A Fractional Model of Bloch Equation in Nuclear Magnetic Resonance and its Analytic Approximate Solution

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Abstract

The purpose of this paper is to employ an analytical approach to the time fractional Bloch Nuclear Magnetic Resonance (NMR) flow equations. A comparative study of the numerical solutions and the well-known analytical solutions are discussed. Absolute error has been calculated to show the accuracy of the applied method. The numerical solutions show that only a few iterations are needed to obtain accurate approximate solutions. The fractional derivatives are described in the Caputo sense. Numerical results are presented graphically.

Keywords: Bloch equation, Caputo derivative, analytical solution, homotopy perturbation method

Introduction

In physics and chemistry, specifically in nuclear magnetic resonance (NMR), magnetic resonance imaging (MRI), and electron spin resonance (ESR), the Bloch equations are a set of macroscopic equations that are used to calculate the nuclear magnetization \( \mathbf{M} = \{M_x, M_y, M_z\} \) in the laboratory frame \((x,y,z)\). \( T_1 \) and \( T_2 \) are known respectively as the spin lattice and sin-spin relaxation times which measure the interaction of the nuclei with their surroundings molecular environment and those between close nuclei. The MRI is a powerful tool for obtaining spatially localized information from the NMR of atoms within a sample. Sometimes they are called the equations of motion of nuclear magnetization. These equations were introduced by Felix Bloch [1]. In 1956, Torrey modified the Bloch equations by incorporating a diffusion term by Torrey [2]. The dynamics of an ensemble of spins without mutual couplings is usually well described by the Bloch equations [3,4], which can be viewed as mathematical descriptions of precession of the macroscopic magnetization vector around a (possibly time-dependent) magnetic field. Recently, Petras [5] and Bhalekar et al. [6] solved the fractional Bloch equation. The Bloch equations can be expressed in the following form:

\[
\begin{align*}
\frac{dM_x}{dt} &= \omega_0 M_y(t) \frac{M_y(t)}{T_2}, \\
\frac{dM_y}{dt} &= \omega_0 M_x(t) \frac{M_x(t)}{T_2}, \\
\frac{dM_z}{dt} &= \frac{M_0 - M_z(t)}{T_1}.
\end{align*}
\] (1)
Fractional Model of Bloch Equation in Nuclear Magnetic Resonance

Sunil KUMAR et al.

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with initial conditions $M_x(0) = 0$, $M_y(0) = 100$ and $M_z(0) = 0$, where $\omega_0 = \gamma B_0$ and $\omega_0 = 2\pi f_0$ (e.g. gyromagnetic ratio $\gamma/2\pi = f_0/B_0 = 42.57\text{MHz/T}$ for water protons) and $M_0$ is the equilibrium magnetization. The complete set of analytic solutions of the system of Eq. (1) is given as [6]:

$$
\begin{align*}
M_x(t) &= e^{-\gamma t/M} \left( M_x(0) \cos \omega_0 t + M_y(0) \sin \omega_0 t \right), \\
M_y(t) &= e^{-\gamma t/M} \left( M_y(0) \cos \omega_0 t - M_x(0) \sin \omega_0 t \right), \\
M_z(t) &= M_z(0) e^{-\gamma t/M} + M_0 (1 - e^{-\gamma t/M}).
\end{align*}
$$

Recently, many experts have paid great attention to construct the solutions of the Bloch equations by different methods from exact solutions to the Bloch equations by Bain et al. [7], analytical solution of the time dependent Bloch NMR by Awojoyogber [8], a solution to Bloch NMR flow equations by Awojoyogber and Boubaker [9], numerical solutions to the time dependent Bloch equations by Murase and Tanki [10], fast approximate solution of Bloch equation by Balac and Chupin [11], some Solutions of the Bloch equations by Leyte [12], solution of the Bloch equation by Hoult [13], approximate solutions of the Bloch equations by Yan et al. [14], exact solutions of the Bloch equations by Schotland and Leigh [15], approximate solution to the Bloch equations with symmetric rf pulses by Sivers [16], and a Near-Resonance Solution to the Bloch equations by Xu and Chan [17].

