Computers and Mathematics with Applications 64 (2012) 3367–3376

Contents lists available at SciVerse ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

Transient chaos in fractional Bloch equations

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ARTICLE INFO

Keywords:
Fractional calculus
Bloch equation
Chaos

ABSTRACT

The Bloch equation provides the fundamental description of nuclear magnetic resonance (NMR) and relaxation (T_1 and T_2). This equation is the basis for both NMR spectroscopy and magnetic resonance imaging (MRI). The fractional-order Bloch equation is a generalization of the integer-order equation that interrelates the precession of the x, y and z components of magnetization with time- and space-dependent relaxation. In this paper we examine transient chaos in a non-linear version of the Bloch equation that includes both fractional derivatives and a model of radiation damping. Recent studies of spin turbulence in the integer-order Bloch equation suggest that perturbations of the magnetization may involve a fading power law form of system memory, which is concisely embedded in the order of the fractional derivative. Numerical analysis of this system shows different patterns in the stability behavior for α near 1.00. In general, when α is near 1.00, the system is chaotic, while for $0.98 \geq \alpha \geq 0.94$, the system shows transient chaos. As the value of α decreases further, the duration of the transient chaos diminishes and periodic sinusoidal oscillations emerge. These results are consistent with studies of the stability of both the integer and the fractional-order Bloch equation. They provide a more complete model of the dynamic behavior of the NMR system when non-linear feedback of magnetization via radiation damping is present.

1. Introduction

Nuclear magnetic resonance (NMR) is a versatile technique used by chemists to analyze the structure of molecules and by radiologists to image the composition of tissues and organs [1]. Magnetic resonance spectroscopy (MRS), however, can be impeded by non-linear effects such as radiation damping, which involves the feedback of a macroscopic reaction field [2–8]. Magnetic resonance imaging (MRI) also is susceptible to non-linear Eddy current effects when the imaging gradients are rapidly cycled during the echo-planer imaging sequence used in functional MRI and in diffusion-weighted tensor imaging (DTI) [9]. Such effects distort images in MRI and broaden spectral lines in MRS. In addition to the loss of image and spectral information, non-linear feedback in NMR can also induce chaotic system behavior. Such behavior is inherent in the Bloch equations when non-linear terms are included. This situation is of particular concern in NMR because data acquisition is typically done in an open loop manner with multiple radiofrequency (RF) pulses or images acquired serially over a time period ranging from milliseconds to tens of seconds. Any disruption of the underlying NMR data acquisition pattern will in these cases be unobserved and indistinguishable from system noise, hence it is very important to study the non-linear Bloch equation in order to better understand the conditions that affect the development of chaos.

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0898-1221/$ – see front matter
doi:10.1016/j.camwa.2012.01.069

Analysis of the time dependent data obtained from MRS and MRI thus requires a mathematical model to correlate the precession and relaxation of the NMR signal with the composition and compartmentalization of the source molecules (e.g., water in MRI and typically hydrogen and carbon nuclei in MRS). The relationship between the measurable NMR parameters (spectral splitting, chemical shifts, T_1 and T_2 relaxation times, and diffusion coefficients) and the tissue or sample heterogeneity is increasingly being viewed in terms of a fractional-order version of the Bloch equation, which appears in many cases to more accurately account for tissue or emulsion complexity [10,11]. This is due in part to the fact that the physical processes that underlie the observed spectral or image intensity parameters span multiple time and length scales in biological tissues. In diffusion, for example, the time scale can extend from milliseconds to tens of seconds, while for imaging the field of view can extend from that of a single cell to the entire human brain. Fractional-order models for polymers, dielectrics, and viscoelastic have been shown to provide a concise way to describe such multi-scale phenomena [12–14]. Thus, we anticipate that such models can provide a new way to interpret NMR phenomena, particularly in complex, heterogeneous, and anisotropic materials such as biological tissue.

In previous studies the Bloch equation was generalized to fractional order to account for the anomalous relaxation and diffusion observed in NMR studies of complex materials—typically gels, emulsions, porous composites and biological tissues [15–18]. A common feature of such materials is their "mesoscopic" structure, which is intermediate in scale between the molecular and the macroscopic domains. In using NMR to probe the organization (ordered/disordered) and dynamics (phase transitions, diffusion, permeability) of mesoscopic structures assumptions must be made about the form of the underlying Bloch equation. The proper form for MR microscopy, for example, is one that incorporates the gradient and RF pulses needed for high resolution and contrast, while for NMR diffusion analysis diffusion-weighted imaging pulses are needed to provide a high signal-to-noise in order to obtain a measure of material porosity and tortuosity. In such studies the fractional order Bloch equation has been found to be useful [10,11,19].

The work in this paper describes a new fractional-order model for NMR relaxation developed through a generalization of the Bloch equation to include the effects of non-linear feedback due to phenomena such as radiation damping. The goal of this work is to analyze the stability of fractional order Bloch equation when its variable order, typically α, the fractional-order dynamics is changed to reflect behavior often observed in experimental data. In the following, we first present our model for NMR relaxation in the presence of feedback, and show analytically that it provides a new way to capture the transient NMR dynamics as a function of time and for a range of α.

The organization of this paper is as follows: in Section 2 we introduce the Bloch equation and we discuss briefly its fractional generalization; in Section 3 we present the asymptotic stability of the commensurate and incommensurate fractional ordered system; in Section 4 the investigated system is presented; in Section 5 we present our findings for examples selected to span a range of fractional orders and acquisition time; and in the last two sections we discuss our contribution by comparing and contrasting it with previous work.

