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Procuring Analytical Solution of Nonlinear Nuclear Magnetic Resonance Model of Fraction Order

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Abstract: Bloch system is mainly employed with attainment of the basic explanation of relaxation T_1 and T_2 and nuclear magnetic resonance (NMR). This equation is said to be the heart of both magnetic resonance imaging (MRI) and NMR spectroscopy. The major goal of this paper is to obtain an analytical solution of Fractional Nuclear Magnetic Resonance (NMR) flow equations. In this study, the use of Laplace transform and the Pade approximation has been ascertained to handle the truncated series that were obtained through the Perturbation Iteration Method for further advancement of the approximation. The fractional derivatives in this work are understood to be in the Caputo sense. The results achieved through this paper will prove that the algorithm is fit to be used for more general kinds of fractional differential equations.

Keywords: Magnetic Resonance Imaging (MRI), Laplace transform, Pade Approximation, Fractional Perturbation Iteration Algorithm, Caputo derivative.

1 Introduction

NMR establishes the physical base for a huge selection of technique that is primarily use to study the dynamics of cells and structure, tissues and entire animals [1]. For example, Magnetic Resonance Spectroscopy (MRS) is used often by chemists for studying bio-molecules and the analysis of their structure. Also magnetic resonance imaging is an imperative requirement of radiology departments in hospitals. MRI scans can form an image of the structures of soft tissue of human spine and brain down to a resolution in sub-millimeter, while MRS can identify individual bio-molecular configurations by a resolution of sub-nanometer. This vast choice of scale offers chemists a tool that makes molecular synthesis more accurate and make physicians to diagnose diseases and their stages by secure means, such as cancer. Spectroscopic and imaging information is important for discovering the molecular basis of abnormal cell growth. In addition to its use of scrutinizing a unique tumors reaction to radiation therapy or drug treatments. The usual definition of nuclear magnetic resonance is “the phenomenon that makes up the inner workings of magnetic resonance imaging is presented in form of vector below by the help of Bloch system [1,2].”

$$\frac{d\mathbf{M}}{dt} = \gamma(\mathbf{M}\times\mathbf{B}) - \frac{M_z - M_o}{T_1}\hat{i}_z - \frac{M_x\hat{i}_x + M_y\hat{i}_y}{T_2} \qquad (1)$$

where time changeable magnetization is $\mathbf{M}(M_x, M_y, M_z)$, stability magnetization is M_o, the useful radio frequency RF is $\mathbf{B}(B_x, B_y, B_z)$, γ is the gyromagnetic ratio, slope and stationary magnetic fields (Tesla), T_1 and T_2 shows the spin lattice relaxation time and spin-spin relaxation time respectively. In case of homogeneous isotropic substances with one spin component, the Bloch system is employed to stipulate the dynamic equilibrium that lies among outwardly apply interior trial relaxation times and magnetic fields. This dynamic equilibrium is the base of many scientific processes, such as image reconstruction, signal acquisition and pulse sequence design in the case of MRI, contrast of tissue [3,4,5] etc.

Recently, marvelous development have been made in the theory and application of the Fractional Differential Equations. FDE’s are being used more and more to deal ideal problems in research area as varied in fluid mechanics, mechanical systems, population dynamics, continuous-time random walks fiber optics, chaos, sub-diffusive systems and anomalous diffusive, wave

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propagation phenomenon and unification of diffusion etc. Generality of the fractional order Bloch system has been embarked by numerous groups to provide a reason for the irregular diffusion and atypical relaxation experiential in Nuclear Magnetic Resonance study of complex materials - usually porous composites, gels, biological tissues and emulsions [6,7,8,9,10,11,12,13].

