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DYNAMICS OF THE TIME DEPENDENT BLOCH NMR EQUATIONS FOR COMPLEX rF $B_1(t)$ MAGNETIC FIELD

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Abstract

This study examines the dynamical changes produced by a complex time-dependent rF $B_1(t)$ magnetic field in an initially unperturbed magnetic resonance system. The analysis uses the Green's function algorithm as a tool to solve the transverse component of the time-dependent Bloch NMR equations with complex rF $B_1(t)$ field. The time development of the system is studied in the Hersenberg picture in which the operators are subject to unitary transformation as the applied rF $B_1(t)$ field changes the state of the NMR system from its initial ground state into another coherent state. The detailed features of the rF $B_1(t)$ field essentially affect the evolution of the state during its application. The state of the system after the complete cessation of the radio-frequency field is determined exclusively by a Fourier component which is in resonance with the NMR system. The unitary operator allows us to determine all the physically relevant information about the system in terms of a NMR relaxation parameter.

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INTRODUCTION

Many techniques in magnetic resonance have been analyzed based on different classical approaches [1-6]. While such novel approaches are very useful and provide the present innovations, it is necessary to have recourse to the Green-functional analysis of the time dependent Bloch NMR equation to fully understand the physics of nuclear magnetic resonance.
Magnetic resonance is a process that should be treated analytically in terms of density matrix calculations for possible NMR pulse experiments. Fortunately the coupling of the nuclear spins mutually and with surrounding matter is weak. This allows a classical treatment on the basis of the Bloch NMR equations extended to the terms describing the relaxation in a phenomenological way. In this presentation we have studied the dynamics of the Bloch NMR equations to explore how the interaction of a complex rf B_1 field with certain nuclei leads among others to the detailed feature of density matrix calculations for the simulation of the effect of rF pulses, J-coupling and precession in a magnetic field variable in space.

Over the years, the density matrix formalism has been developed to suitably simulate the behavior of two spins system of different nuclei when a pulse sequence is applied. These may be very useful to simulate the effect of rF pulses, J-coupling and precession in a magnetic field variable in space. Quite a number of computer programs of sophisticated versions have been written to deal with such simulations [7-16]. It may be appreciated that these several computer programs have contributed greatly to the understanding of NMR experiments. Some of the drawbacks of these mathematical packages are the fact that the user cannot include relaxation parameters and the program execution may take a considerable long time if the pulse sequences involved are long.

Therefore, there is a need to develop a mathematical algorithm for better understanding of the properties of magnetic resonance so that the design of the best mathematical package for the calculations of the effects of pulse sequences on spins exactly can be achieved without critical drawbacks. This need can be satisfied by solving the transverse component of time dependent Bloch NMR flow equations because of the fundamental role the Bloch equations play in the analysis of the properties of Magnetic Resonance Imaging (MRI). In this work, we choose the Green's function approach to solve the time-dependent Bloch NMR equation, because it has proved very useful even in many similar but more difficult problems.

MATHEMATICAL METHOD

For this investigation, we assumed that resonance condition exists at Larmor frequency

$$f_o = \gamma B - \omega = 0$$

The NMR signal is the emf induced by the precessing transverse magnetization, M_y. M_y results from the combined effect of the static magnetic field B_o and the radiofrequency field rF $B_1(t)$, on blood spins. The following are made

(i) The excitor coil is fixed and the detector coil overlaps coaxially in a cross coil mode with the excitor coil and is movable axially.

(ii) The detector coil length, L_D, is greater than the excitor coil length.

(iii) It is further assumed that resonance condition exists within the excitor as well as the detector coils.

(iv) Spins are magnetized by the static B_o field to an equilibrium magnetization, M_o, before entering the excitor coil.

The z axis in the rotating frame coincides with the laboratory Z axis; the x axis makes an angle `ωt' at any instant of time 't' with laboratory X axis. X=0 position could be such that the transverse magnetic field at the end of the detector coil is negligible.