2. Bloch equation

The classical description of nuclear magnetic resonance (NMR) is summarized in vector form by the Bloch equation [1,20],

$$\frac{d\vec{M}}{dt} = \gamma\, \vec{M} \times \vec{B} - \frac{(M_z - M_0)}{T_1}\hat{i}_z - \frac{\left(M_x\hat{i}_x + M_y\hat{i}_y\right)}{T_2}, \tag{2.1}$$

where $\vec{M}$ (M_x, M_y, M_z) represents the time-varying magnetization (Amps/s), M_0 the equilibrium magnetization, $\vec{B}$ $\left(B_x, B_y, B_z\right)$ the applied radiofrequency (RF), gradient and static magnetic fields (Tesla), γ is the gyromagnetic ratio (42.57 MHz/T, for spin 1/2 protons), and T_1, T_2 are the spin–lattice and the spin–spin relaxation times, respectively. For homogeneous (e.g., over a 1–2 mm^3 voxel), and isotropic materials with a single spin component (typically water protons), the Bloch equation represents the dynamic balance between externally applied magnetic fields and internal sample relaxation times. This dynamic balance is the basis for pulse sequence design, signal acquisition, image reconstruction and, in the case of MRI, tissue contrast [9,21–23].

Fractional order generalization of the Bloch equation with delay was the subject of a previous work by this group [10,11, 15–19,24]. In those studies the fractional order of the time derivative was balanced by the precession and relaxation terms —to account for the anomalous relaxation observed in NMR studies of complex materials. In this study we extend this model by introducing feedback into the precessional terms. The new model is non-linear, and hence is potentially chaotic. Such models have different stability and sensitivity properties and we seek here to explore them in the case of NMR phenomena, such as that observed in radiation damping [25].

3. Preliminaries

The basic definitions and properties of the fractional calculus used in this manuscript can be found in [26,27]. Numerical methods used for solving ODEs have to be modified for solving fractional differential equations (FDEs). A modification of Adams–Bashforth–Moulton algorithm is proposed by Diethelm et al. in [28–30] to solve FDEs.

The method we have used (fractional Adams–Bashforth–Moulton scheme) is proposed by Diethelm et al. [28–30]. The algorithm is used by many researchers to study the chaos in fractional order systems.

This is a particularly well understood algorithm for which the detailed theoretical analysis is available [31].

Moreover, it has been shown to be stable and reliable also in cases where the differential equation to be solved was considered to be difficult [32], and comparative studies [33] have demonstrated that its performance compares favorably with other methods.

3.1. Asymptotic stability of the commensurate fractional ordered system

Consider the following commensurate fractional ordered dynamical system

$$D^{\alpha}x_i = f_i(x_1, x_2, x_3), \quad 1 \le i \le 3. \tag{3.1}$$

Let $p \equiv \left(x_1^*, x_2^*, x_3^*\right)$ be an equilibrium point of the system (3.1) i.e. $f_i(p) = 0$, $1 \le i \le 3$ and $\xi_i = x_i - x_i^*$ a small disturbance from a fixed point. Then

$$\begin{aligned} D^{\alpha}\xi_i &= D^{\alpha}x_i, \\ &= f_i\left(x_1, x_2, x_3\right) = f_i\left(\xi_1 + x_1^*, \xi_2 + x_2^*, \xi_3 + x_3^*\right) \\ &= f_i\left(x_1^*, x_2^*, x_3^*\right) + \xi_1\frac{\partial f_i(p)}{\partial x_1} + \xi_2\frac{\partial f_i(p)}{\partial x_2} + \xi_3\frac{\partial f_i(p)}{\partial x_3} + \text{ higher ordered terms} \\ &\approx \xi_1\frac{\partial f_i(p)}{\partial x_1} + \xi_2\frac{\partial f_i(p)}{\partial x_2} + \xi_3\frac{\partial f_i(p)}{\partial x_3}. \end{aligned} \tag{3.2}$$

System (3.2) can be written as

$$D^{\alpha}\xi = J\xi, \tag{3.3}$$

where $\xi = (\xi_1, \xi_2, \xi_3)^t$ and

$$J = \begin{pmatrix} \partial_1 f_1(p) & \partial_2 f_1(p) & \partial_3 f_1(p) \\ \partial_1 f_2(p) & \partial_2 f_2(p) & \partial_3 f_2(p) \\ \partial_1 f_3(p) & \partial_2 f_3(p) & \partial_3 f_3(p) \end{pmatrix}. \tag{3.4}$$

The linear autonomous system

$$D^{\alpha}\xi = J\xi, \qquad \xi(0) = \xi_0, \tag{3.5}$$

where J is $n \times n$ matrix and $0 < \alpha < 1$ is asymptotically stable if and only if $|\arg(\lambda)| > \alpha\pi/2$ for all eigenvalues λ of J. In this case, each component of solution $\xi(t)$ decays towards 0 like $t^{-\alpha}$ [34,35].

This shows that if $|\arg(\lambda)| > \alpha\pi/2$ for all eigenvalues λ of J then the solution $\xi_i(t)$ of the system (3.3) tends to 0 as $t \to \infty$. Thus the equilibrium point p of the system is asymptotically stable if $|\arg(\lambda)| > \alpha\pi/2$, for all eigenvalues λ of J i.e. if

$$\min_i |\arg(\lambda_i)| > \alpha\pi/2. \tag{3.6}$$

3.2. Asymptotic stability of the incommensurate fractional ordered system

Consider the incommensurate fractional ordered dynamical system [36]

$$D^{\alpha_i}x_i = f_i(x_1, x_2, x_3), \quad 1 \le i \le 3, \tag{3.7}$$

where $0 < \alpha_i < 1$, $\alpha_i = v_i/u_i$, $(u_i, v_i) = 1$, u_i, v_i are positive integers. Define M to be the least common multiple of u_i's. Let $p \equiv \left(x_1^*, x_2^*, x_3^*\right)$ be an equilibrium point of the system (3.7) and $\xi_i = x_i - x_i^*$, $1 \le i \le 3$ a small perturbation from a fixed point. Using similar analysis as in Section 3.1,

$$D^{\alpha_i}\xi_i \approx \xi_1\frac{\partial f_i(p)}{\partial x_1} + \xi_2\frac{\partial f_i(p)}{\partial x_2} + \xi_3\frac{\partial f_i(p)}{\partial x_3}, \quad 1 \le i \le 3. \tag{3.8}$$