A commonly found aspect in some complex materials is a “meso-scopic structure” existing in the range of macroscopic regimes and the molecular. MRI and NMR spectroscopy both are dominant tools for experimentation on inquiring the disordered and structured organization and dynamics (like transition of phase, diffusion and permeability of the meso-scopic structures). Extraordinary resolution of magnetic resonance microscopy yields macromolecular coalescence, images of high contrast particle aggregation and separation of phase. Studies of nuclear magnetic resonance diffusion provide a direct determination of material’s tortsituoy plus porosity. Nevertheless, the appliance of these types of tools and the investigation of the acquired information are extremely reliant upon the theoretical assumption that underlies the Bloch system such as the Brownian particle motion, Gaussian spins dynamics and exponential relaxation of first order. The dependence goes so far that these assumptions are valid for an exacting material for a transition involving phases of dissimilar material, conventional nuclear magnetic resonance analysis is legitimate and suitable.

However, collecting experimental proof on complex materials suggests an atypical dynamic activity. This anomalous performance apparently reflects the distributions of multi-scale phenomenon and relaxation times that sometimes recommend a structure of fractal-like, nonlocal relations, memory of fading and age. Ergo, it is estimated that nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) of complex materials measurements through meso-scopic configurations or states will display like ? dynamic behavior and fractional order. The most unanswered question regarding the “generalized” Bloch system is to relate the operators of the fractional order at the molecular to the spin dynamics and macroscopic scale and how to modify it? From the precession of spin (nanosecond) to the reorientation of molecular (microsecond) then to the dephasing of spin?spin (millisecond), up and around to the relaxation of spin lattice (second) and diffusion. NMR is a broadly used procedure of experimentation for the reason that it’s effectiveness in probing time scales. Nuclear magnetic resonance analysis assigns to each area of concern (pixel) particular experimental data values for example correlation coefficient, chemical shift, coefficient of diffusion, relaxation times (spin?spin and spin?lattice), by using images or localized spectroscopy. This procedure works excellently for imaging macroscopic region that is voxels at the order or for spectroscopy on untainted samples in unvarying magnetic fields that is $1D$ & $2D$ nuclear magnetic resonance spectra. Nonetheless, approaching the resolution of imaging into the meso-scopic regime or microscopic or pulling complex spectrum from tissues or macroscopic mixtures expose elementary restrictions in either spectral resolution or signal-to-noise (SNR).

The application of extremely high field nuclear magnetic resonance systems of these problems, regrettably can’t be overcome all the time by taking further signal averages. The aim of fractional order nuclear magnetic resonance modeling is to widen the experimental casement of nuclear magnetic resonance techniques for time,space and bandwidth. It does not only simply raise the resolution in system, but appending the governing equations for the observed phenomena a fractional order interpretation. The command of fractional calculus is that, it suitably assimilates into the operator?s order a fractal set-up of lacunae extend more a diffusion coefficients or a large distribution of relaxation times. Such preciseness come at the rate of relinquish the particular sub compartment value for entity diffusion constants or relaxation times, but provide the advantage of capture hierarchical, multi-scale phenomena in time and space.

This paper introduces a new technique for the analytical solution of the Bloch System of fractional-order. It has been arranged as follows: Section 2 outlines the Hybrid Laplace Fractional Perturbation Pade Transform Method ($HLFPPTM$). Section 3 demonstrates the application of this method on the Fractional order Bloch equation obtains of the exact solution. In the last section, a conclusive summary has been presented.

2 Research Methodology

In this research, Hybrid Laplace Fractional Perturbation Pade Transform Method ($HLFPPTM$) is implemented for solving Bloch equation of Fractional order.

2.1 Pade Approximate

For any power series $f(t)$, the Pade approximate of order $[L,M]$ is represented by $R_{L,M}(t)$ and is defined as

$$R_{L,M}(t) = \frac{\sum_{k=0}^{L} p_k t^k}{1+\sum_{k=0}^{M} q_k t^k} \quad such\ that\ f(t) - R_{L,M}(t) = O(t^{L+M+1}) \tag{2}$$

By considering only first $(L+M+1)$ terms of the power series of $R_{L,M}(t)$ and $f(t)$. Next correspondence of only those terms of $R_{L,M}(t)$ and $f(t)$ of $(L+M+1)$ is considered. The coefficients p_k and q_k is being multiplied by the denominator of $R_{L,M}(t)$ and then obtained result is compared bt the coefficients of t^k, for $k=0,1,2,...,L+M$.