Mathematical modeling of many physical systems leads to linear and nonlinear fractional differential equations in various fields of physics and engineering. The use of fractional differentiation for the mathematical modeling of real world physical problems has been widespread in recent years, e.g. modeling of earthquakes, fluid dynamic traffic models with fractional derivatives, measurement of viscoelastic material properties, etc. The book by Oldham and Spanier [18] has played a key role in the development of the subject. Some fundamental results related to solving fractional differential equations may be found in books [19-21].

The main aim of this article presents a mathematical model of Bloch equations with fractional time derivative $\alpha, \beta, \gamma$ $(0 < \alpha, \beta, \gamma \leq 1)$ in the form of a rapidly convergent series with easily computable components. This method was first proposed and applied by He [22-25] and was successfully applied to solve many problems related to fractional calculus [26-31].

Basic Idea of Homotopy Perturbation Method (HPM)

To illustrate the basic ideas of the HPM for fractional differential equations, the following problem is considered:

$$
D^\alpha_t \xi(x,t) = \nu(x,t) - L \xi(x,t) - N \xi(x,t), m-1 < \alpha < m, m \in N, t \geq 0, x \in R^n,
$$

subject to the initial and boundary conditions:

$$
\xi^{(i)}(0,0) = c_i, B \left( \xi, \frac{\partial \xi}{\partial x_j}, \frac{\partial \xi}{\partial t} \right) = 0, i = 0,1,..., m-1, j = 1,2,...n,
$$

where $L$ is a linear operator, while $N$ is a nonlinear operator, $\nu$ is a known analytical function and $D^\alpha_t$ denotes the fractional derivative in the Caputo sense. $\xi$ is assumed to be a causal function of time, i.e.,

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274  Walailak J Sci & Tech 2014; 11(4)
vanishing for $t < 0$. Also $\xi^{(i)}(x,t)$ is the $ith$ derivative of $\xi$, $c_i, i = 0,1,\ldots, m-1$ are the specified initial conditions, and $B$ is a boundary operator.

In view of He’s homotopy perturbation technique, the following simple homotopy can be constructed.

$$(1 - p)D^\alpha_t \xi(x,t) + p(D^\alpha_t \xi(x,t) + L \xi(x,t) + N \xi(x,t) - \nu(x,t)) = 0, \quad p \in [0,1],$$  \hspace{1cm} (5)

or

$$D^\alpha_t \xi(x,t) + p(L \xi(x,t) + N \xi(x,t) - \nu(x,t)) = 0, \quad p \in [0,1].$$  \hspace{1cm} (6)

The homotopy parameter $p$ always changes from zero to unity. In case $p = 0$ Eq. (5) and Eq. (6) becomes;

$$D^\alpha_t \xi(x,t) = 0,$$  \hspace{1cm} (7)

where $p = 1$, Eq. (5) and Eq. (6) turns out to be the original fractional differential equation. In view of the homotopy perturbation method, the homotopy parameter $p$ is used to expand the solution in the following form.

$$\xi(x,t) = \xi_0(x,t) + p\xi_1(x,t) + p^2\xi_2(x,t) + p^3\xi_3(x,t) + \ldots$$  \hspace{1cm} (8)

For a nonlinear problem, set $N\xi(x,t) = S(x,t)$ Substituting Eq. (8) into Eq. (6) or Eq. (5) and equating the terms with identical power of $p$, a series of equations of the form is obtained.

$$p^0 : D^\alpha_t \xi_0(x,t) = 0,$$

$$p^1 : D^\alpha_t \xi_1(x,t) = -L \xi_0(x,t) - S_0(\xi_0(x,t)) + \nu(x,t),$$

$$p^2 : D^\alpha_t \xi_2(x,t) = -L \xi_1(x,t) - S_1(\xi_0(x,t), \xi_1(x,t)),$$

$$p^3 : D^\alpha_t \xi_3(x,t) = -L \xi_2(x,t) - S_2(\xi_0(x,t), \xi_1(x,t), \xi_2(x,t)), $$

where the functions $S_0, S_1, S_2,\ldots$ satisfy the following equation.