System (3.8) is equivalent to

$$\begin{pmatrix} D^{\alpha_1}\xi_1 \\ D^{\alpha_2}\xi_2 \\ D^{\alpha_3}\xi_3 \end{pmatrix} = J\begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix}, \tag{3.9}$$

where J is the Jacobian matrix as defined in (3.4) evaluated at point p. Define

$$\Delta(\lambda) = \text{diag}\left(\left[\lambda^{M\alpha_1}\lambda^{M\alpha_2}\lambda^{M\alpha_3}\right]\right) - J. \tag{3.10}$$

Then the solution of the linear system (3.9) is asymptotically stable if all the roots of the equation $\det(\Delta(\lambda)) = 0$ satisfy the condition $|\arg(\lambda)| > \pi/(2M)$ [37]. This condition is equivalent to the following inequality

$$\frac{\pi}{2M} - \min_i \{|\arg(\lambda_i)|\} < 0. \tag{3.11}$$

Table 1
Equilibrium point and corresponding eigenvalues.

Equilibrium point	Eigenvalues	Nature
$E_1(0.031698, 0.0049, 0.9980)$	$-0.19961, 4.75331 \pm 30.7485\imath$	Saddle point

Thus an equilibrium point p of the system (3.7) is asymptotically stable if the condition (3.11) is satisfied. The term $\frac{\pi}{2M} - \min_i \{|\arg(\lambda_i)|\}$ is called as the instability measure for equilibrium points in fractional order systems (IMFOSs). Hence, a necessary condition for fractional order system (3.7) to exhibit chaotic attractor is [36]

$$\text{IMFOS} \geq 0. \tag{3.12}$$

In the subsequent section we demonstrate that the condition (3.12) is not sufficient for chaos to exist.

4. System description

In this article we study the following nonlinear fractional order system

$$\begin{aligned} D^{\alpha_1}x &= \delta y + \lambda z\,(x\sin(\psi) - y\cos(\psi)) - \frac{1}{T_2}x \\ D^{\alpha_2}y &= -\delta x - z + \lambda z\,(y\sin(\psi) + x\cos(\psi)) - \frac{1}{T_2}y \\ D^{\alpha_3}z &= y - \lambda\sin(\psi)\left(x^2 + y^2\right) - \frac{1}{T_1}(z-1) \end{aligned} \tag{4.1}$$

where $\alpha_i \in (0, 1)$, $\delta = -0.4\pi$, $\lambda = 30$, $\psi = 0.173$, $T_1 = 5$ and $T_2 = 2.5$.

We are using the Caputo fractional derivative (defined by the fractional integral of an ordinary derivative). In NMR problems the spin system is perturbed by a series of RF pulses applied for short duration (typically less than a millisecond), which is long with respect to the period of the resonance frequency (approx 10 ns for 3 T MRI at 127 MHz), but short compared with the T_1 and T_2 relaxation times (300 and 100 ms, respectively). So we must be able to model the Bloch equation with a derivative that we can turn on and off in a pulse- or step-like manner. The Caputo is well defined under such conditions, the Riemann–Liouville is not, and furthermore requires fractional order initial conditions, which we cannot prescribe.

If $\alpha_1 = \alpha_2 = \alpha_3 = \alpha$ then the system (4.1) is called commensurate otherwise incommensurate.

The system (4.1) has three equilibrium points out of which two are complex *viz.* $(0.0777 \pm 0.3405\imath, -0.308 \pm 0.0664\imath, -0.0379 \pm 0.0223\imath)$. The real equilibrium point and the eigenvalues of corresponding Jacobian matrix

$$J = \begin{pmatrix} -0.4 + 5.16415z & -1.25664 - 29.5522z & 30(0.172138x - 0.985073y) \\ 1.25664 + 29.5522z & -0.4 + 5.16415z & -1 + 30(0.985073x + 0.172138y) \\ -10.3283x & 1 - 10.3283y & -0.2 \end{pmatrix} \tag{4.2}$$

are given in Table 1. An equilibrium point p of the system is called as saddle point if the Jacobian matrix at p has at least one eigenvalue with negative real part (stable) and one eigenvalue with non-negative real part (unstable). A saddle point is said to have index one (/two) if there is exactly one (/two) unstable eigenvalue/s. It is established in the literature [38–42] that, scrolls are generated only around the saddle points of index two. Saddle points of index one are responsible only for connecting scrolls.

It is clear from Table 1 that the equilibrium point E_1 is a saddle point of index two.