This will yield M simultaneous equations for q_k. $\sum_{k=1}^{min(r-M)} q_k C_{r-k} = -C_r;\ r = (L+1,...,L+M)$ and $L+1$ expression for the p_k, $k = 0,1,2,...,L$ $p_k = C_k + \sum_{s=1}^{min(k-M) q_s C_{k-s}} = -C_r;\ k = 0,1,2,...,L.$

2.2 Fractional Perturbation Iteration Algorithm

For any system of fractional differential equation

$$G_k(D_t^{\alpha} u_k, u_k, t) = 0,\ m-1 < \alpha \le m,\ t > 0,\ u \in \mathbb{R} \quad (3)$$

Comprising of initial conditions $\frac{d^{\alpha}}{dt^{\alpha}} u(t,0) = u_k(t)$, $k = 0,1,2,3,\ldots,m-1$. Eq.(3) can also be given in the form

$$D_t^{\alpha} u_k + A[u(t)] = 0$$

where A refers to a general differential operator which consists of linear operator $L(u)$ and nonlinear operator $N(u)$. D_t^{α} is the caputo fractional derivative operator of order α. Introducing small perturbation parameter in above equation yield

$$D_t^{\alpha} u_k + L[u(t)] + \epsilon N[u(t)] = 0 \quad (4)$$

By considering the nonlinear term in Eq.(4) as perturbation, we assume that solution can be presented as a power series of small perturbation

$$u = u_{\circ} + \epsilon u_1 + \epsilon^2 u_2 + \epsilon^3 u_3 + \ldots \quad (5)$$

By substituting Eq.(5) into Eq.(4) and equating identical power of ϵ, we attain a number of differential equation, that can be integrated recursively, to discover the value of $u_{\circ}, u_1, u_2, u_3, \ldots$

2.3 Hybrid Laplace Fractional Perturbation Pade Transforms

Now, the use of Laplace Transform and Pade approximation is giving to be discussed. There is a need to deal with the truncated series obtained with the help of Fractional Perturbation Iteration Algorithm for improving the approximation. Foremost, the Laplace Transform is applied to a series solution obtained by the Fractional Perturbation Iteration technique, then $\frac{1}{\epsilon}$ replaces s in the equation under question. After that, Pade approximation [2/2] is used with $\frac{1}{s}$ instead of ϵ. Finally, through the inverse Laplace Transformation, we attain the modified approximate solution.

3 Analytical Solution of the Bloch System by Hybrid Laplace Fractional Perturbation Pade Transform Method

Modified nonlinear fractional Bloch System that governs the magnetization evolution:

$$\begin{aligned} D_t^{\alpha_1} M_x(t) &= \omega_{\circ} M_y(t) - \frac{M_x(t)}{T_2} \\ D_t^{\alpha_2} M_y(t) &= -\omega_{\circ} M_x(t) - \frac{M_y(t)}{T_2} \\ D_t^{\alpha_3} M_z(t) &= \frac{M_{\circ} - M_z(t)}{T_1} \end{aligned} \quad (6)$$

with initial conditions $M_x(0) = A$, $M_y(0) = B$, $M_z(0) = C$. The complete set of exact solutions for the Bloch System is presented as:

$$\begin{aligned} M_x(t) &= exp(\frac{-t}{T_2})\Big(A\cos(\omega_{\circ} t) + B\sin(\omega_{\circ} t)\Big) \\ M_y(t) &= exp(\frac{-t}{T_2})\Big(A\cos(\omega_{\circ} t) - B\sin(\omega_{\circ} t)\Big) \\ M_z(t) &= exp(\frac{-t}{T_1})(C - M_{\circ}) + M_{\circ} \end{aligned} \quad (7)$$

