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Operational matrix approach for approximate solution of fractional model of Bloch equation

Harendra Singh

Department of Mathematical Sciences, Indian Institute of Technology, Banaras Hindu University, Varanasi 221005, India

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Abstract In present paper operational matrix of integration for Laguerre polynomial is used to solve fractional model of Bloch equation in nuclear magnetic resonance (NMR). The operational matrix converts the Bloch equation in a system of linear algebraic equations. Solving system we obtain the approximate solutions for fractional Bloch equation. Results are compared with existing methods and exact solution. Graphs are plotted for different fractional values of time derivatives.

1. Introduction

The fractional Bloch equations are used in physics, chemistry, nuclear magnetic resonance (NMR), electron spin resonance (ESR) and magnetic resonance imaging (MRI). The fractional Bloch equation is generalization of standard Bloch equation and obtained by replacing integer order time derivative to fractional order Caputo derivative. Fractional calculus has many real applications in science and engineering such as fluid-dynamic traffic (He, 1999), biology (Robinson, 1981), viscoelasticity (Bagley and Torvik, 1983a,b, 1985), signal processing (Panda and Dash, 2006), bioengineering (Magin, 2004) and control theory (Bohannan, 2008). The fractional model of Bloch equation is given as,

$$\begin{aligned} \frac{d^{\alpha}M_x(t)}{dt^{\alpha}} &= \omega_0 M_y(t) - \frac{M_x(t)}{T_2}, \\ \frac{d^{\beta}M_y(t)}{dt^{\beta}} &= -\omega_0 M_x(t) - \frac{M_y(t)}{T_2}, \\ \frac{d^{\gamma}M_z(t)}{dt^{\gamma}} &= \frac{M_0 - M_z(t)}{T_1}, \end{aligned} \tag{1}$$

where $0 < \alpha, \beta, \gamma \leqslant 1$, with initial conditions $M_x(0) = 0$, $M_y(0) = 100$ and $M_z(0) = 0$.

Where $M_x(t), M_y(t)$ and $M_z(t)$ represent the system magnetization in x, y and z component respectively, M_0 is the equilibrium magnetization, ω_0 is the resonant frequency given by theLarmor relationship $\omega_0 = \gamma B_0$, where B_0 is the static magnetic field in z -component, T_1 is spin-lattice relaxation time, T_2 is spin-spin relaxation time. The set of analytical solutions for integer order Bloch equation is given as,

$$\begin{aligned} M_x(t) &= e^{-t/T_2}(M_x(0)\cos\omega_0 t + M_y(0)\sin\omega_0 t), \\ M_y(t) &= e^{-t/T_2}(M_y(0)\cos\omega_0 t - M_x(0)\sin\omega_0 t), \\ M_z(t) &= M_z(0)e^{-t/T_1}M_0(1 - e^{-t}/T_1). \end{aligned} \tag{2}$$

The fraction in time derivative suggests a modulation—or weighting—of system memory (West et al., 2003; Magin et al., 2008), the assumption of fractional derivatives plays an important role affecting the spin dynamics described by the Bloch equations in Eq. (1). More recently, time fractional

E-mail addresses: harendra059@gmail.com, harendrasingh.rs.apm12@iitbhu.ac.in
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model of Bloch equation was resolved using Homotopy perturbation method (Kumar et al., 2014) and Petráš (2011) used iterative method to solve fractional model of Bloch equation. A generalization of the fractional Bloch equation by taking delay in the time was reported through numerical solution (Bhalekar et al., 2011). Recently Yu et al. (2014), gave an implicit numerical method to solve fractional Bloch equation in NMR. Some other existing methods to solve Bloch equation in NMR are reported in the literature (Hoult, 1979; Sivers, 1986; Yan et al., 1987; Xu and Chan, 1999; Balac and Chupin, 2008; Magin et al., 2009; Murase and Tanki, 2011; Sun et al., 2016). In this paper we are using operational matrix of fractional integration of Laguerre polynomial to solve fractional model of Bloch equation as Laguerre polynomials are more convenient for computational purpose. Recent investigations report the application of operational matrices to solve fractional differential equations (Wu, 2009; Yousefi et al., 2011; Kazem et al., 2013; Tohidi et al., 2013; Heydari et al., 2014; Zhou and Xu, 2014; Bhrawy and Zaky, 2015; Singh and Singh, 2016). Using operational matrix we convert the Bloch equation into a system of linear algebraic equation whose solution gives approximate solution for Bloch equation in NMR.

2. Preliminaries and operational matrix

In this paper, the fractional order differentiations and integrations are in well-known Caputo and Riemann-Liouville sense respectively (Miller and Ross, 1993; Diethelm et al., 2005).

