag{9}$$

where

$$c_r = \frac{1}{\sigma_r^{c,d}}\int_0^1 \nu_r(\xi)\, f(\xi)w^{(c,d)}(\xi)d\xi \tag{10}$$

Eq. (9), for the finite dimensional approximation, is expressed in the subsequent form

$$f \cong \sum_{r=0}^{m} c_r\nu_r(\xi) = C^T q_m(\xi) \tag{11}$$

where C in addition $q_m(\xi)$ are $(m+1)\times 1$ matrices expressed by $C = [c_0, c_1, \cdots, c_m]^T$ and $q_m(\xi) = [\nu_0, \nu_1, \cdots, \nu_m]^T$.

3. Operational matrix for Caputo-Fabrizio fractional integration

Theorem 1. If $q_m(\xi) = [\nu_0, \nu_1, \cdots, \nu_m]^T$ represents shifted Jacobi vector in addition if $\beta > 0$, then ${}_0^{CF}I_\xi^\beta \nu_r(\xi) = {}_0^{CF}I_\xi^{(\beta)} q_m(\xi)$. Where ${}_0^{CF}I_\xi^{(\beta)} = \eta_\beta(r, s)$, is the $(m+1)\times(m+1)$ operational matrix of Caputo-Fabrizio fractional integral of order β, and its (r, s) th element expressed by

$$\eta_\beta(r,s)=\sum_{k=0}^{r}\sum_{f=0}^{s}(-1)^{r+s-k-f}\frac{\Gamma(r+d+1)\Gamma(r+k+c+d+1)(2s+c+d+1)s!\Gamma(s+f+c+d+1)\Gamma(c+1)}{\Gamma(k+d+1)\Gamma(r+c+d+1)(r-k)!k!(s+c+1)\Gamma(f+d+1)(s-f)!f!}\left[\frac{(1-\beta)\Gamma(f+k+d+1)}{\Gamma(f+k+c+d+2)}+\frac{\beta}{(k+1)}\frac{\Gamma(f+k+d+2)}{\Gamma(f+k+c+d+3)}\right]$$

Proof. The analytical form of $\nu_r(\xi)$ *of degree, r is given by Eq. (6). Using Eq. (5) we get*

$$
\begin{aligned}
{}_{0}^{CF}I_{\xi}^{\beta}(\nu_r(\xi))&={}_{0}^{CF}I_{\xi}^{\beta}\left(\sum_{k=0}^{r}(-1)^{r-k}\frac{\Gamma(r+d+1)\Gamma(r+k+c+d+1)}{\Gamma(k+d+1)\Gamma(r+c+d+1)(r-k)!k!}\xi^{k}\right)=\sum_{k=0}^{r}(-1)^{r-k}\frac{\Gamma(r+d+1)\Gamma(r+k+c+d+1)}{\Gamma(k+d+1)\Gamma(r+c+d+1)(r-k)!k!}{}_{0}^{CF}I_{\xi}^{\beta}(\xi^{k})\\
&=\sum_{k=0}^{r}(-1)^{r-k}\frac{\Gamma(r+d+1)\Gamma(r+k+c+d+1)}{\Gamma(k+d+1)\Gamma(r+c+d+1)(r-k)!k!}\left[(1-\beta)\xi^{k}+\beta\int_{0}^{\xi}s^{k}ds\right]\\
&=\sum_{k=0}^{r}(-1)^{r-k}\frac{\Gamma(r+d+1)\Gamma(r+k+c+d+1)}{\Gamma(k+d+1)\Gamma(r+c+d+1)(r-k)!k!}\left[(1-\beta)\xi^{k}+\beta\frac{\xi^{k+1}}{k+1}\right]
\end{aligned}
\tag{12}
$$

