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Research Article

Solution of the Bloch Equations including Relaxation

Eric R. Johnston

Department of Chemistry and Biochemistry, The University of North Carolina at Greensboro, Greensboro, NC, USA 27412

Correspondence should be addressed to Eric R. Johnston; erj3681@hotmail.com

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The magnetization differential equations of Bloch are integrated using a matrix diagonalization method. The solution describes several limiting cases and leads to compact expressions of wide validity for a spin ensemble initially at equilibrium.

1. Introduction

In 1949 Torrey used Laplace transforms to provide [1] the first solution of the differential equations proposed by Bloch [2] for the magnetization components of a spin ensemble. His results are somewhat cumbersome and contain some errors. Although the problem is fundamental, a general solution including relaxation does not appear in any of the standard NMR texts, with one partial exception [3]. The problem has been revisited several times employing third-order differential equations [4, 5] and Laplace transforms [6] to give unwieldy solutions using somewhat opaque derivations. The first-order differential equations are directly integrated here using a matrix diagonalization method.

2. Bloch Equations and Their Integration

The Bloch equations for a collection of identical spins $-(1/2)$ in the frame rotating at ω_{rf} are

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix} = -\mathbf{K}\begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ R_1 M_0 \end{pmatrix}, \quad (1)$$

where

$$\mathbf{K} = \begin{pmatrix} R_2 & \Delta & 0 \\ -\Delta & R_2 & \omega_1 \\ 0 & -\omega_1 & R_1 \end{pmatrix}. \quad (2)$$

R_1 and R_2 are the longitudinal and transverse relaxation rates in s^{-1}, and $\Delta = |\omega_0 - \omega_{rf}|$ and $\omega_1 = \gamma B_1$ are the resonance frequency offset and the rf amplitude for a B_1 field along the x-axis, in radians/s. γ is the (positive) gyromagnetic ratio, and M_0 is the equilibrium magnetization.

Defining a magnetization vector $V = \begin{pmatrix} M_x & M_y & M_z \end{pmatrix}^T$, the integrated solution of equation (1) is

$$V(t) = \exp(-\mathbf{K}t)[V(0) - V(ss)] + V(ss) = \mathbf{X} \cdot \exp(-\mathbf{D}t)\mathbf{X}^{-1}[V(0) - V(ss)] + V(ss), \quad (3)$$

where $\mathbf{K} = \mathbf{X}\,\mathbf{D}\mathbf{X}^{-1}$. The problem is, thus, deducing the roots of $\mathbf{K}(=\mathbf{D})$, the matrix $\mathbf{X}$ and inverse $\mathbf{X}^{-1}$ which diagonalize $\mathbf{K}$ and the steady-state magnetization vector $V(ss)$.

2.1. Evaluation of Roots. $|\mathbf{K} - \lambda \mathbf{1}| = 0$ gives the following cubic equation:

$$\lambda^3 - (R_1 + 2R_2)\lambda^2 + \left(R_2^2 + 2R_1R_2 + \Delta^2 + \omega_1^2\right)\lambda - \left(R_1R_2^2 + R_1\Delta^2 + R_2\omega_1^2\right) = 0. \quad (4)$$

Choosing roots of the form $\lambda_1 = a$, $\lambda_{2,3} = b \pm i\Omega$ gives the corresponding cubic equation:

$$(\lambda - a)\left(\lambda^2 - 2b\lambda + b^2 + \Omega^2\right) = \lambda^3 - (a + 2b)\lambda^2 + \left(b^2 + 2ab + \Omega^2\right)\lambda - a\left(b^2 + \Omega^2\right) = 0. \quad (5)$$

Equating the last term in equations (4) and (5), and with $R_2 < \omega_1$ and/or Δ in (4) and $b < \Omega$ in (5),

$$a = R_1 \cos^2\theta + R_2 \sin^2\theta \equiv R_\theta, \quad (6)$$

using $\tan\theta = (\omega_1/\Delta)$ and $\Omega \equiv (\Delta^2 + \omega_1^2)^{1/2}$.

b is obtained by equating the coefficients of the second term in equations (4) and (5):

$$b = \frac{1}{2}\left(R_1 + 2R_2 - R_\theta\right) = R_2 - \frac{1}{2}\left(R_2 - R_1\right)\sin^2\theta. \quad (7)$$

These expressions agree with Torrey ([1], equation 59) and with Abragam ([3]. p. 70).