5. Results

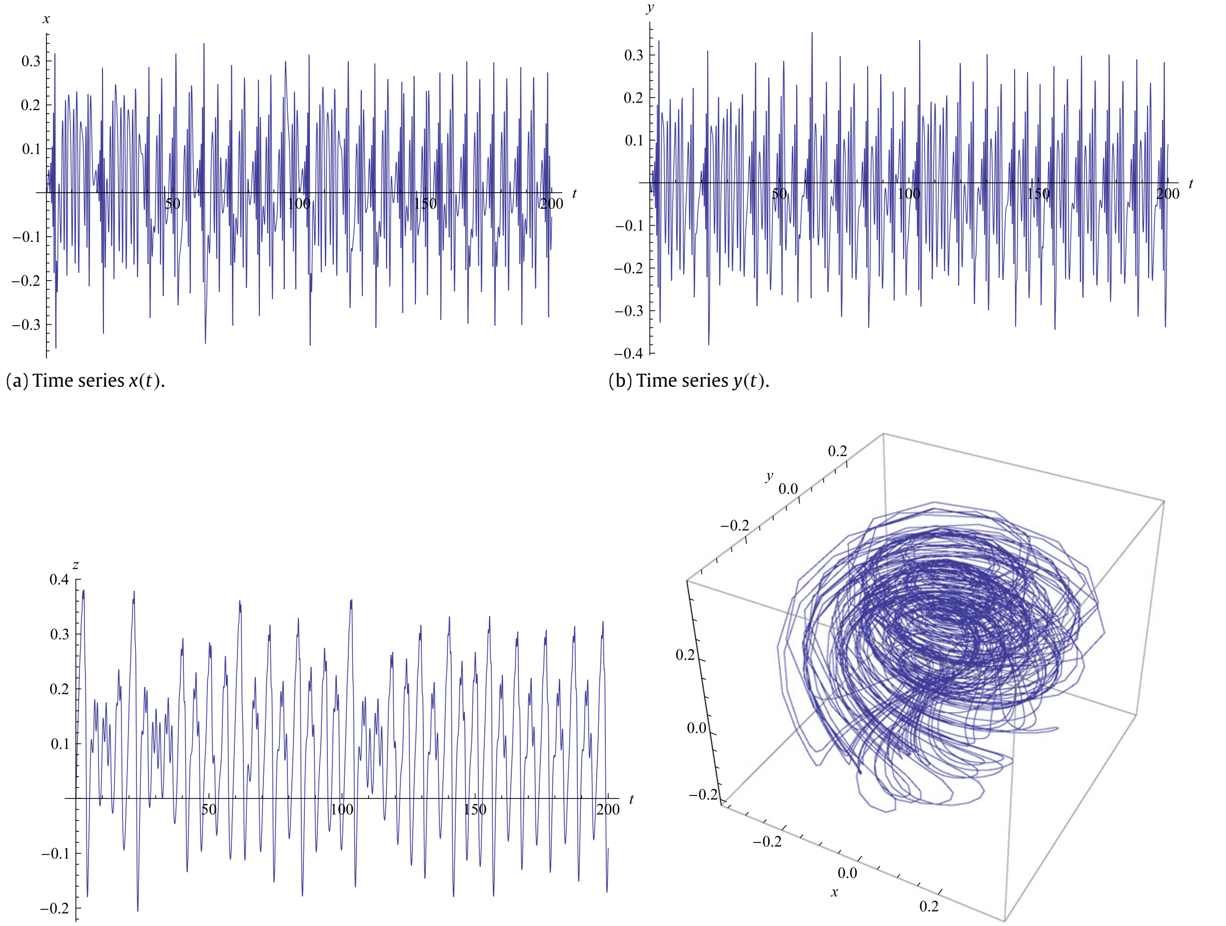
5.1. Commensurate ordered system

Consider the system (4.1) with $\alpha_1 = \alpha_2 = \alpha_3 = \alpha$ (commensurate order). The system (4.1) shows regular behavior if it satisfies (3.6). i.e.

$$\alpha < \frac{2}{\pi}\min_i |\arg(\lambda_i)| \approx 0.90236. \tag{5.1}$$

The condition (5.1) is sufficient and not necessary for stability of the system. We have employed the method discussed in [28–30] to study the behavior of system (4.1) for different values of fractional order α.

- For $1 \geq \alpha \geq 0.99$, the system is chaotic. Fig. 1 (a)–(c) show time series $x(t)$, $y(t)$ and $z(t)$ respectively, for $\alpha = 0.99$. For the same value of α, the chaotic phase portraits in xyz-space, xy-plane, yz-plane and xz-plane are plotted in Fig. 1(d)–(g) respectively.



(a) Time series $x(t)$.

(b) Time series $y(t)$.

(c) Time series $z(t)$.

(d) xyz-phase portrait.

Fig. 1. Time series and different phase portraits for the case $\alpha = 0.99$.

- For $0.98 > \alpha \geq 0.94$, the system shows *transient chaos* i.e. the trajectory is chaotic initially for some time and then becomes periodic. We have considered $\alpha = 0.97$ and drawn time series in Fig. 2(a)–(c).
- System exhibits periodic oscillations for sufficiently larger values of t and for $\alpha \leq 0.93$. Periodic oscillations and limit cycles are shown in Fig. 3, for $\alpha = 0.89$. This shows that the condition (5.1) is not necessary for stability.

5.2. Incommensurate ordered system

In this subsection we study the incommensurate order system (4.1). We fix any two α_i to 1 and vary the third $\alpha_i \in (0, 1)$.