Now approximate $(1-\beta)\xi^{k}+\beta\frac{\xi^{k+1}}{k+1}$ by $m+1$ terms of the shifted Jacobi series, it yields

$$(1-\beta)\xi^{k}+\beta\frac{\xi^{k+1}}{k+1}=\sum_{s=0}^{m}c_s\sigma_s(\xi). \tag{13}$$

where c_s is given from Eq. (10) and

$$c_s=\frac{(2s+c+d+1)s!}{\Gamma(s+c+1)}\sum_{f=0}^{s}(-1)^{s-f}\frac{\Gamma(s+f+c+d+1)\Gamma(c+1)}{\Gamma(f+d+1)(s-f)!f!}\left[\frac{(1-\beta)\Gamma(f+k+d+1)}{\Gamma(f+k+c+d+2)}+\frac{\beta}{(k+1)}\frac{\Gamma(f+k+d+2)}{\Gamma(f+k+c+d+3)}\right]. \tag{14}$$

By Eqs. (12) and (13), we get

$${}_{0}^{CF}I_{\xi}^{\beta}(\nu_r(\xi))=\sum_{s=0}^{m}\eta_\beta(r,s)\nu_s(\xi),\ \ r=0,1,m \tag{15}$$

where

$$\eta_\beta(r,s)=\sum_{k=0}^{r}\sum_{f=0}^{s}(-1)^{r+s-k-f}\frac{\Gamma(r+d+1)\Gamma(r+k+c+d+1)(2s+c+d+1)s!\Gamma(s+f+c+d+1)\Gamma(c+1)}{\Gamma(k+d+1)\Gamma(r+c+d+1)(r-k)!k!(s+c+1)\Gamma(f+d+1)(s-f)!f!}$$

$$\left[\frac{(1-\beta)\Gamma(f+k+d+1)}{\Gamma(f+k+c+d+2)}+\frac{\beta}{(k+1)}\frac{\Gamma(f+k+d+2)}{\Gamma(f+k+c+d+3)}\right]. \tag{16}$$

In this way, Eq. (15) can be written in the following manner

$${}_{0}^{CF}I_{\xi}^{\beta}(\nu_r(\xi))=[\eta_\beta(r,0),\eta_\beta(r,1),\eta_\beta(r,2),\ldots\ldots\ldots\ldots\ldots,\eta_\beta(r,n)]q_m(\xi) \tag{17}$$

4. Computational procedure of the method

Here, we discuss a computational scheme to obtain the approximate solutions of FBE. By utilizing it we can find magnetisation in each direction.

First of all, we take the subsequent approximation

$${}_{0}^{CF}D_{\xi}^{\alpha}P_x(\xi)=C_1^{T}q(\xi),\quad {}_{0}^{CF}D_{\xi}^{\beta}P_y(\xi)=C_2^{T}q(\xi),\quad {}_{0}^{CF}D_{\xi}^{\gamma}P_z(\xi)=C_3^{T}q(\xi) \tag{18}$$

and

$$P_x(0)=E^{T}q(\xi),P_y(0)=F^{T}q(\xi),P_x(0)=G^{T}q(\xi),\ \frac{P_0}{T_1}=H^{T}q(\xi). \tag{19}$$

From Eqs. (18) and (19), we have

$$P_x(\xi)=C_1^{T}\,{}_{0}^{CF}I_{\xi}^{\alpha}q(\xi)+E^{T}q(\xi), \tag{20}$$

$$P_y(\xi)=C_2^{T}\,{}_{0}^{CF}I_{\xi}^{\beta}q(\xi)+F^{T}q(\xi), \tag{21}$$

$$P_z(\xi)=C_3^{T}\,{}_{0}^{CF}I_{\xi}^{\gamma}q(\xi)+G^{T}q(\xi), \tag{22}$$

Using Eqs. (18)–(22) in Eq. (3), we have

$$C_1^{T}\left(I+\frac{1}{T_2}{}_{0}^{CF}I_{\xi}^{\alpha}\right)-\mu_0C_2^{T}\,{}_{0}^{CF}I_{\xi}^{\beta}=\mu_0F^{T}-\frac{1}{T_2}E^{T} \tag{23}$$