For $R_2 = 1s^{-1}$ and ω_1 and/or $\Delta = 2\pi \times 10\,\text{Hz}$, for example, the above approach is valid and avoids the explicit solution of the cubic equation (4).

2.2. Calculation of **X**. **X** is obtained by evaluating the three cofactors of $\mathbf{K} - \lambda\mathbf{1}$ for $\lambda_1 = R_\theta$ and $\lambda_{2,3} = b \pm i\Omega$. Choosing the third row of $\mathbf{K} - \lambda\mathbf{1}$, the cofactors are

cofactor $1 = \Delta\omega_1$
cofactor $2 = -\omega_1 (R_2 - \lambda)$
cofactor $3 = (R_2 - \lambda)^2 + \Delta^2$

Omitting all (small) relaxation rate difference terms (which are exactly zero for $R_1 = R_2$) and dividing all elements by ω_1 gives **X**:

$$\mathbf{X} = \begin{pmatrix} \Delta & \Delta & \Delta \\ 0 & i\Omega & -i\Omega \\ \dfrac{\Delta^2}{\omega_1} & -\omega_1 & -\omega_1 \end{pmatrix}. \quad (8)$$

2.3. Calculation of $\mathbf{X}^{-1}$. $\mathbf{X}^{-1}$ is formed by constructing the matrix of all cofactors of **X**, taking the transpose, and dividing by the determinant $|\mathbf{X}|$ [7]. The result is

$$\mathbf{X}^{-1} = \frac{1}{2\Omega^2}\begin{pmatrix} \dfrac{2\omega_1^2}{\Delta} & 0 & 2\omega_1 \\ \Delta & -i\Omega & -\omega_1 \\ \Delta & i\Omega & -\omega_1 \end{pmatrix}. \quad (9)$$

These may be rewritten in a more compact form using $\tan\theta = (\omega_1/\Delta)$ and Ω:

$$\mathbf{X} = \begin{pmatrix} \cos\theta & \cos\theta & \cos\theta \\ 0 & i & -i \\ \dfrac{\cos\theta}{\tan\theta} & -\sin\theta & -\sin\theta \end{pmatrix}, \quad (10)$$

$$\mathbf{X}^{-1} = \frac{1}{2}\begin{pmatrix} 2\sin\theta\tan\theta & 0 & 2\sin\theta \\ \cos\theta & -i & -\sin\theta \\ \cos\theta & i & -\sin\theta \end{pmatrix}. \quad (11)$$

Finally, we calculate the matrix $\mathbf{A} = \mathbf{X}\exp(-\mathbf{D}t)\mathbf{X}^{-1}$:

$$\mathbf{A} = \mathbf{X}\begin{pmatrix} \exp - R_\theta t & & \\ & \exp - bt\,(c - is) & \\ & & \exp - bt\,(c + is) \end{pmatrix} \mathbf{X}^{-1}, \text{ where } \begin{matrix} c = \cos\Omega t \\ s = \sin\Omega t \end{matrix}. \quad (12)$$

The elements of **A** are

$$\begin{aligned} A_{11} &= \sin^2\theta \exp - R_\theta t + \cos^2\theta \exp - bt\cos\Omega t, \\ A_{22} &= \exp - bt\cos\Omega t, \\ A_{12} &= -A_{21} = -\cos\theta \exp - bt\sin\Omega t, \\ A_{23} &= -A_{32} = -\sin\theta \exp - bt\sin\Omega t, \\ A_{13} &= A_{31} = \sin\theta\cos\theta\left(\exp - R_\theta t - \exp - bt\cos\Omega t\right), \\ A_{33} &= \cos^2\theta \exp - R_\theta t + \sin^2\theta \exp - bt\cos\Omega t. \end{aligned} \quad (13)$$