- $\alpha_2 = \alpha_3 = 1$:

  Consider $\alpha_1 = 0.79 = 79/100$, $M = LCM(100, 1, 1) = 100$. Since $\Delta(\lambda) = \text{diag}\left(\lambda^{79}\lambda^{100}\lambda^{100}\right) - J(E_1)$,

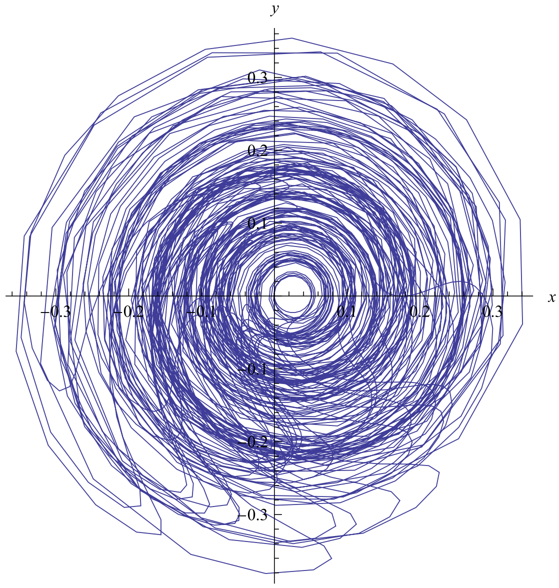
$$\det(\Delta(\lambda)) = \lambda^{279} - 4.7535\lambda^{200} - 4.5535\lambda^{179} + 967.084\lambda^{100} - 0.91467\lambda^{79} + 193.236. \tag{5.2}$$

  The IMFOS of the system is

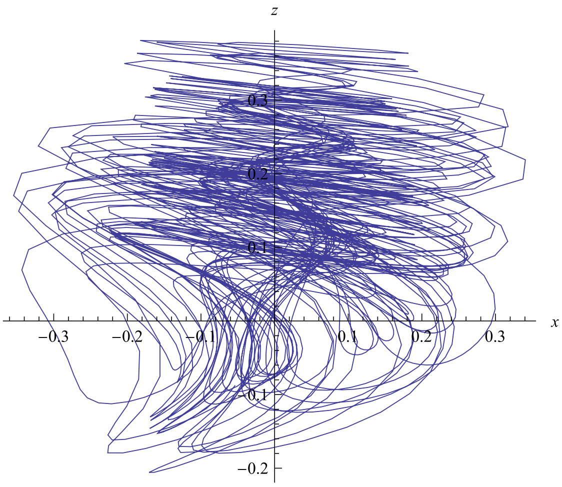
$$\frac{\pi}{200} - 0.0157192 = -0.0000112544 < 0. \tag{5.3}$$

  It is observed that the IMFOS < 0 for $\alpha_1 \leq 0.79$ and hence the system is stable for these values. For $\alpha_1 > 0.79$, the IMFOS > 0. Numerical simulations show the transient chaos for some values such as $\alpha_1 = 0.98$ (cf. Fig. 4(a)) or a periodic limit cycle e.g. $\alpha_1 = 0.99$ (cf. Fig. 4(b)). Chaos is not observed in this case.
- $\alpha_1 = \alpha_3 = 1$:

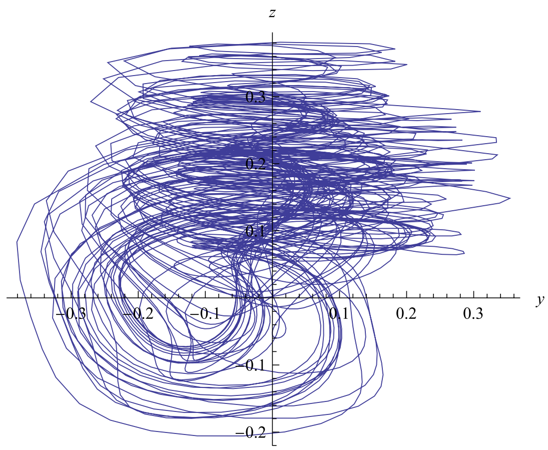
  Consider $\alpha_2 = 0.79 = 79/100$, $M = LCM(1, 100, 1) = 100$. In this case $\Delta(\lambda) = \text{diag}\left(\lambda^{100}\lambda^{79}\lambda^{100}\right) - J(E_1)$ and the IMFOS $= -0.0000112544 < 0$. Hence the system is stable for the values $\alpha_2 \leq 0.79$. We have observed from numerical experiments that the system does not show chaotic behavior for these values of parameters. The behavior is



(e) *xy*-phase portrait.



(f) *yz*-phase portrait.



(g) *xz*-phase portrait.

Fig. 1. (*continued*)

either transient chaos or periodic. Fig. 5(a) shows state $x(t)$ for $\alpha_2 = 0.97$ with transient chaos and Fig. 5(b) shows a limit cycle in case $\alpha_2 = 0.99$.