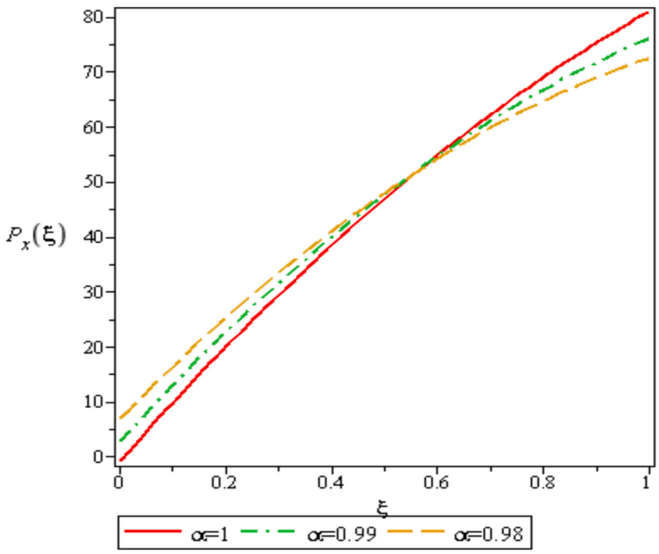

Fig. 1. Response of the solution of $P_x(\xi)$ at $\alpha = 0.98,\ 0.99$ and 1, with parameter: $\mu_0 = 1,\ T_1 = 1,\ T_2 = 20,\ c = 1, d = 1$.

$$\mu_0 C_1^T\, {}_0^{CF}I_\xi^\alpha + C_2^T\left(I + \frac{1}{T_2}\,{}_0^{CF}I_\xi^\beta\right) = -\mu_0 E^T - \frac{1}{T_2}F^T \tag{24}$$

$$C_3^T\left(I + \frac{1}{T_{10}}\,{}^{CF}I_\xi^\gamma\right) = H^T - \frac{1}{T_1}G^T \tag{25}$$

where ${}_0^{CF}I_\xi^\alpha$, ${}_0^{CF}I_\xi^\beta$ and ${}_0^{CF}I_\xi^\gamma$ are indicating operational matrices of Caputo-Fabrizio integral of α, β as well as γ orders and I stand for an identity matrix.

From Eqs. (23)–(25), we have

$$C_1^T U_1 - C_2^T U_5 = S_1 \tag{26}$$

$$C_1^T U_4 + C_2^T U_2 = S_2 \tag{27}$$

$$C_3^T U_3 = S_3 \tag{28}$$

where

$$U_1 = I + \frac{1}{T_{20}}\,{}^{CF}I_\xi^\alpha \tag{29}$$

$$U_2 = I + \frac{1}{T_{20}}\,{}^{CF}I_\xi^\beta \tag{30}$$

$$U_3 = I + \frac{1}{T_{10}}\,{}^{CF}I_\xi^\gamma \tag{31}$$

$$U_4 = \mu_0\,{}_0^{CF}I_\xi^\alpha \tag{32}$$

$$U_5 = \mu_0\,{}_0^{CF}I_\xi^\beta \tag{33}$$

$$S_1 = \mu_0 F^T - \frac{1}{T_2}E^T \tag{34}$$

$$S_2 = -\mu_0 E^T - \frac{1}{T_2}F^T \tag{35}$$

$$S_3 = H^T - \frac{1}{T_1}G^T \tag{36}$$

Matrix $U_1, U_2, U_3, U_4, U_5, S_1, S_2$ and S_3 are known matrices since these are expressed in terms of known values.

On solving Eqs. (26)–(28)

$$C_1^T = \left(S_1U_5^{-1} + S_2U_2^{-1}\right)\left(U_1U_5^{-1} + U_4U_2^{-1}\right)^{-1} \tag{37}$$

$$C_2^T = \left\{\left(S_1U_5^{-1} + S_2U_2^{-1}\right)\left(U_1U_5^{-1} + U_4U_2^{-1}\right)^{-1}U_1 - S_1\right\}W_5^{-1} \tag{38}$$