The following symbols are defined; γ denotes the gyromagnetic ratio of the spins; $\omega/2\pi$ is the rF excitation frequency, f_o/γ is the off- resonance field in the rotating frame of reference and T_2 is the spin-spin relaxation time. The time dependent transverse magnetization $M_{y,}$ of the Bloch NMR equations is given by [1-6]

$$\frac{dM_y}{dt} = \gamma M_o B_1(t) - \frac{M_y}{T_2} \tag{1}$$

In this application, we shall be interested in the dynamical, changes produced by the complex time dependent rF B_1 (t) magnetic field in an initially unperturbed magnetic resonance system. We assumed that outside the time interval $t_1 < t < t_2$, the Hamiltonian H, is defined by the time dependent Bloch NMR equation and that the (disturbance) rF $B_1(t) \neq 0$ is applied only during a finite time interval $t_1 < t < t_2$. The time development of the system is conveniently studied in the Hersenberg picture in which the operators are subject to a unitary transformation as they change from the initial regime before t_1 to a final regime after t_2. The relevant commutation relations for M_y and $M_y^{\oplus}$, taken at equal time, are defined as

$$[M_y(t), M_y^{\oplus}(t)] = 1$$

Equation (1) is the equation of motion for the transverse magnetization $M_y(t)$.

A Green's function appropriate to equation (1) is a solution of the equation

$$\frac{dG(t-t')}{dt} + \frac{1}{T_2} G(t-t') = \delta(t-t') \tag{2}$$

because such a function permits us to write a particular solution of equation (1) as

$$M_y(t) = \gamma M_o \int_{-\infty}^{\infty} G(t-t') B_1(t') dt' \tag{3a}$$

where δ is a delta function.

Obviously, for $t \neq t'$ the Green's function is proportional to $e^{-\frac{(t-t')}{T_2}}$, but at $t = t'$ there is a discontinuity. By integrating equation (2) over an interval which includes t', we derive the condition

$$\lim_{\lambda \to 0} [G(+\lambda) - G(-\lambda) = 1 \tag{3b}$$

for $\lambda > 0$

Two particular Green's functions are useful:

$$G_R(t-t') = \eta(t-t') e^{-\frac{(t-t')}{T_2}} \tag{4}$$

and

$$G_A(t-t') = \eta(t'-t)e^{-\frac{(t-t')}{T_2}} \tag{5}$$

In addition to the delta function, it is convenient to introduce the unit step function η(t) defined by

$$\eta(t) = \int_{-\infty}^{\infty} \delta(t')dt' = \begin{cases} 0 & t<0 \\ 1 & t>0 \end{cases} \tag{6}$$

Equations (4) and (5) are known as the retarded and advanced Green's functions, respectively.
If we denote by $M_{y(in)}(t)$ and $M_{y(out)}(t)$ those solutions of the homogenous equation

$$\frac{dM_y(t)}{dt} + \frac{1}{T_2} M_y(t) = 0$$

which coincide with the solution $M_y(t)$ of equation (1) for $t > t_1$ and $t > t_2$ respectively, we can write

$$M_y(t) = M_{y(in)}(t) + \gamma M_o \int_{-\infty}^{+\infty} G_R(t-t')B_1(t')dt' \tag{7}$$

$$= M_{y(in)}(t) + \gamma M_o \int_{-\infty}^{t} e^{-\frac{(t-t')}{T_2}} B_1(t')dt'$$

Or, equivalently

$$M_y(t) = M_{y(out)}(t) + \gamma M_o \int_{-\infty}^{+\infty} G_A(t-t')B_1(t')dt' \tag{8}$$

$$= M_{y(out)}(t) - \gamma M_o \int_{t}^{+\infty} e^{-\frac{(t-t')}{T_2}} B_1(t')dt'$$

By equating the right-hand sides of equations (7) and (8), we obtain the relation

$$M_{y(out)}(t) = M_{y(in)}(t) + \gamma M_o \int_{-\infty}^{+\infty} e^{-\frac{(t-t')}{T_2}} B_1(t')dt' \tag{9}$$