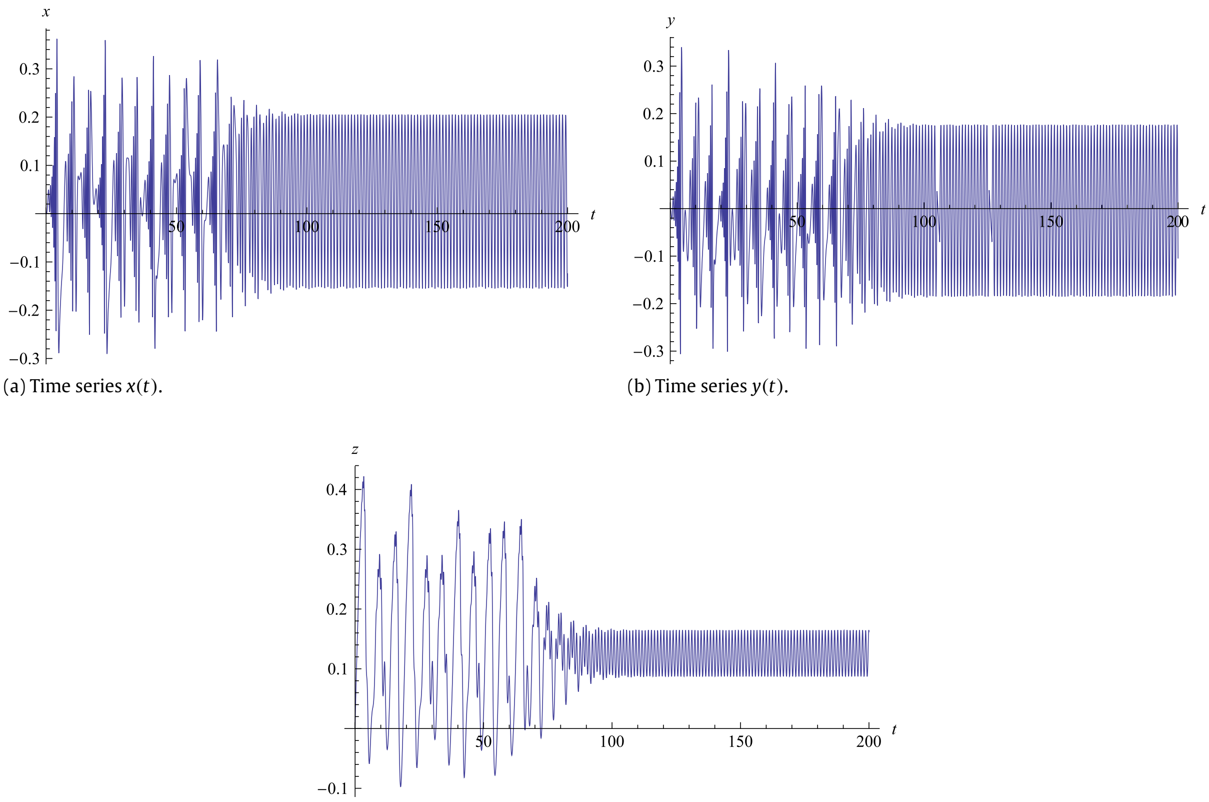
- $\alpha_1 = \alpha_2 = 1$:

    In this case, we did not get any value of the parameter α_3 for which the IMFOS < 0, (e.g. IMFOS $= 0.0306137$, for $\alpha_3 = 0.2$). Numerical experiments, in this case show that the system is regular (or transient chaotic) for all values of parameter α_3 (cf. Fig. 6(a),(b)).

    In the previous work [43,44] we have shown that the condition (3.12) i.e. IMFOS > 0 is not sufficient for chaos but still there were some parameter values where the system becomes chaotic. In this example the IMFOS is never negative as well as the system is never chaotic. According to authors' knowledge, this type of example is observed for the first time in the literature.

6. Discussion

A key aspect in the development of magnetic resonance imaging and spectroscopy is the quest to develop new technologies with higher sensitivity and specificity. Such technology is needed to detect and diagnose the changes in the tissue structure that underlie the appearance of neurodegenerative diseases such as Alzheimer's. Changes in the tissue structure of the brain arise through shifts in tissue components and compartments (organelles, cells, extra-cellular matrix,



(a) Time series $x(t)$. (b) Time series $y(t)$. (c) Time series $z(t)$.

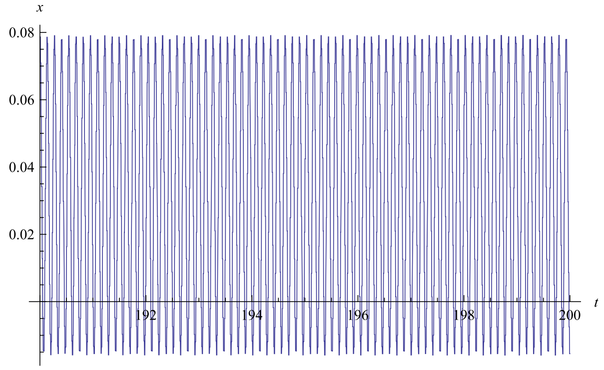
Fig. 2. Time series showing transient chaos for the case $\alpha = 0.97$.

and vascular/lymphatic networks), all of which directly impact the fundamental biochemical and biophysical processes, but only indirectly affect observable relaxation times and diffusion coefficients. For example, while T_1 and T_2 contrasts and diffusion-weighted images can often identify small centimeter diameter regions of plaque in Alzheimer's disease, tissue classification and disease staging are still dependent upon biopsy, histology and pathological analysis.

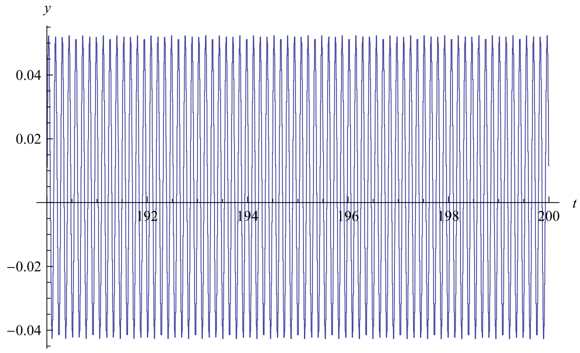
Improving MRI technology requires improvements not only in the hardware and software, but also in the development of new models for NMR phenomena that more accurately reflect the tissue (and disease) microenvironments. Thus, for a given temperature, static field strength, observation time and sample volume, MR physics establishes minimal voxel size, SNR and k-space sampling rate, which unfortunately limits the ability to use MRI to acquire, analyze and assess complex biological structures that extend in space over at least six orders of magnitude—from nanometers to millimeters. Since imaging voxels are typically in the order of cubic millimeters while cells and the extra-cellular matrix exhibit structure at the cubic micron scale and below; and given the relatively slow acquisition and sampling rate of existing NMR technology (typically seconds for high resolution images), the impetus for higher field magnets, multiple transmit and up to 128 received channels, and phased array coils is clear. Nevertheless, signal acquisition takes time and biological systems place constraints on the safe level of applied fields (particularly RF power and fast changing gradients). Therefore, in seeking to improve the capabilities of MR technology to uncover key aspects of complex tissue structure we have sought to extend the fundamental mathematical model of NMR – the Bloch equation – through generalization of the time derivative to non-integer or fractional order through the techniques of fractional calculus.