2.4. Steady States. The steady-state magnetizations are found by setting equation (1) to zero and using Cramer's rule [7]:

$$M_x(\text{ss}) = \frac{R_1\Delta\omega_1 M_0}{d}, \quad (14)$$

$$M_y(\text{ss}) = \frac{-R_1 R_2 \omega_1 M_0}{d}, \quad (15)$$

$$M_z(\text{ss}) = \frac{R_1\left(R_2^2 + \Delta^2\right)M_0}{d}, \quad (16)$$

where $d = R_1 R_2^2 + R_1\Delta^2 + R_2\omega_1^2$.

For $R_2 < \omega_1$ and/or Δ, these may be simplified using equation (6):

$$M_x(\text{ss}) \longrightarrow \left(\frac{R_1}{R_\theta}\right)\sin\theta\cos\theta M_0, \quad (17)$$

$$M_y(\text{ss}) \longrightarrow -\frac{R_1 R_2 \sin\theta}{R_\theta \Omega} M_0 \approx 0, \quad (18)$$

$$M_z(\text{ss}) \longrightarrow \left(\frac{R_1}{R_\theta}\right)\cos^2\theta M_0. \quad (19)$$

The integrated solution equation (3) for the initial condition $M_z(0) = M_0$ is

$$M_x(t) = A_{13}M_0 - A_{11}M_x(\mathrm{ss}) - A_{12}M_y(\mathrm{ss}) - A_{13}M_z(\mathrm{ss}) + M_x(\mathrm{ss}), \quad (20)$$

$$M_y(t) = A_{23}M_0 - A_{21}M_x(\mathrm{ss}) - A_{22}M_y(\mathrm{ss}) - A_{23}M_z(\mathrm{ss}) + M_y(\mathrm{ss}), \quad (21)$$

$$M_z(t) = A_{33}M_0 - A_{31}M_x(\mathrm{ss}) - A_{32}M_y(\mathrm{ss}) - A_{33}M_z(\mathrm{ss}) + M_z(\mathrm{ss}). \quad (22)$$

In the absence of relaxation, these are the well-known Bloch equations [8, 9]:

$$M_x(t) = A_{13}M_0 = \sin\theta\cos\theta M_0(1 - \cos\Omega t), \quad (23)$$

$$M_y(t) = A_{23}M_0 = -\sin\theta M_0 \sin\Omega t, \quad (24)$$

$$M_z(t) = A_{33}M_0 = \cos^2\theta M_0 + \sin^2\theta M_0 \cos\Omega t. \quad (25)$$

3. Results

Limiting forms of equation (3) are discussed in this section.

3.1. Case 1: Resonant Nutation $\Delta = \cos\theta = 0, b = (R_1 + R_2)/2$, and $M_z(0) = M_0$.

$$\begin{aligned} A_{11} &= \exp - R_2 t, \\ A_{12} &= A_{21} = A_{13} = A_{31} = 0, \\ A_{22} &= A_{33} = \exp - bt\cos\omega_1 t, \\ A_{23} &= -A_{32} = -\exp - bt\sin\omega_1 t, \end{aligned} \quad (26)$$

$$\begin{aligned} M_x(\mathrm{ss}) &= M_x(t) = 0, \\ M_y(\mathrm{ss}) &= -\left(\frac{R_1}{\omega_1}\right)M_0, \\ M_z(\mathrm{ss}) &= \left(\frac{R_1R_2}{\omega_1^2}\right)M_0, \end{aligned} \quad (27)$$

$$M_y(t) = A_{23}M_0 + M_y(\mathrm{ss})[1 - A_{22}] - A_{23}M_z(\mathrm{ss}), \quad (28)$$

$$M_z(t) = A_{33}M_0 + M_z(\mathrm{ss})[1 - A_{33}] - A_{32}M_y(\mathrm{ss}). \quad (29)$$

M_y and M_z interconvert at rate ω_1 and decay to (small) steady states.