The free operators $M_{y(in)}$ and $M_{y(out)}$ have the simple time dependence

$$M_{y(in)} = M_{y(in)} e^{-\frac{(t-t')}{T_2}}$$

$$M_{y(out)} = M_{y(out)} e^{-\frac{(t-t')}{T_2}}$$

Hence, from equation (9), we get

$$M_{y(out)} = M_{y(in)} + \gamma M_0 g^*(T_2) \tag{10}$$

where

$$g(T_2) = \int_{-\infty}^{+\infty} e^{-\frac{(t-t')}{T_2}} B_1^*(t')dt'$$

is the Fourier transform of the radiofrequency field $B_1(t)$. We now seek to determine the unitary operator S which transforms $M_{y(in)}$ into $M_{y(out)}$ such that

$$M_{y(out)} = S^{\oplus} M_{y(in)} S \tag{11}$$

The operator S provides the vital link between the description of the NMR system before t_1 and after t_2. The operator S can be determined quite easily if we note the simple identity

$$e^{-\alpha M_y^{\oplus} + \alpha^{\otimes} M_y} M_y e^{\alpha M_y^{\oplus} + = -\alpha^{\otimes} M_y} = M_y + \alpha \tag{12}$$

for any complex number α.

Comparison of equations (10), (11) and (12) shows that the unitary transformation we seek is

$$S = \exp(\alpha M_y^{\oplus} - \alpha^{\otimes} M_y)$$

with

$$\alpha = \gamma M_o g^*(T_2) \tag{13}$$

We note that

$$\int_{-\infty}^{+\infty} [B_1^*(t) M_{y(in)}(t) + B_1(t) M_{y(in)}^{\oplus}(t)] dt = g(T_2) M_{y(in)} + g^*(T_2) M_{y(in)}^{\oplus} \tag{14a}$$

Hence, we may express S as

$$S = \exp \int_{-\infty}^{\infty} [B_1(t) M_{y(in)}(t) + B_1(t) M_{y(in)}^{\oplus}(t)] dt \tag{14b}$$

An equivalent expression for S is obtained by replacing $M_{y(in)}$ and $M^{\oplus}_{y(in)}$ by $M_{y(out)}$ and $M^{\oplus}_{y(out)}$.

The operator S allows us to determine all the physically relevant information about the NMR system after time t_2 from the knowledge of its conditions before t_1. The simplest initial condition assumes that the system is in the ground state of Hamiltonian H_{in}, so that its energy before the onset of rF field is a minimum.

COHERENT STATES

An intriguing consequence of the formalism can be read off equation (10) if it is applied to the state

$$|0\rangle_{in} = S|0\rangle_{out}$$

This vector satisfies the relation

$$M_{y(out)}|0\rangle_{in} = \alpha|0\rangle_{in} \tag{15}$$

showing that $|0\rangle_{in}$ is an eigenvector of $M_{y(out)}$ with eigenvalue of α. Since M_y is not a normal operator, its eigenvectors are not subject to any orthogonality requirement, and since $g(T_2)$ is arbitrary, any complex number is an allowed eigenvalue of M_y. From equation (15) it follows immediately that

$${}_{in}\langle 0|M_{y(out)}^{\oplus} M_{y(out)}|0\rangle_{in} = {}_{in}\langle 0|M_{y(out)}^{\oplus}|0\rangle_{in}\, {}_{in}\langle 0|M_{y(out)}|0\rangle_{in} \tag{16}$$

These special states are called ***Coherent States***. Further insight is gained if we construct the time-dependent states vector in the Schrodinger picture for $t > t_2$. From equation (11) it follows that for all t

$$M_{y(out)}(t) = S^{\oplus} M_{y(in)}(t) S \tag{17a}$$

since both $M_{y(out)}(t)$ and $M_{y(in)}(t)$ depend on the time through the same factor $e^{-\frac{t}{T_2}}$.
We can write equation (17a) in term of the ground state Hamiltonian H_{in}, as

$$M_{y(out)}(t) = S^{\oplus} e^{-\gamma M_o H_{in} t} M_{y(in)} e^{\gamma M_o H_{in} t} S \qquad (17b)$$