The classical description of NMR is complete, concise and well established both in terms of the underlying theory (vector and quantum mechanical) and over 50 years of successful applications. However, the classical analysis while molecular (or more precisely, nuclear), in its origin is in fact quite course grained in its implementation. NMR assumes, in most cases, an averaging process over an immense number of nuclear spins—many of which are not directly observable. This spatial and temporal averaging is not a particular problem for mm-scale resolution, as seen in most clinical and animal MRI. The problem is confounded, however, when we seek more specific or more localized information on the structure, substructure or compartmentalization of the water that carries the NMR-visible nuclear magnetic moments.

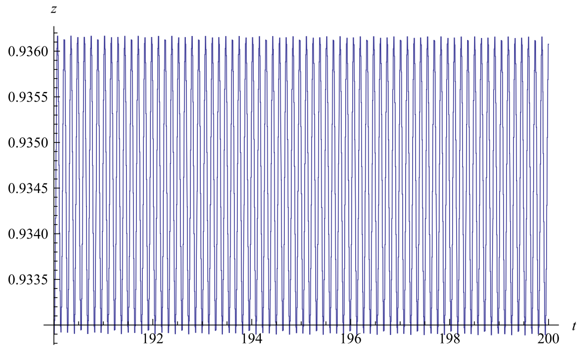
In the theory section of this paper we presented a generalized model of the dynamics of a single magnetic species in NMR by assuming a fractional order fading memory kernel. This extension via convolution is significant in that it adds (memory) while retaining linearity, causality, time-invariance from the classical model. This extension of the Bloch equation to fractional order is under active investigation by several research groups [12–14]. Fractional order generalization of the



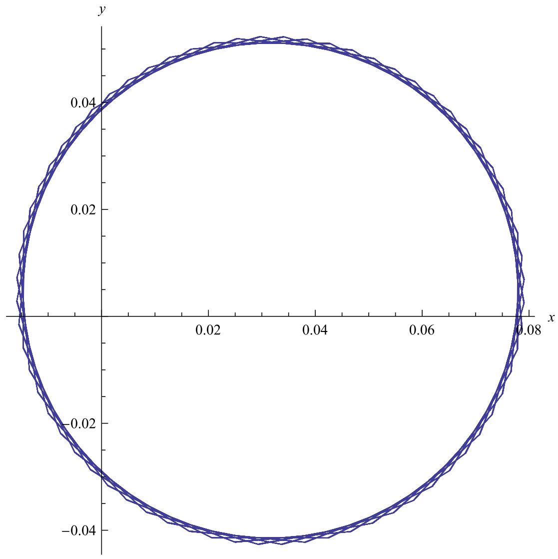
(a) Time series $x(t)$.



(b) Time series $y(t)$.

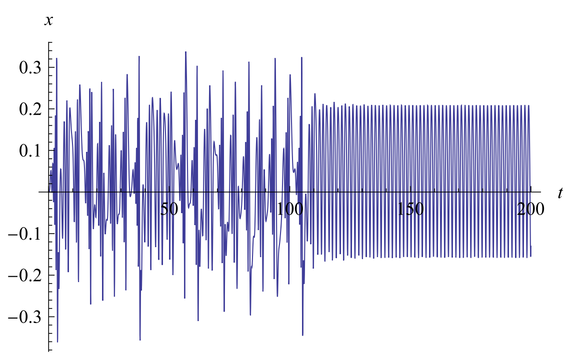


(c) Time series $z(t)$.

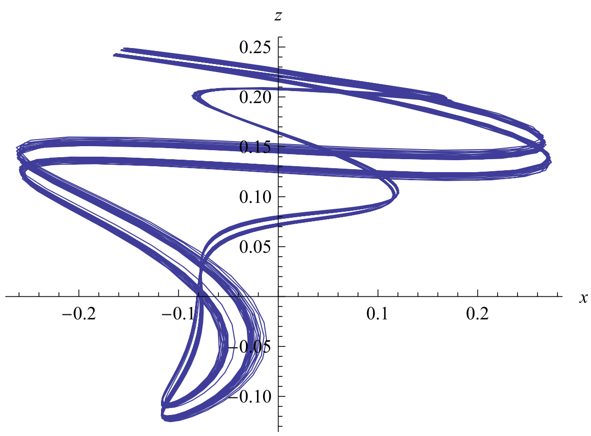


(d) xy-phase portrait.

Fig. 3. Periodic behavior of the system for $\alpha = 0.89$.

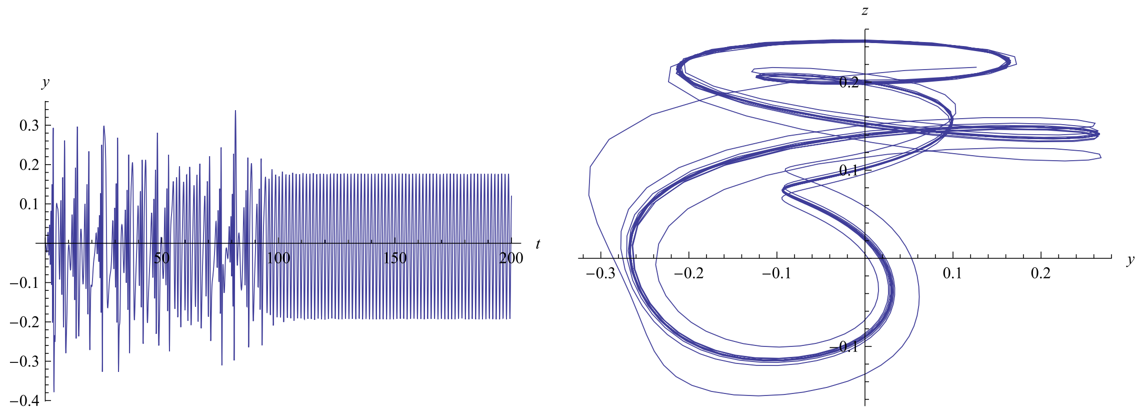


(a) Transient chaos $\alpha_1 = 0.98$.