$$C_3^T = S_3W_3^{-1} \tag{39}$$

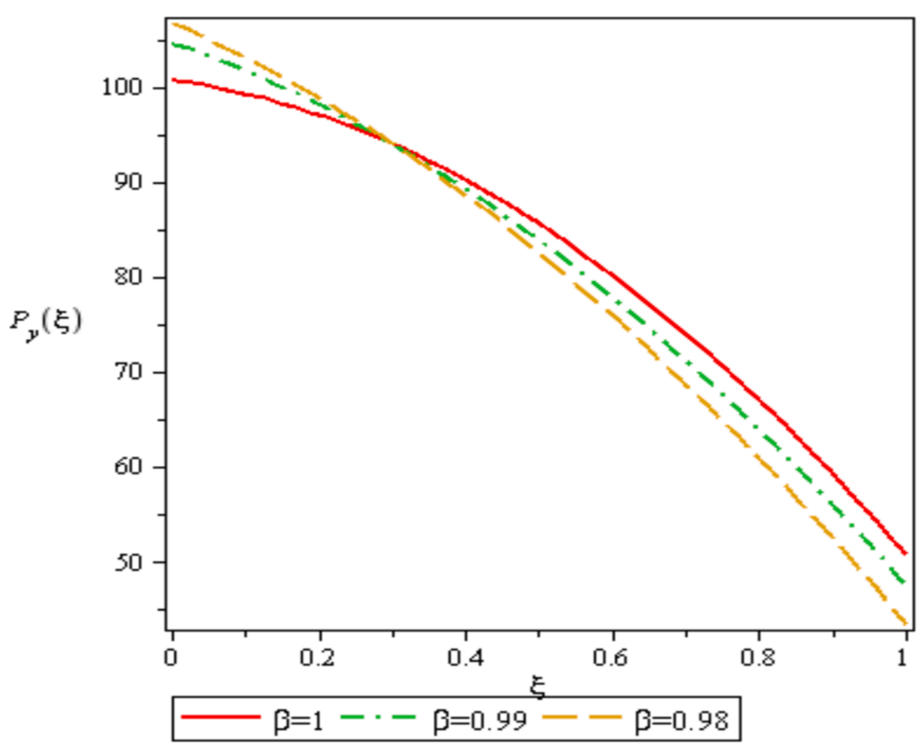

Fig. 2. Response of the solution of $P_y(\xi)$ at $\beta = 0.98,\ 0.99$ and 1, with parameter: $\mu_0 = 1,\ T_1 = 1,\ T_2 = 20,\ c = 1, d = 1$.

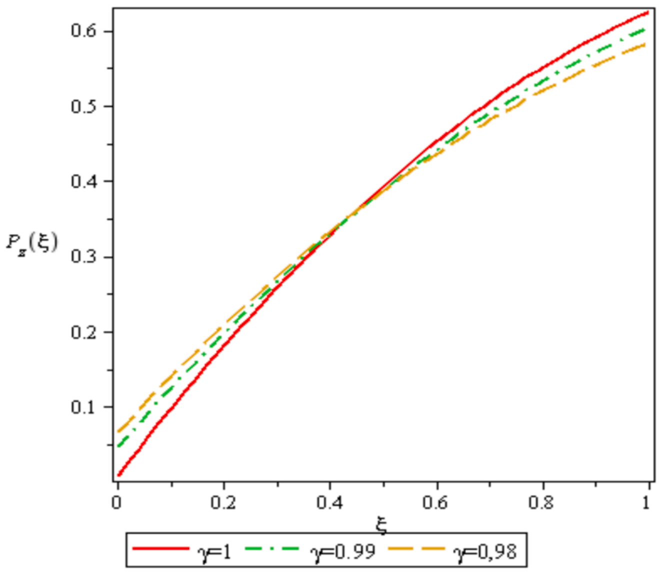

Fig. 3. Response of the solution of $P_z(\xi)$ at $\gamma = 0.98, 0.99$ and 1, with parameter:$\mu_0 = 1, T_1 = 1, T_2 = 20, c = 1, d = 1$.

Table 1
Comparison with the approximate solutions of the scheme in (Singh, 2017; Kumar et. al, 2014), present technique and exact solution of P_x, P_y and P_z.