$$S(\xi_0(x,t) + p\xi_1(x,t) + p^2\xi_2(x,t) + p^3\xi_3(x,t) + \ldots) = S_0(\xi_0(x,t)) + pS_1(\xi_0(x,t), \xi_1(x,t)) + p^2S_2(\xi_0(x,t), \xi_1(x,t), \xi_2(x,t)) + \ldots$$  \hspace{1cm} (10)

Applying the inverse operator on both sides of the equation and considering the initial and boundary conditions, the terms of the series solution can be given by;
\[\xi_0(x,t) = \sum_{i=0}^{n} c_i t^i,\]
\[\xi_1(x,t) = -I_1^{\alpha} (L \xi_0(x,t)) + I_1^{\delta} \nu(x,t),\]
\[\xi_j(x,t) = -I_1^{\alpha} (L \xi_{j-1}(x,t)) + I_1^{\delta} S_j \xi_0(x,t), j = 2, 3, \ldots.\]

Hence, an accurate approximate in the following form is obtained.
\[\xi(x,t) = \sum_{i=0}^{n} \xi_i(x,t).\]

**Basic definitions of fractional calculus**

In this section, some basic definitions and properties of fractional calculus theory are given which are used in this paper:

**Definition 2.1.** A real function \( f(t), t > 0 \) is said to be in the space \( C_{\alpha}, \mu \in \mathbb{R} \) if there exists a real number \( p > \mu \), such that \( f(t) = t^p f_1(t) \) where \( f_1(t) \in C(0, \infty) \) and it is said to be in the space \( C_\mu \) if and only if \( f^{(n)} \in C_{\mu}, n \in \mathbb{N} \).

**Definition 2.2.** The Riemann–Liouville fractional integral \( (J^\alpha_t) \) of order \( \alpha \) of a function \( f \in C_{\mu}, \mu \geq -1 \) is defined as:
\[J^\alpha_t f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \tau)^{\alpha-1} f(\tau) d\tau, (\alpha > 0, t > 0),\]
\[J^\alpha_t f(t) = f(t).\]

where \( \Gamma(.) \) is the well-known Gamma function. Some of the properties of the operator \( (J^\alpha_t) \), can be found in [18-21]; only the following are considered. For \( f \in C_{\mu}, \mu \geq -1, \alpha, \beta \geq 0 \) and \( \gamma \geq -1;\)

1. \( J^\alpha_t J^\beta_t f(t) = J^{\alpha+\beta}_t f(t),\)
2. \( (J^\alpha_t J^\beta_t) f(t) = (J^\beta_t J^\alpha_t) f(t),\)
3. \( J^\alpha_t t^\gamma = \frac{\Gamma(\gamma + 1)}{\Gamma(\gamma + \alpha + 1)} t^{\gamma + \alpha}.\)

The Riemann–Liouville derivative has certain disadvantages when trying to model real world phenomena with fractional differential equations.

**Definition 2.3.** The fractional derivative \( D^\alpha_t \) of \( f(t) \) in the Caputo sense defined as:
\[D^\alpha_t f(t) = \frac{1}{\Gamma(m - \alpha)} \int_0^t f^{(m)}(\tau)(t - \tau)^{\alpha-1-m} d\tau,\]
\[where \ m - 1 < \alpha \leq m, m \in \mathbb{N}, t > 0, f \in C^{m}_m.\]
The following are 2 basic properties of the Caputo’s fractional derivative;

**Lemma 2.1.** If \( m - 1 < \alpha \leq m \), \( m \in \mathbb{N} \) and \( f \in C^m, \mu \geq -1 \), then:

\[
(D^\alpha)^n f(t) = f(t),
\]

\[
(J^n D^\alpha)^n f(t) = f(t) - \sum_{i=0}^{\frac{m-1}{\mu}} f^{i}(0^+) \frac{t^i}{i!},
\]

(15)

**Definition 2.6.** The Mittag-Leffler function \( E_{\alpha}(z) \) with \( \alpha > 0 \) is defined by the following series representation, valid in the whole complex plane [32];

\[
E_{\alpha}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}, \quad \alpha > 0, \quad z \in \mathbb{C}.
\]

(16)