(b) Limit cycle $\alpha_1 = 0.99$.

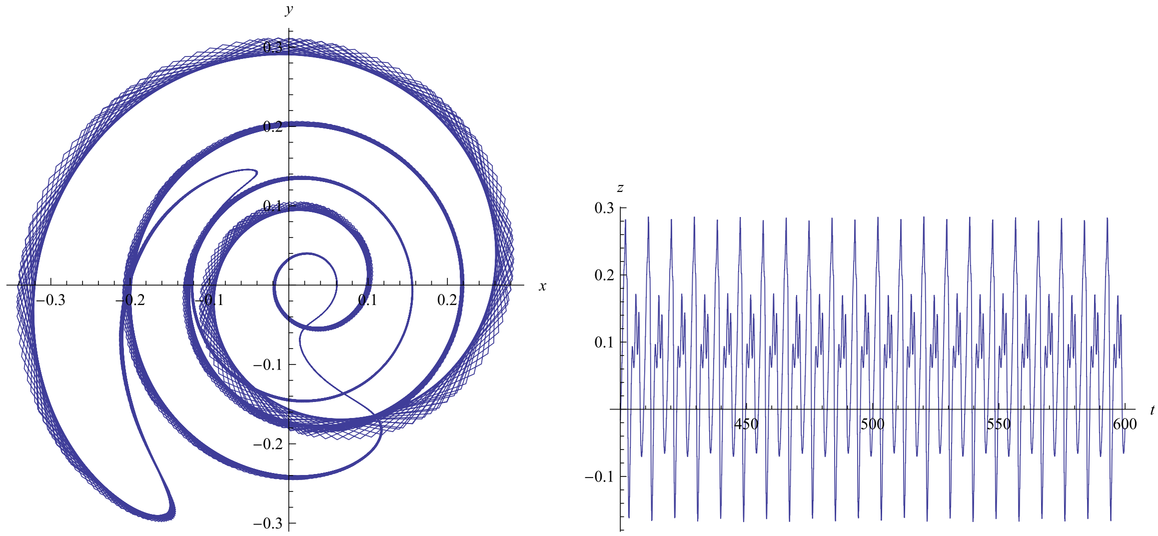
Fig. 4. Behavior of the system for $\alpha_2 = \alpha_3 = 1$ and $\alpha_1 \in (0, 1)$.



(a) Transient chaos $\alpha_2 = 0.97$.

(b) Limit cycle $\alpha_2 = 0.99$.

Fig. 5. Behavior of the system for $\alpha_1 = \alpha_3 = 1$ and $\alpha_2 \in (0, 1)$.



(a) Limit cycle $\alpha_3 = 0.98$.

(b) Periodic orbit $\alpha_3 = 0.99$.

Fig. 6. Behavior of the system for $\alpha_1 = \alpha_2 = 1$ and $\alpha_3 \in (0, 1)$.

Bloch equation has been undertaken by several groups [10,11,15–19] to account for the anomalous relaxation and anomalous diffusion observed in NMR studies of complex materials - typically gels, emulsions, porous composites and biological tissues.

The still unresolved question regarding the fractional or "generalized" Bloch equation is how to modify it to account for the presence of feedback due to phenomena such at radiation damping. Recently fractional order operators in time – with or without delay – were used to incorporate system memory [45]. The delay model investigated modifies the time window for the fractional order time derivative by allowing not only a fading memory of an earlier state or time, but also by introducing averaged or extended information about the previous conditions at a time specified by the time delay. The rationale for this approach is that it may extend the modeling capabilities of the Bloch equation so that transient mesoscopic structures in complex materials can be better visualized. But, the presence of feedback is another concern in building a better or more complete model of complex materials.

The results presented in this paper demonstrate that solutions to the generalized fractional order Bloch equation with feedback exhibit novel behavior dependent upon the selected system parameters. In general, for values of α near 1.00, the system exhibits chaos. This phenomena disappears when α falls below 0.90 and is transient in the intermediate range from 0.9 to 1.00. The appearance of such behavior in experimental systems is known and as such can contribute to spin turbulence and loss of information.

There are three time scales in NMR: resonance (nanosecond), RF pulse durations (microseconds), and relaxation (milliseconds to seconds). Thus, we can set the delay in our model in such a way as to couple to each of these processes. Chaos could result from coupling between or at any of these time scales.

Further work is needed to connect this new fractional order model with delay to the NMR behavior of complex molecules and materials.

7. Conclusion

We introduced in this paper a new model for T_1 and T_2 relaxation in NMR in the presence of feedback. The model arises by replacing the ordinary time derivative in the Bloch equation with a fractional-order operator and by introducing feedback in the corresponding precessional dynamics. This extension results in numerical solutions that exhibit transient chaos. These models are still in their early stages of development. The results, based upon assessment of the perturbed NMR system dynamics, demonstrate a wide range of new phenomena. A key aspect of this work is the development of a dynamic formulation for the NMR relaxation problem that has its foundation in the physics of the material.

Acknowledgment

V. Daftardar-Gejji acknowledges the Department of Science and Technology, N. Delhi, India for the Research Grants [Project No. 1SR/S2/HEP-024/2009].

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