3.2. Case 2: Free Precession/M_z Relaxation $\omega_1 = \sin\theta = 0$ and $M_x(0) = M_z(\mathrm{ss}) = M_0$.

$$\begin{aligned} A_{11} &= A_{22} = \exp - R_2 t\cos\Delta t, \\ A_{12} &= -A_{21} = -\exp - R_2 t\sin\Delta t, \\ A_{13} &= A_{31} = A_{23} = A_{32} = 0, \\ A_{33} &= \exp - R_1 t, \end{aligned} \quad (30)$$

$$\begin{aligned} M_x(t) &= A_{11}M_0 = M_0\exp - R_2 t\cos\Delta t, \\ M_y(t) &= A_{21}M_0 = M_0\exp - R_2 t\sin\Delta t, \\ M_z(t) &= -A_{33}M_0 + M_z(\mathrm{ss}) = M_0(1 - \exp - R_1 t). \end{aligned} \quad (31)$$

M_x and M_y interconvert at rate Δ and decay to zero as M_z returns to equilibrium.

3.3. Case 3: Spin-Locked Relaxation $M_x(0) = \sin\theta M_0$, $M_z(0) = \cos\theta M_0$, and $M_y(\mathrm{ss}) \approx 0$.

$$\begin{aligned} M_x(t) &= A_{11}\sin\theta M_0 + A_{13}\cos\theta M_0 - A_{11}M_x(\mathrm{ss}) - A_{13}M_z(\mathrm{ss}) + M_x(\mathrm{ss}), \\ M_y(t) &= A_{21}\sin\theta M_0 + A_{23}\cos\theta M_0 - A_{21}M_x(\mathrm{ss}) - A_{23}M_z(\mathrm{ss}), \\ M_z(t) &= A_{31}\sin\theta M_0 + A_{33}\cos\theta M_0 - A_{31}M_x(\mathrm{ss}) - A_{33}M_z(\mathrm{ss}) + M_z(\mathrm{ss}). \end{aligned} \quad (32)$$

Employing the steady states of equations (17)–(19), these become

$$\begin{aligned} M_x(t) &= \sin\theta M_0\exp - R_\theta t + \left(\frac{R_1}{R_\theta}\right)\sin\theta\cos\theta M_0[1 - \exp - R_\theta t], \\ M_y(t) &= 0, \\ M_z(t) &= \cos\theta M_0\exp - R_\theta t + \left(\frac{R_1}{R_\theta}\right)\cos^2\theta M_0[1 - \exp - R_\theta t]. \end{aligned} \quad (33)$$

The magnetization vector relaxes to a steady state along the effective field $B_{\mathrm{eff}} = (\Omega/\gamma)$ [10, 11].

3.4. Case 4: General Solution $M_z(0) = M_0$.

Equations (20)–(22) may be recast using the steady states of equation (17)–(19) as

$$\begin{aligned} M_x(t) &= A_{13}M_0 + M_x(\mathrm{ss})[1 - \exp - R_\theta t], \\ M_y(t) &= A_{23}M_0, \\ M_z(t) &= A_{33}M_0 + M_z(\mathrm{ss})[1 - \exp - R_\theta t]. \end{aligned} \quad (34)$$

These expressions agree with equations (60)–(62) of Torrey [1] and with Abragam [3].

For a weak rf field $\omega_1 < \Delta$ $(\cos\theta \longrightarrow 1, \sin^2\theta \longrightarrow 0)$, they reduce to

$$M_x(t) = \left(\frac{\omega_1}{\Delta}\right) M_0 (1 - \exp - R_2 t \cos \Delta t),$$
$$M_y(t) = -\left(\frac{\omega_1}{\Delta}\right) M_0 \exp - R_2 t \sin \Delta t, \quad (35)$$
$$M_z(t) \approx M_0,$$

in agreement with Slichter ([12], p. 35).