**Solution of the given problem by HPM**

The fractional-order Bloch equations are considered where integer order derivatives are replaced by fractional order as;

\[
\begin{align*}
D^\alpha M_x(t) &= \omega_x M_y(t) - \frac{M_y(t)}{T_2}, & 0 < \alpha \leq 1, \\
D^\beta M_y(t) &= \omega_y M_x(t) - \frac{M_x(t)}{T_2}, & 0 < \beta \leq 1, \\
D^\gamma M_z(t) &= M_0 - \frac{M_z(t)}{T_1}, & 0 < \gamma \leq 1,
\end{align*}
\]

(17)

where \( \alpha, \beta \) and \( \gamma \) are the derivative orders. The total order of the system is \( (\alpha, \beta, \gamma) \). Here, all parameters \( \omega_x, T_2 \) and \( T_1 \) have units of \((s)^{-\theta}\) to maintain a consistent set of units for the magnetization.

The following homotopy is constructed.

\[
\begin{align*}
D^\alpha M_x(t) &= p \left( \omega_x M_y(t) - \frac{M_y(t)}{T_2} \right), & 0 < \alpha \leq 1, \\
D^\beta M_y(t) &= p \left( -\omega_y M_x(t) - \frac{M_x(t)}{T_2} \right), & 0 < \beta \leq 1, \\
D^\gamma M_z(t) &= p \left( M_0 - \frac{M_z(t)}{T_1} \right), & 0 < \gamma \leq 1,
\end{align*}
\]

(18)

with appropriate initial conditions \( M_x(0) = 0, M_y(0) = 100 \) and \( M_z(0) = 0 \).

Assuming the solution of the fractional-order Bloch equations (18) to be in the following form;

\[
\begin{align*}
M_x(t) &= \lim_{N \to \infty} \sum_{i=0}^{N} p^i M_{x,i}(t), & M_y(t) &= \lim_{N \to \infty} \sum_{i=0}^{N} p^i M_{y,i}(t), & M_z(t) &= \lim_{N \to \infty} \sum_{i=0}^{N} p^i M_{z,i}(t).
\end{align*}
\]

(19)
Substituting Eq. (19) into Eq. (18) and collecting terms of the same power of \( P \), the following set of differential equations is obtained.

\[
p^0 : \begin{cases} 
D^\alpha_t M_{x,0}(t) = 0, \\
D^\beta_t M_{y,0}(t) = 0, \\
D^\gamma_t M_{z,0}(t) = 0,
\end{cases}
\]

\[
p^1 : \begin{cases} 
D^\alpha_t M_{x,1}(t) = \alpha_0 M_{x,0}(t) - \frac{M_{x,0}(t)}{T_2}, \\
D^\beta_t M_{y,1}(t) = -\alpha_0 M_{y,0}(t) - \frac{M_{y,0}(t)}{T_2}, \\
D^\gamma_t M_{z,1}(t) = \frac{M_0 - M_{x,0}(t)}{T_1},
\end{cases}
\]

Consequently, the above system of nonlinear equations can be easily solved by applying the operator \( J^\gamma_p \) to (20) - (21), giving the various components \( M_{x,0}(t), M_{y,0}(t) \) and \( M_{z,0}(t) \), thus enabling the series solution to be entirely determined. The first few components of the homotopy perturbation solution for Eq. (19) are derived as follows.

\[
M_{x,0}(t) = M_x(0) = 0, \quad M_{y,0}(t) = M_y(0) = 100, \quad M_{z,0}(t) = M_z(0) = 0,
\]

\[
M_{x,1}(t) = \frac{100 \alpha_0 t^\alpha}{\Gamma(\alpha + 1)}, \quad M_{y,1}(t) = -\frac{100 t^\beta}{T_2 \Gamma(\beta + 1)}, \quad M_{z,1}(t) = \frac{M_0}{T_1 t^\gamma \Gamma(\gamma + 1)},
\]