Now, by applying Fractional Perturbation Iteration Algorithm first. For FPIA(1,1), only one correction term for each variable is considered that is

$$\begin{aligned} M_{x,n+1}(t) &= M_{x,n}(t) + \epsilon M_{x,n}^c(t) \\ M_{y,n+1}(t) &= M_{y,n}(t) + \epsilon M_{y,n}^c(t) \\ M_{z,n+1}(t) &= M_{z,n}(t) + \epsilon M_{z,n}^c(t) \end{aligned} \quad (8)$$

$$\begin{aligned} D_t^{\alpha_1} M_x(t) - \epsilon\Big(\omega_{\circ} M_y(t) - \frac{M_x(t)}{T_2}\Big) &= 0 \\ D_t^{\alpha_2} M_y(t) - \epsilon\Big(\omega_{\circ} M_x(t) - \frac{M_y(t)}{T_2}\Big) &= 0 \\ D_t^{\alpha_3} M_z(t) - \epsilon\Big(\frac{M_{\circ} - M_z(t)}{T_1}\Big) &= 0 \end{aligned} \quad (9)$$

With appropriate initial conditions $\Big(M_x(0), M_y(0), M_z(0)\Big) = (A, B, C)$. Assuming the solution of the Bloch system Eq.(6) in the following form

$$\begin{aligned} M_x(t) &= \lim_{i\to\infty} M_{x,i}(t) \\ M_y(t) &= \lim_{i\to\infty} M_{y,i}(t) \\ M_z(t) &= \lim_{i\to\infty} M_{z,i}(t) \end{aligned} \quad (10)$$

$$\epsilon^{\circ} = \begin{cases} D_t^{\alpha_1} M_{x,\circ}(t) = 0 \\ D_t^{\alpha_2} M_{y,\circ}(t) = 0 \\ D_t^{\alpha_3} M_{z,\circ}(t) = 0 \end{cases} \quad (11)$$

with initial conditions $M_{x,0}(0)=A$, $M_{y,0}(0)=B$, $M_{z,0}(0)=C$. Then, the obtained correction term for each iteration are

$$\epsilon^1=\begin{cases} D_t^{\alpha_1}M_{x,n}^c(t)=-D_t^{\alpha_1}M_{x,n}(t)+\omega_\circ M_y(t)-\dfrac{M_x(t)}{T_2}\\ D_t^{\alpha_2}M_{y,n}^c(t)=-D_t^{\alpha_2}M_{y,n}(t)-\omega_\circ M_x(t)-\dfrac{M_y(t)}{T_2}\\ D_t^{\alpha_3}M_{z,n}^c(t)=-D_t^{\alpha_3}M_{z,n}(t)+\dfrac{M_\circ-M_z(t)}{T_1}\end{cases} \tag{12}$$

with initial condition $\left(M_{x,0}^c(0),M_{y,0}^c(0),M_{z,0}^c(0)\right)=(0,0,0)$
Let the first solution be

$$\begin{aligned} M_{x,0}(t)&=A\\ M_{y,0}(t)&=B\\ M_{z,0}(t)&=C\end{aligned} \tag{13}$$

$$\begin{aligned} M_{x,1}(t)&=A+\frac{Bt^{\alpha_1}\omega_\circ}{\Gamma 1+\alpha_1}-\frac{At^{\alpha_1}}{T_2\Gamma 1+\alpha_1}\\ M_{y,1}(t)&=B-\frac{At^{\alpha_2}\omega_\circ}{\Gamma 1+\alpha_2}-\frac{Bt^{\alpha_2}}{T_2\Gamma 1+\alpha_2}\\ M_{z,0}(t)&=C-\frac{Ct^{\alpha_3}}{T_1\Gamma 1+\alpha_3}+\frac{M_\circ t^{\alpha_3}}{T_1\Gamma 1+\alpha_3}\end{aligned} \tag{14}$$