Definition 2.1. The Riemann-Liouville fractional order integral operator is given by

$$I^{\alpha}f(x) = \frac{1}{\Gamma\alpha}\int_0^x (x-t)^{\alpha-1}f(t)dt \quad \alpha > 0, \quad x > 0,$$

$$I^0 f(x) = f(x).$$

Definition 2.2. The Caputo fractional derivative of order β are defined as

$$D^{\beta}f(x) = I^{m-\beta}D^m f(x) = \frac{1}{\Gamma(m-\beta)}\int_0^x (x-t)^{m-\beta-1}\frac{d^m}{dt^m}f(t)dt,$$

$$m-1 < \beta < m, \quad x > 0.$$

The Laguerre polynomial is defined by Ali et al. (2015) and Bhrawy et al. (2014)

$$L_k(t) = \sum_{i=0}^{k}\frac{(-1)^i}{i!}\binom{k}{i}t^i, \quad k = 0,1,2,\ldots,n. \tag{3}$$

The set of Laguerre polynomial $\{L_0(t), L_1(t), \ldots, L_n(t)\}$ forms an orthonormal basis with respect to weight function $w(t) = e^{-t}$ on the interval $[0, \infty)$ with the following property,

$$\int_0^{\infty} L_i(t)L_j(t)w(t)dt = \delta_{ij}, \quad \forall i,j \geqslant 0, \tag{4}$$

where δ_{ij} is the kronecker delta function.

A function $f(t)$, square integrable in $[0, \infty)$ may be expressed as sum of Laguerre polynomial as follows:

$$f(t) = \lim_{n\to\infty}\sum_{i=0}^{n} c_i L_i(t), \tag{5}$$

where $c_i = \int_0^{\infty} f(t)w(t)L_i(t)dt$.

If the series is truncated at $n = m$, then we have

$$f \cong \sum_{i=0}^{m} c_i L_i = F^T\psi(t), \tag{6}$$

where F and $\psi(t)$ are $(m+1)\times 1$ matrices given by,

$$F = [c_0, c_1, \ldots, c_m]^T \quad \text{and} \quad \psi(t) = [L_0(t), L_1(t), \ldots, L_m(t)]^T.$$

Theorem 2.1. *Let $\psi(t) = [L_0(t), L_1(t), \ldots, L_n(t)]^T$, be Laguerre vector and consider $\alpha > 0$, then*

$$I^{\alpha}L_i(t) = I^{(\alpha)}\psi(t), \tag{7}$$

where $I^{(\alpha)} = (\theta(i,j))$, is $(n+1)\times(n+1)$ operational matrix of fractional integral of order α and its (i,j) th entry is given by

$$\theta(i,j) = \sum_{k=0}^{i}\sum_{r=0}^{j}(-1)^{k+r}\frac{i!r!\Gamma(k+\alpha+r+1)}{(i-k)!(k)!(j-r)!(r!)^2\Gamma(\alpha+k+1)}$$

$$0 \leqslant i,j \leqslant n. \tag{8}$$

Proof. Pl see (Bhrawy and Taha, 2012). □

3. Outline of method

In this section, we describe the outline of the method for the construction of approximate solution of the Bloch equation.

Consider the following approximations:

$$\frac{d^{\alpha}M_x(t)}{dt^{\alpha}} = F_1^T\psi(t), \quad \frac{d^{\beta}M_y(t)}{dt^{\beta}} = F_2^T\psi(t), \quad \frac{d^{\gamma}M_z(t)}{dt^{\gamma}} = F_3^T\psi(t). \tag{9}$$

Taking integral of order α, β and γ in component M_x, M_y and M_z respectively in Eq. (9) we get,

$$M_x(t) = F_1^T I^{(\alpha)}\psi(t) + M_x(0), \tag{10}$$

$$M_y(t) = F_2^T I^{(\beta)}\psi(t) + M_y(0), \tag{11}$$

$$M_z(t) = F_3^T I^{(\gamma)}\psi(t) + M_z(0). \tag{12}$$

Let

$$M_x(0) = P^T\psi(t), \quad M_y(0) = Q^T\psi(t), \quad M_z(0) = R^T\psi(t). \tag{13}$$

From Eqs. (10)–(13) we get,

$$M_x(t) = (F_1^T I^{(\alpha)} + P^T)\psi(t), \tag{14}$$

$$M_y(t) = (F_2^T I^{(\beta)} + Q^T)\psi(t), \tag{15}$$

$$M_z(t) = (F_3^T I^{(\gamma)} + R^T)\psi(t). \tag{16}$$

Using Eqs. (9), (14), (15) and (16) in Eq. (1) we get following equations,