\[
M_{x,2}(t) = -\frac{100 \alpha_0}{T_2} \left( \frac{t^{2\alpha}}{\Gamma(2\alpha + 1)} + \frac{t^{2\alpha + \beta}}{\Gamma(\alpha + \beta + 1)} \right) M_{x,1}(t) + 100 \left( \frac{t^{\gamma \beta}}{T_1^2 \Gamma(2\beta + 1)} - \frac{\alpha_0 t^{\gamma \beta}}{\Gamma(\alpha + \beta + 1)} \right) M_{z,2}(t) = -\frac{M_0}{T_1} \frac{t^{2\gamma \beta}}{\Gamma(2\gamma + 1)},
\]

\[
M_{x,3}(t) = \frac{100 \alpha_0}{T_2} \left( \frac{t^{3\alpha}}{\Gamma(3\alpha + 1)} + \frac{t^{3\alpha + 2\beta}}{\Gamma(\alpha + 2\beta + 1)} + \frac{t^{2\alpha + 3\beta}}{\Gamma(2\alpha + \beta + 1)} \right) M_{x,2}(t) - 100 \alpha_0 \frac{t^{3\gamma \beta}}{T_1^2 \Gamma(2\gamma + 1)},
\]

\[
M_{y,3}(t) = \frac{100 \alpha_0 t^2}{T_2} \left( \frac{2t^{\alpha + 2\beta}}{\Gamma(\alpha + 2\beta + 1)} + \frac{t^{2\alpha + 2\beta}}{\Gamma(2\alpha + \beta + 1)} \right) M_{y,2}(t) - 100 \frac{t^{3\gamma \beta}}{T_1^2 \Gamma(3\gamma + 1)}, \quad M_{z,3}(t) = \frac{M_0}{T_1} \frac{t^{3\gamma \beta}}{\Gamma(3\gamma + 1)},
\]

and so on. In this manner, the rest of components of the homotopy perturbation solution can be obtained. The approximate solutions \( \tilde{M}_x(t), \tilde{M}_y(t) \) and \( \tilde{M}_z \), by truncating the respective solutions series at level \( N = 14 \), are given by:

\[
\tilde{M}_x(t) = \sum_{n=0}^{14} M_{x,n}(t), \quad \tilde{M}_y(t) = \sum_{n=0}^{14} M_{y,n}(t), \quad \tilde{M}_z(t) = \sum_{n=0}^{14} M_{z,n}(t),
\]

hence,
The series solution converges very rapidly. The rapid convergence means only a few terms are required to get the approximate solutions.

\[
\begin{align*}
\tilde{M}_x(t) &= 100 \alpha (t^\nu \Gamma(\alpha + 1) - t^{2\alpha} \Gamma(\alpha + 1)) + 100 \alpha^2 (t^{3\alpha} \Gamma(3\alpha + 1) + t^{2\alpha} \Gamma(2\alpha + 1)) - \frac{\alpha \Gamma(2\alpha + 1)}{T_1 (\alpha + 2\beta + 1)} + \ldots \\
\tilde{M}_y(t) &= 100 \alpha (t^{\nu} \Gamma(\alpha + 1) - t^{2\alpha} \Gamma(\alpha + 1)) + 100 \alpha^2 (t^{3\alpha} \Gamma(3\alpha + 1) + t^{2\alpha} \Gamma(2\alpha + 1)) + \ldots \\
\tilde{M}_z(t) &= \frac{M_z}{T_1} \left[1 - E_x(-t^\nu)\right]
\end{align*}
\]

Figure 1: The Exact $M_x$ (solid line), $M_y$ (solid line) and the approximate solution $\tilde{M}_x$ (Red dotted line) and $\tilde{M}_y$ (Blue dotted) at $\omega = 1$ and $T_2 = 20$ (ms).
The observations are depicted through **Figures 1 - 8.** **Figure 1 - 2** shows the comparison between the exact solutions and approximate solutions (by HPM) for the standard Bloch equation, i.e. for $\alpha = \beta = \gamma = 1$. It can be seen from **Figures 1 - 2** that the approximate solutions $\tilde{M}_x(t), \tilde{M}_y(t), \tilde{M}_z(t)$ obtained by the present method are nearly identical to the exact solutions $M_x(t), M_y(t), M_z(t)$ with high accuracy. All graphical result have parameters $\omega = 1, T_1 = 1(s)^g$ and $T_2 = 20 (ms)^g$.