$$\begin{aligned} M_{x,2}(t)&=A+\frac{Bt^{\alpha_1}\omega_\circ}{\Gamma 1+\alpha_1}-\frac{At^{2\alpha_1}\omega_\circ^2}{\Gamma 1+2\alpha_1}+\frac{At^{2\alpha_1}}{T_2^2\Gamma 1+2\alpha_1}-\\ &\quad\frac{At^{\alpha_1}}{T_2\Gamma 1+\alpha_1}-\frac{2Bt^{2\alpha_1}\omega_\circ}{T_2\Gamma 1+2\alpha_1}\\ M_{y,2}(t)&=B-\frac{At^{\alpha_2}\omega_\circ}{\Gamma 1+\alpha_2}-\frac{Bt^{2\alpha_2}\omega_\circ^2}{\Gamma 1+2\alpha_2}+\frac{Bt^{2\alpha_2}}{T_2^2\Gamma 1+2\alpha_2}-\\ &\quad\frac{Bt^{\alpha}}{T_2\Gamma 1+\alpha_2}+\frac{2At^{2\alpha_2}\omega_\circ}{T_2\Gamma 1+2\alpha_2}\\ M_{z,2}(t)&=C+\frac{Ct^{2\alpha_3}}{T_1^2\Gamma 1+2\alpha_3}-\frac{t^{2\alpha_3}M_\circ}{T_1^2\Gamma 1+2\alpha_3}-\\ &\quad\frac{Ct^{\alpha_3}}{T_1\Gamma 1+\alpha_3}+\frac{M_\circ t^{\alpha_3}}{T_1\Gamma 1+\alpha_3}\end{aligned} \tag{15}$$

$$\begin{aligned} M_{x,3}(t)&=A+\frac{Bt^{\alpha_1}\omega_\circ}{\Gamma 1+\alpha_1}-\frac{At^{2\alpha_1}\omega_\circ^2}{\Gamma 1+2\alpha_1}-\frac{Bt^{3\alpha_1}\omega_\circ^3}{\Gamma 1+3\alpha_1}-\\ &\quad\frac{At^{3\alpha_1}}{T_2^3\Gamma 1+3\alpha_1}+\frac{At^{2\alpha_1}}{T_2^2\Gamma 1+2\alpha_1}+\frac{3Bt^{3\alpha_1}\omega_\circ}{T_2^2\Gamma 1+3\alpha_1}-\\ &\quad\frac{At^{\alpha_1}}{T_2\Gamma 1+\alpha_1}-\frac{2Bt^{2\alpha_1}\omega_\circ}{T_2\Gamma 1+2\alpha_1}+\frac{3At^{3\alpha_1}\omega_\circ^2}{T_2\Gamma 1+3\alpha_1}\\ M_{y,3}(t)&=B-\frac{At^{\alpha_2}\omega_\circ}{\Gamma 1+\alpha_2}-\frac{Bt^{2\alpha_2}\omega_\circ^2}{\Gamma 1+2\alpha_2}+\frac{At^{3\alpha_2}\omega_\circ^3}{\Gamma 1+3\alpha_2}-\\ &\quad\frac{Bt^{3\alpha_2}}{T_2^3\Gamma 1+3\alpha_2}+\frac{Bt^{2\alpha_2}}{T_2^2\Gamma 1+2\alpha_2}-\frac{3At^{3\alpha_2}\omega_\circ}{T_2^2\Gamma 1+3\alpha_2}-\\ &\quad\frac{Bt^{\alpha_2}}{T_2\Gamma 1+\alpha_2}+\frac{2At^{2\alpha_2}\omega_\circ}{T_2\Gamma 1+2\alpha_2}+\frac{3Bt^{3\alpha_2}\omega_\circ^2}{T_2\Gamma 1+3\alpha_2}\end{aligned} \tag{16}$$

$$\begin{aligned} M_{z,3}(t)&=C-\frac{Ct^{3\alpha_3}}{T_1^3\Gamma 1+3\alpha_3}+\frac{M_\circ t^{3\alpha_3}}{T_1^3\Gamma 1+3\alpha_3}+\frac{Ct^{2\alpha_3}}{T_1^2\Gamma 1+2\alpha_3}+\\ &\quad\frac{M_\circ t^{2\alpha_3}}{T_1^2\Gamma 1+2\alpha_3}-\frac{Ct^{\alpha_3}}{T_1\Gamma 1+\alpha_3}+\frac{M_\circ t^{\alpha_3}}{T_1\Gamma 1+\alpha}\end{aligned}$$