If we choose the initial time 0 to precede and the final time t to follow the external perturbation, $0 < t_1 < t_2 < t$, we may then identify $M_{y(in)} = M_y(0)$ and $M_{y(out)}(t) = M_y(t)$ and conclude that the time development operator is (except for a constant phase factor)

$$T(t,0) = e^{\gamma M_o H_{in} t} S$$

The Schrödinger operators M_y and $M_y^{\oplus}$ may be equated with the Heisenberg operators $M_y(t)$ and $M_y^{\oplus}(t)$ evaluated at t = 0. Hence, the notation $M_y = M_y(0) = M_{y(in)}$ is appropriate.
For times $t > t_2$ the state vector is given by

$$\psi(t) = e^{\gamma M_o H_{in} t} S \psi(0) \qquad (18)$$

where H_o is the unperturbed Hamiltonian. If the initial state is the ground state,

$$\psi(0) = |0\rangle,$$

after the rF field is terminated the state develops in time as

$$\psi(t) = e^{-\frac{(|\alpha|^2 + \frac{t}{T_2})}{2}} \exp(\alpha M_y^{\oplus} e^{-\frac{t}{T_2}}) |0\rangle \qquad (19)$$

UNITARY TRANSFORMATION

If the state of the NMR system is described by ψ and if the system admits rotations as symmetry operations, a particular rotation R produces a new state ψ′, related to ψ by a unitary transformation S_R:

$$\psi' = S_R \psi \qquad (20)$$

Three rotations m_x, m_y, m_z are said to be the Cartesian components of a vector operator $\mathbf{M_y}$ if under every rotation, the expectation values transforms like the components of a vector. It is required of a vector operator that for any ψ, the old and new expectation values $\mathbf{M_y}$ may be related by

$$(\psi', m_i \psi') = \sum_{j=1}^{3} R_{ij} (\psi, m_j \psi) \qquad (i = 1,2,3) \qquad (21)$$

where R_{ij} represents the real orthogonal matrix which characterizes the rotation of the Cartesian coordinates x, y, z. It follows that a rotation about the z-axis by an angle θ would, according to the rules of analytical geometry, be written as

$$R = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (22)$$

The matrices R constitute an irreducible representation of the rotation group. Substituting ψ′ from equation (20) into equation (21) taking note that the resulting relation should hold for arbitrary state ψ, we obtain the condition

$$S_R^{\oplus} m_i S_R = \sum_{j=1}^{3} R_{ij} m_j \tag{23}$$

as the fundamental criterion for whether $\mathbf{M_y}$ is a vector or not. A necessary and sufficient condition for a vector operator can be derived by applying equation (23) to the special case of an infinitesimal rotation. For such a rotation, R is very close to the identity matrix, and S_R is very close to the identify operator. We can write

$$R_{ij} = \sigma_{ij} + \varepsilon_{ij} \tag{24}$$

where σ and ε are vector operator and angle of rotation respectively. Applying the orthogonality of the matrix and setting $\varepsilon_{12} = -\varepsilon_x$, $\varepsilon_{23} = -\varepsilon_z$ and $\varepsilon_{31} = -\varepsilon_y$, we can write for the infinitesimal rotation

$$\boldsymbol{R} = \begin{pmatrix} \mathbf{1} & -\varepsilon_z & \varepsilon_y \\ \varepsilon_z & \mathbf{1} & -\varepsilon_x \\ -\varepsilon_y & -\varepsilon_x & \mathbf{1} \end{pmatrix} \tag{25}$$

