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ORIGINAL ARTICLE

A new numerical algorithm for fractional model of Bloch equation in nuclear magnetic resonance

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Abstract This paper presents a new algorithm based on operational matrix of fractional integrations for fractional Bloch equation in Nuclear Magnetic Resonance (NMR). For construction of operational matrix Legendre scaling functions are used as a basis. Using this operational matrix in the equations, we obtain approximate solutions for fractional Bloch equation. Convergence as well as error of the proposed method is given. Results are also compared with known solution. Absolute errors graph are plotted to show the accuracy of proposed new algorithm.

1. Introduction

The Bloch equations, namely

$$\begin{aligned} \frac{dM_x(t)}{dt} &= \omega_0 M_y(t) - \frac{M_x(t)}{T_2}, \\ \frac{dM_y(t)}{dt} &= -\omega_0 M_x(t) - \frac{M_y(t)}{T_2}, \\ \frac{dM_z(t)}{dt} &= \frac{M_0 - M_z(t)}{T_1}, \end{aligned} \tag{1}$$

with initial conditions

$$M_x(0) = 0, \quad M_y(0) = 100 \text{ and } M_z(0) = 0.$$

are used in physics, chemistry, nuclear magnetic resonance (NMR), electron spin resonance (ESR) and magnetic resonance imaging (MRI).

Where $M_x(t), M_y(t)$ and $M_z(t)$ represent the system magnetisation in x, y and z component respectively, M_0 is the equilibrium magnetisation, ω_0 is the resonant frequency given by the Larmor relationship $\omega_0 = \gamma B_0$, where B_0 is the static magnetic field in z-component, T_1 is spin-lattice relaxation time, and T_2 is spin-spin relaxation time. Well posed-ness of this equation is known when derivatives are of integer order. The set of analytic solution of the system of Eq. (1) with initial conditions in Eq. (2) 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 aim of this paper was to study Eq. (1) by replacing integer order time derivatives to fractional order derivatives because some physical quantity depends on the past so it is physically very important to study such systems. The fractional model of Bloch equation is given as follows:

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$$\frac{d^{\alpha}M_x(t)}{dt^{\alpha}} = \omega_0 M_y(t) - \frac{M_x(t)}{T_2},$$
$$\frac{d^{\beta}M_y(t)}{dt^{\beta}} = -\omega_0 M_x(t) - \frac{M_y(t)}{T_2}, \tag{3}$$
$$\frac{d^{\gamma}M_z(t)}{dt^{\gamma}} = \frac{M_0 - M_z(t)}{T_1},$$

where $0 < \alpha, \beta, \gamma \leqslant 1$.

The fraction in time derivative suggests a modulation—or weighting—of system memory, and the assumption of fractional derivatives plays an important role affecting the spin dynamics described by the Bloch equations in Eq. (3), see [1,2]. In addition, it is known that fractional derivative is strongly dependent on the initial conditions; therefore, we should choose the fractional derivative most appropriate for handling the initial conditions of our physical problem. In NMR the initial state of the system is specified by the components of the magnetisation, and hence these need to be clearly recognised. The physical meaning of the fractional Bloch equations goes back to the basic formulation of the fractional Schrodinger equation in quantum mechanics.

There are several methods to obtain approximate solution for Bloch equation in NMR [3–10]. Recently some authors solve mathematical model of Bloch equation with fractional time derivative [11–13].

In this paper we present a new algorithm based on operational matrix of integration for the approximate solution of time fractional model of Bloch equation. Operational matrix has several applications in fractional calculus. For the construction of operational matrices and their applications in fractional calculus see [14–25]. Using operational matrix in Bloch model we obtain unknown coefficients for approximated parameter in model. Using these coefficients we obtain approximate solution for fractional model of Bloch equation in NMR. Convergence as well as error of the proposed method is given.

The present paper is organised as follows. In Section 2, we describe basic preliminaries. In Section 3, we construct operational matrix using Legendre scaling functions as basis. In Section 4, we describe the algorithm for the construction of approximate solutions. In Section 5, we show the convergence of approximate solution to the exact solution. In Section 6, we give error bound for the proposed method. In Section 7, we give numerical experiments and discussion for different cases of time derivative to show the effectiveness of the proposed method.