Three considered iterations are:

$$\begin{aligned} M_x(t)&=M_{x,3}(t)\\ M_y(t)&=M_{y,3}(t)\\ M_z(t)&=M_{z,3}(t)\end{aligned} \tag{17}$$

Consider $M_x(t)$. Taking Laplace Transform, the following equation is obtained:

$$\begin{aligned} L[M_x(t)]&=\frac{A}{s}+Bs^{-1-\alpha_1}\omega_\circ-As^{-1-2\alpha_1}\omega_\circ^2-Bs^{-1-3\alpha_1}\omega_\circ^3-\\ &\quad\frac{As^{-1-3\alpha_1}}{T_2^3}+\frac{As^{-1-2\alpha_1}}{T_2^2}+\frac{3Bs^{-1-3\alpha_1}\omega_\circ}{T_2^2}-\\ &\quad\frac{As^{-1-\alpha_1}}{T_2}-\frac{2Bs^{-1-2\alpha_1}\omega_\circ}{T_2}+\frac{3As^{-1-2\alpha_1}\omega_\circ^2}{T_2}\end{aligned} \tag{18}$$

Using transformation $s=\dfrac{1}{\epsilon}$ and $\alpha_1=1$, we get

$$\begin{aligned} L[M_x(t)]&=A\epsilon+B\epsilon^2\omega_\circ-A\epsilon^3\omega_\circ^2-B\epsilon^4\omega_\circ^3-\frac{A\epsilon^4}{T_2^3}+\\ &\quad\frac{A\epsilon^3}{T_2^3}+\frac{3B\epsilon^4\omega_\circ}{T_2^2}-\frac{A\epsilon^2}{T_2}-\frac{2B\epsilon^3\omega_\circ}{T_2}+\frac{3A\epsilon^4\omega_\circ^2}{T_2}\end{aligned} \tag{19}$$

Pade Approximant of [2/2] yields

$$L[M_x(t)]=\frac{A\epsilon+\dfrac{(A+BT_2\omega_\circ)\epsilon^2}{T_2}}{1+\dfrac{2\epsilon}{T_2}+\dfrac{(1+T_2^2\omega_\circ^2)\epsilon^2}{T_2^2}} \tag{20}$$

Using reverse transformation $\epsilon=1/s$ gives

$$L[M_x(t)]=\frac{\dfrac{A}{s}+\dfrac{(A+BT_2\omega_\circ)}{T_2s^2}}{1+\dfrac{2}{T_2s}+\dfrac{(1+T_2^2\omega_\circ^2)}{T_2^2s^2}} \tag{21}$$

Now applying Laplace Inverse

$$M_x(t)=exp(\frac{-t}{T_2})\Big(A\cos(\omega_\circ t)+B\sin(\omega_\circ t)\Big) \tag{22}$$

Similarly applying above procedure to $M_y(t)$ and $M_z(t)$, set the following results:

$$\begin{aligned} M_y(t)&=exp(\frac{-t}{T_2})\Big(A\cos(\omega_\circ t)-B\sin(\omega_\circ t)\Big)\\ M_z(t)&=exp(\frac{-t}{T_1})(C-M_\circ)+M_\circ\end{aligned} \tag{23}$$

4 Perspective

In this paper, the method called “Hybrid Laplace Fractional Perturbation Pade Transform Method ($HLFPPTM$)” has been applied adequately for the derivation of analytical solutions of the nonlinear Fractional Bloch System. The results yields in this paper recommend that this algorithm is sufficiently equipped to be applied on more complex and disordered systems. Moreover, general kinds of linear and nonlinear differential equations as well as fractional ones.

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