For the case of an infinitesimal rotation about the z-axis this agrees with equation (22) if we set θ = εz. Generally, the rotation shown in equation (25) takes place in a plane perpendicular to the vector ε (εx, εy, εz): |ε| is the angle of rotation, and the rotation is such that it forms a right-handed screw advancing in the direction of **ε**. The unitary operator which corresponds to such a rotation is

$$S_R = 1 + \gamma N M_0 \varepsilon . J + \gamma M_0 \tag{26}$$

where N = θ/ε represents infinitesimal rotations and **J** is the operator which represents the total angular momentum of the NMR system. If we substitute equations (24) and (26) into equation (23), we obtain

$$\begin{aligned} (1 - \gamma M_0 \varepsilon . J)\, m_i\, (1 + \gamma M_0 \varepsilon . J) &= m_i + \varepsilon_{ij} m_j + \varepsilon_{ik} m_k \\ &= m_i - \varepsilon_k m_j\ \varepsilon_j m_k \end{aligned} \tag{27}$$

By comparing the two sides of equation (27) to first order in ε, we obtain the relation

$$m_x J_y - J_y m_x = \frac{m_z}{\gamma M_o}, \qquad m_x J_z - J_z m_x = -\frac{m_y}{\gamma M_o} \tag{28a}$$

$$m_y J_z - J_z m_y = \frac{m_x}{\gamma M_o}, \qquad m_y J_x - J_x m_y = -\frac{m_z}{\gamma M_o} \tag{28b}$$

$$m_z J_x - J_x m_z = \frac{m_y}{\gamma M_o}, \qquad m_z J_y - J_y m_z = -\frac{m_x}{\gamma M_o} \tag{28c}$$

and

$$m_x J_x - J_x m_x = m_y J_y - J_y m_y = m_z J_z - J_z m_z = 0 \tag{29}$$

For the infinitesimal rotations these commutation relations are equivalent to the condition expressed in equation (23). They are also sufficient to ensure that equation (23) is satisfied for finite rotations. If the condition in equation (23) holds for two different rotations R and U, we can write

$$S_R^{\oplus} m_i S_R = \sum_j R_{ij} m_j$$

and

$$S_U^{\oplus} m_i S_U = \sum_j U_{ij} m_j$$

It follows that for the compound rotation RU

$$S_{RU}^{\oplus} m_i S_{RU} = S_R^{\oplus} S_U^{\oplus} m_i S_U S_R = S_R^{\oplus} \sum_j U_{ij} m_j S_R$$

Hence, if the condition in equation (23) holds for all infinitesimal rotations, as is guaranteed by the commutation relations in equations (27) and (29), then equation (23) will also hold for any finite rotation.

If **J** is the operator which represents the total angular momentum of the NMR system about a given origin 0, then the operators D(**u**,dθ) and D(**u**, θ) which represent an infinitesimal rotation dθ of the system, and a finite rotation θ, respectively, about an axis through 0 in the direction of the unit vector **u**, can be written in the form

D(**u**,dθ) = 1 - idθ(**J.u**) ; D(**u**, θ) = exp(-iθ(**J.u**) (30)

For a rotation R(α,β,ζ,) about the origin, given by the Euler angles α, β, ξ, we have

$$D(\alpha,\beta,\xi) = e^{-i\alpha J_x} e^{-i\beta J_y} e^{-i\xi J_z} \tag{31a}$$

The operator D(α, β, ξ) has the following matrix representation

$$D^{(j)}_{mm'}(\alpha,\beta,\xi) \equiv \langle jm | B(\alpha,\beta,\xi) | jm' \rangle = e^{-i\alpha m_x} d^{(j)}_{mm'}(\beta) e^{-i\xi m'} \tag{31b}$$

where

$$d^{(j)}_{mm'}(\beta) = \langle jm | e^{-i\beta J_y} | jm' \rangle \tag{32}$$

are the coefficients.

DENSITY MATRIX CALCULATIONS

Our goal, the construction of S corresponding to a given rotation R, will be considerably facilitated if we consider infinitesimal rotations, and thus for a small rotation we write to a first approximation the first two terms in a Taylor's series

S = 1 - i/2 ε **n. σ** (33)

where **n** is the axis of rotation, ε the angle of rotation about the axis and **σ** represents three constant matrices σx, σy, σz whose detailed structure is yet to be determined. The factor i/2 is introduced so that **σ** will have certain simple and desirable properties. In particular, the imaginary coefficient ensures that, if S is to be unitary to first order in ε, then **σ** must be Hermitian. If we carry out N = θ/ε infinitesimal rotations in succession, we get for the final product