**Numerical result and discussion**

In this section, the error analysis between the exact solutions and approximate solutions are depicted through **Figures 3 – 5**, and **Figures 6 - 8** shows the approximate solutions for different fractional Brownian motions and standard motions. During numerical computation, only 14 terms of the series solution are considered. The accuracy of the result can be improved by introducing more terms of the approximate solutions.

The simplicity and accuracy of the proposed method is illustrated by computing the absolute errors $e_{x}(t) = |M_x(t) - \tilde{M}_x(t)|$, $e_{y}(t) = |M_y(t) - \tilde{M}_y(t)|$, and $e_{z}(t) = |M_z(t) - \tilde{M}_z(t)|$, where $M_x(t), M_y(t), M_z(t)$ are the exact solutions and $\tilde{M}_x(t), \tilde{M}_y(t), \tilde{M}_z(t)$ are the approximate solutions of (3) obtained by truncating the respective solutions series (21) at level $N = 14$. **Figures 3 - 5** represent absolute errors between the exact solutions $M_x(t), M_y(t), M_z(t)$ and the approximate solutions $\tilde{M}_x(t), \tilde{M}_y(t), \tilde{M}_z(t)$ respectively, which show high accuracy of the approximate solutions. **Figures 3 - 5** show that the series solution (by HPM) converges to the exact solution very rapidly.

**Figure 3** Absolute error $e_x = |M_x(t) - \tilde{M}_x(t)|$ at $\omega = 1$ and $T_2 = 20 (ms)^g$. 

280 Walailak J Sci & Tech 2014; 11(4)
Figure 4 Absolute error \( e_y = |M_y(t) - \tilde{M}_y(t)| \) at \( \omega = 1 \) and \( T_z = 20 \ (ms)^p \).

Figure 5 Absolute error \( e_z = |M_z(t) - \tilde{M}_z(t)| \) at \( \omega = 1 \) and \( T_i = 1 \ (ms)^p \).
Figure 6 Approximately, solution $\tilde{y}_{1}(t)$ for different values of $\alpha$ at $\omega = 1$ and $T_z = 20 (ms)^{\ell}$.

Figure 7 Approximately, solution $\tilde{y}_{1}(t)$ for different values of $\beta$ at $\omega = 1$ and $T_z = 20 (ms)^{\ell}$.
Figures 6 - 8 show the evolution of results for the approximate solutions $\tilde{M}_x(t)$, $\tilde{M}_y(t)$ and $\tilde{M}_z(t)$ of Eq. (3) obtained for different values $\alpha, \beta$ and $\gamma$ respectively, by using the HPM. It is seen from Figures 6 and 8 that the approximate solutions $\tilde{M}_x(t)$ and $\tilde{M}_z(t)$ increase with the increases in $t$ for different value of $\alpha = \beta = 0.7, 0.8, 0.9$, and also for the standard Bloch equation i.e. for $\alpha = \beta = 1$. It is also seen from Figure 7 that the approximate solution $\tilde{M}_y(t)$ decreases with the increases in $t$ for different values of $\gamma = 0.7, 0.8, 0.9, 1$. It is to be noted that only 14 terms of the homotopy perturbation series were used in evaluating the approximate solutions in all figures.

Conclusions

The present case studied the effect of different orders of fractional time for the Bloch NMR flow equations, which are a set of macroscopic equations that are used for modeling of nuclear magnetization as a function of time by homotopy perturbation method. The following observations have been made.

1) $\tilde{M}_x(t)$ and $\tilde{M}_z(t)$ increase with the increases in $t$ for different values of $\alpha = \beta = 0.7, 0.8, 0.9$.

2) For the standard Bloch equation i.e. for $\alpha = \beta = 1$, $\tilde{M}_x(t)$ and $\tilde{M}_z(t)$ increase with the increases in $t$.

3) Absolute errors between the exact solutions $M_x(t), M_y(t), M_z(t)$ and approximate solutions $\tilde{M}_x(t), \tilde{M}_y(t), \tilde{M}_z(t)$ respectively show high accuracy of the approximate solutions.

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