P_j	ξ	Exact Solution	Present Method	Kumar et al. (2014)	Singh (2017)
$P_x(\xi)$	0.2	19.6693	19.7950	19.6677	19.6528
	0.4	38.1707	38.3376	38.1413	38.1798
	0.6	54.7955	54.7148	54.6270	54.8107
	0.8	68.9228	68.9267	68.3307	68.9246
	1	80.0432	80.0292	78.4583	80.0270
$P_y(\xi)$	0.2	97.0315	97.0346	97.0783	97.1108
	0.4	90.2823	90.2021	90.3399	90.3047
	0.6	80.0943	80.1943	79.8246	80.0340
	0.8	66.9388	67.0111	65.5723	66.8616
	1	51.3951	51.3826	47.6269	51.3626
$P_z(\xi)$	0.2	0.1813	0.1802	0.1813	0.1813
	0.4	0.3297	0.3285	0.3297	0.3297
	0.6	0.4512	0.4520	0.4512	0.4512
	0.8	0.5507	0.5508	0.5507	0.5507
	1	0.6321	0.6321	0.6321	0.6321

Using Eqs. (37)–(39) in Eqs. (20)–(22) respectively, we get a system of magnetisation $P_x(\xi), P_y(\xi)$ and $P_z(\xi)$ for fractional Bloch model.

5. Results and discussions

We will numerically simulate our outcomes in this section. To compute numerical results, we take $P_x(0) = 0$, $P_y(0) = 100$ and $P_z(0) = 0$. The behaviour of the solutions of $P_x(\xi)$, $P_y(\xi)$ and $P_z(\xi)$ shown in Figs. 1-3 at distinct values α, β and γ, respectively.

It is evident from these outcomes of the study that the obtained solution regularly changes from fractional order to integer order. From Fig. 1, we observe that the value of $P_x(\xi)$ increases with increasing time ξ. Decreasing the order of non-integer order derivatives leads to increase in the value of $P_x(\xi)$ initially, after some time its nature is opposite. From Fig. 2, we notice that the value of $P_y(\xi)$ decrease with increasing time on ξ. Decreasing the order of arbitrary order derivatives leads to diminution in the value of $P_y(\xi)$ initially, after some time its nature is opposite. From Fig. 3 we inspect that value of $P_z(\xi)$ increase with increasing time ξ. On decreasing the order of fractional derivatives leads to an enhancement in the value of $P_z(\xi)$ initially, after some time its nature is opposite.

It is evident that the results vary continuously from arbitrary order to classical order. Both the exact solution as well as the approximate solutions obtained by using our proposed scheme is presented in the Table 1. We have compared outcomes obtained by Jacobi polynomial, exact solution and method (Singh, 2017; Kumar et al., 2014). Table 1 reveals that the results of the described technique are faithful for practical implementations of FBE.

6. Conclusions

In this study, we have suggested a computational scheme for arbitrary order Bloch equation pertaining to the Caputo −Fabrizio operator. The proposed method offers notable advantages in terms of simplicity and user-friendliness compared to alternative techniques, primarily due to the straightforward construction of the operational matrix for differential equations. Specifically, we develop an operational matrix for Caputo-Fabrizio integration by utilizing the Jacobi polynomial. When α, $\beta, \gamma = 1$, we observe strong agreement between the solution obtained through operational matrix techniques and the exact solution of the Bloch equation of arbitrary order. These findings underscore the suitability and accuracy of our proposed approach for analyzing fractional order models employing the Caputo-Fabrizio operator. Future endeavors will delve into the utilization of various special functions such as Bernstein and Vieta Lucas, alongside the operational matrix method, while also exploring the impacts of arbitrary orders on the dynamics of the Bloch equation.

CRediT authorship contribution statement

Jagdev Singh: Writing – review & editing, Supervision, Software, Conceptualization. **Jitendra Kumar:** Writing – original draft, Software, Methodology, Conceptualization. **Dumitru Baleanu:** Visualization, Validation, Investigation, Formal analysis.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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