2. Preliminaries

There are several definitions of fractional order derivatives and integrals. These are not necessarily equivalent. In this paper, the fractional order differentiations and integrations are in well-known Caputo and Riemann-Liouville sense respectively [26,27].

The Legendre scaling functions $\{\phi_i(t)\}$ in one dimension are defined by

$$\phi_i(t) = \begin{cases} \sqrt{(2i+1)}P_i(2t-1), & \text{for } 0 \leqslant t < 1. \\ 0, & \textit{otherwise}, \end{cases}$$

where $P_i(t)$ is Legendre polynomials of order i on the interval $[-1, 1]$, given explicitly by the following formula:

$$P_i(t) = \sum_{k=0}^{i}(-1)^{i+k}\frac{(i+k)!}{(i-k)!}\frac{t^k}{(k!)^2}. \tag{4}$$

Legendre scaling functions are constructed normalising the shifted Legendre polynomials. So the collection $\{\phi_i(t)\}$ forms an orthonormal basis for $L^2[0,1]$. The Legendre scaling function of degree i is given by

$$\phi_i(t) = (2i+1)^{\frac{1}{2}}\sum_{k=0}^{i}(-1)^{i+k}\frac{(i+k)!}{(i-k)!}\frac{t^k}{(k!)^2} \tag{5}$$

A function $f \in L^2[0,1]$, with bounded second derivative $|f''(t)| \leqslant M$, expanded as infinite sum of Legendre scaling function and the series converges uniformly to the function $f(t)$,

$$f(t) = \lim_{n\to\infty}\sum_{i=0}^{n}c_i\phi_i(t), \tag{6}$$

where $c_i = \langle f(t), \phi_i(t)\rangle$, and $\langle .,. \rangle$ is standard inner product on $L^2[0,1]$.

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

$$f \cong \sum_{i=0}^{m}c_i\phi_i = C^T\phi(t), \tag{7}$$

where C and $\phi(t)$ are $(m+1)\times 1$ matrices given by

$C = [c_0, c_1, \ldots, c_m]^T$ and $\phi(t) = [\phi_0(t), \phi_1(t), \ldots, \phi_m(t)]^T$.

3. Operational matrix

Theorem 3.1. *Let* $\phi(x) = [\phi_0(x), \phi_1(x), \ldots, \phi_n(x)]^T$, *be Legendre scaling vector and consider* $\alpha > 0$, *then*

$$I^{\alpha}\phi_i(x) = I^{(\alpha)}\phi(x), \tag{8}$$

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

$$\omega(i,j) = (2i+1)^{1/2}(2j+1)^{1/2}\sum_{k=0}^{i}\sum_{l=0}^{j}(-1)^{i+j+k+l} \times \frac{(i+k)!(j+l)!}{(i-k)!(j-l)!(k)!(l!)^2(\alpha+k+l+1)\Gamma(\alpha+k+1)}$$
$$0 \leqslant i,j \leqslant n.$$

Proof. Using the Legendre scaling function of degree i, we get

$$I^{\alpha}\phi_i(x) = (2i+1)^{1/2}\sum_{k=0}^{i}(-1)^{i+k}\frac{(i+k)!}{(i-k)!}\frac{1}{(k!)^2}I^{\alpha}x^k$$
$$= (2i+1)^{1/2}\sum_{k=0}^{i}(-1)^{i+k}\frac{(i+k)!}{(i-k)!(k)!\Gamma(\alpha+k+1)}x^{\alpha+k}$$

using Legendre scaling function approximation for $x^{\alpha+k}$, we have

$$x^{\alpha+k} = \sum_{j=0}^{n}c_j\phi_j(x), \text{ where}$$
$$c_j = (2j+1)^{1/2}\sum_{l=0}^{j}(-1)^{l+j}\frac{(j+l)!}{(j-l)!}\frac{1}{(l!)^2}\frac{1}{(\alpha+k+l+1)}. \tag{9}$$