$\mathbf{S_R} \approx [1 - (i\theta/2N)\ \mathbf{n.\ \sigma}]^N$

In the limit $N \to \infty$

$\mathbf{S_R} = \exp(-i\theta/2\ \mathbf{n.\ \sigma})$ (34)

We consider the special case of an infinitesimal rotation about the z-axis. This implies

$$R=\begin{pmatrix}1 & -\varepsilon & 0\\ \varepsilon & 1 & 0\\ 0 & 0 & 1\end{pmatrix} \tag{35a}$$

and

$$S=1-\frac{i}{2}\varepsilon\sigma_z \tag{35b}$$

Hence, by substituting equation (32) into (23), we obtain the necessary conditions

$$\sigma_z m_x - m_x\sigma_z = 2im_y \tag{36a}$$

$$\sigma_z m_y - m_y\sigma_z = -2im_x \tag{36b}$$

$$\sigma_z m_z - m_z\sigma_z = 0 \tag{36c}$$

Similarly, rotation about x and y-axis gives the rotations

$$\sigma_x m_y - m_y\sigma_x = 2im_z \tag{37a}$$

$$\delta_x m_z - m_z\delta_x = -2im_y \tag{37b}$$

$$\sigma_x m_x - m_x\sigma_x = 0 \tag{37c}$$

and

$$\sigma_y m_z - m_z\sigma_y = 2im_x \tag{38a}$$

$$\sigma_y m_x - m_x\sigma_y = -2im_z \tag{38b}$$

$$\sigma_y m_y - m_y\sigma_y = 0 \tag{38c}$$

Since $\boldsymbol{\sigma}$ is a vector operator, we may make the identification

$$\mathbf{M_y} = \boldsymbol{\sigma} \tag{39}$$

in equations (36)-(38). In this way we obtain a set of fundamental commutation relations which can be combined symbolically in the system equation

$$\boldsymbol{\sigma} \times \boldsymbol{\sigma} = 2i\boldsymbol{\sigma} \tag{40}$$

equation (39) encompasses the restrictions which the δ matrices must obey if matrices of the form expressed in equation (34) are to represent rotations. The matrices σ_x, σ_y, and σ_z are completely determined by the commutation relations and by the selection of the eigen spinors of σ_x as the basis spinors. σ_x, σ_y, and σ_z are the Pauli spin matrices. The spin matrices can be represented as

$$m_x=\sigma_x=\frac{1}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},\quad m_y=\sigma_y=\frac{1}{2}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix},\quad m_z=\sigma_z=\frac{1}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \tag{41}$$

We can obtain the eigenvectors

$$\phi_{m'_x}=\begin{bmatrix}A\\ B\end{bmatrix}\quad of\quad m'_x$$

and

$$\phi_{m'_y}=\begin{bmatrix}C\\ D\end{bmatrix}\quad of\quad m'_y$$

with eigenvalues m'_x and m'_y by solving the matrix eigenvalue equation:

$$\frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} A \\ B \end{bmatrix} = m'_x \begin{bmatrix} A \\ B \end{bmatrix}_x \tag{42a}$$

$$\frac{1}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} C \\ D \end{bmatrix} = m'_y \begin{bmatrix} C \\ D \end{bmatrix}_x \tag{42b}$$

The solutions are

$$\phi_{m'_x} = +\frac{1}{2} = \frac{1}{\sqrt{2}} e^{i\alpha_1}\begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \phi_{m'_x} = -\frac{1}{2} = \frac{1}{\sqrt{2}} e^{i\beta_1}\begin{bmatrix} 1 \\ -1 \end{bmatrix} \tag{43a}$$

$$\phi_{m'_y} = +\frac{1}{2} = \frac{1}{\sqrt{2}} e^{i\alpha_2}\begin{bmatrix} 1 \\ i \end{bmatrix}, \quad \phi_{m'_y} = -\frac{1}{2} = \frac{1}{\sqrt{2}} e^{i\beta_2}\begin{bmatrix} 1 \\ -i \end{bmatrix} \tag{43b}$$

and similarly, for m_z,

$$\phi_{m'_z} = +\frac{1}{2} = \frac{1}{\sqrt{2}} e^{i\alpha_3}\begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \phi_{m'_z} = -\frac{1}{2} = \frac{1}{\sqrt{2}} e^{i\beta_3}\begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{43c}$$

where the $\alpha\mathbf{M_y}$ and the $\beta\mathbf{M_y}$ are arbitrary phase angles.

If $\mathbf{M_y}$ is defined as a matrix

$$M_y = \frac{\beta}{2}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

we can determine the matrix elements of the rotation operator for states having j = ½ directly from equation (31b), where

$$M_y^{2n} = (-1)^n \left(\frac{\beta}{2}\right)^n \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \textit{and} \quad M_y^{2n+1} = (-1)^n \left(\frac{\beta}{2}\right)^{n+1} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \tag{44}$$

and n is an integer. Since, in the $[\mathbf{J}^2, \mathbf{J}_z]$ representation, $i\beta\mathbf{J}_y = M_y$, we have

$$\left\langle jm \left| e^{-i\beta J_y} \right| jm' \right\rangle = \begin{array}{c|cc} M & M' = 1/2 & -1/2 \\ \hline 1/2 & \cos\beta/2 & -\sin\beta/2 \\ -1/2 & \sin\beta/2 & \cos\beta/2 \end{array} \tag{45}$$

and

$$D^{\frac{1}{2}}(\alpha,\beta,\xi)=\begin{bmatrix} e^{-(i\frac{i}{2})\alpha}\cos(\frac{\beta}{2})e^{-(i\frac{i}{2})\xi} & -e^{-(i\frac{i}{2})\alpha}\sin(\frac{\beta}{2})e^{(i\frac{i}{2})\xi} \\ e^{(i\frac{i}{2})\alpha}\sin(\frac{\beta}{2})e^{-(i\frac{i}{2})\xi} & e^{(i\frac{i}{2})\alpha}\cos(\frac{\beta}{2})e^{(i\frac{i}{2})\xi} \end{bmatrix} \tag{46}$$

CONCLUSION

In this work, we have presented a Green's function approach to the solution of the time dependent NMR flow equation where the rf $B_1(t)$ field is treated as a complex valued function. The Fourier transform of the rf $B_1^*(t)$ gives an arbitrary function of the spin-spin relaxation parameter $g(T_2)$. This implies that any complex number is an allowed eigenvalue of the transverse magnetization, M_y. We determine the special states called coherent states for the system. It is very clear that the equilibrium magnetization M_o is complex and has a quantum mechanical value. This ensures a sufficient condition to be satisfied for finite rotations of M_y. It is easy to check from the analysis that the two eigenvectors of each of the operators m_x, m_y and m_z are normal, mutually orthogonal, and form a complex set, i.e. any arbitrary eigenvector can be written as a linear combination of the members of any one of these pairs of eigenvectors. The square moduli of the coefficients of such a linear combination give the probability of obtaining the particular value $\pm$ 1/2 of m'_x of m'_y of m'_z, according to the pair of eigenvector used. Thus, for example, since z - axis and the x - axis are perpendicular to each other, the probability of finding $m'_z = \pm$ 1/2 if a system is known to be in an eigenstate of m_x is equal to 1/2. The solutions to the time dependent NMR Bloch equation as presented by the Green's function approach have allowed us the use of general principle of semi classical mechanics to explore very useful information which can be invaluable in the design of a mathematical package which can include relaxation and other important NMR parameters.

Additionally, it may be noteworthy to mention that, the effects of a complex rf $B_1(t)$ field has deliberately, perhaps unintentionally been omitted in the literature. The actual relation of the density matrix calculations as discussed in an earlier study [16] to the NMR flow analysis can be more appreciated by solving the time dependent Bloch NMR equation with complex rf $B_1(t)$ field via the Green's function algorithm as discussed in this study.

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