3.5. Case 5: Equal Relaxation Rates $R_\theta = b = R$, $M_z(0) = M_0$. An exact solution of the Bloch equations is given by equations (20)–(22) using the full steady-state expressions (14)–(16). Using the steady states of equation (17)–(19), they become

$$M_x(t) = \sin\theta \cos\theta M_0 (1 - \exp - Rt \cos \Omega t),$$
$$M_y(t) = -\sin\theta M_0 \exp - Rt \sin \Omega t, \quad (36)$$
$$M_z(t) = \cos^2\theta M_0 + \sin^2\theta M_0 \exp - Rt \cos \Omega t.$$

4. Discussion

Equation (3) describes a number of experimental situations.

4.1. Case 1: Resonant Nutation. Resonant nutation (equations (28) and (29)) was described by Torrey in his original paper [1]. The effective relaxation rate is the average of the longitudinal and transverse relaxation rates [3].

4.2. Case 2: Free Precession and Relaxation. In the absence of an rf field, the transverse components interconvert and relax to zero (the free induction decay) as the longitudinal component, initially zero, relaxes independently to equilibrium (equation (31)).

4.3. Case 3: Spin-Locked Relaxation. Orientation of the magnetization vector parallel to the effective field suppresses precession and results in a single-exponential approach to equilibrium, affording the longitudinal and transverse relaxation rates using equations (6) and (33) [10, 11].

4.4. Case 4: General Solution. Equation (34) presents in compact form the solutions originally given by Torrey [1] and by Morris and Chilvers [6] as Laplace expressions and the tabulations of Madhu and Kumar [4, 5] for a spin ensemble initially at equilibrium. They are valid provided

$$R_2\left(s^{-1}\right) < \Omega\left(\text{rad}\, s^{-1}\right), \quad (37)$$

which holds for most cases of practical interest. In the example given by Madhu and Kumar [4, 5],

$$R_1 = 10\, s^{-1},$$
$$R_2 = 100\, s^{-1}, \quad (38)$$
$$\Delta = \omega_1 = 2\pi \times 1\, \text{kHz}.$$

Accordingly, from equations (6), (7), and (17)–(19),

$$R_\theta = 55\, s^{-1},$$
$$b = 77.5\, s^{-1},$$
$$\Omega = 2\pi \times 1414\, \text{Hz}, \quad (39)$$
$$M_x(ss) = M_z(ss) = \frac{M_0}{11},$$
$$M_y(ss) = -\frac{M_0}{(110 \times 2\pi)} \approx 0.$$

These values do not appear to reproduce the figures presented in [5].

4.5. Case 5: Equal Relaxation Rates. The solutions (20)–(22) for equal relaxation rates are exact provided the full steady states of equation (14)–(16) are used. The inequality of Case 4 leads to the simpler expressions (36). We note also that setting $\omega_1 = \sqrt{2}\Delta$ results in $R_\theta = b = (R_1 + 2R_2)/3$.

4.6. Neglect of Relaxation. For rf amplitude and precession terms which are large compared to relaxation rates equations (23)–(25) pertain. They are useful, for example, in describing selective (on-resonance) excitation with (off-resonance) signal suppression [9] as in the following example (using Hz units).

4.6.1. On-Resonance Rotation

$$\cos\theta \longrightarrow 0,$$
$$\nu_1 t_p = \frac{1}{4}, \quad (40)$$
$$M_y(t_p) = -M_0,$$
$$M_x(t_p) = M_z(t_p) = 0.$$

4.6.2. Off-Resonance Rotation

$$\Omega t_P = 1,$$
$$M_z(t_P) = M_0,$$
$$M_x(t_P) = M_y(t_P) = 0, \quad (41)$$
$$\Omega t_p = 1 \text{ requires } \Delta t_p = \frac{\sqrt{15}}{4} \text{ so } t_p = \frac{\sqrt{15}}{4\Delta}\text{ sec.}$$

Then, $\nu_1 = (1/4t_p) = (\Delta/\sqrt{15})$Hz.

For a 5 KHz offset $t_p = 193.6\,\mu$sec and $\nu_1 = 1291$Hz.

The on-resonance magnetization is rotated to the $-y$ axis by the rf pulse, whereas the off-resonance magnetization undergoes an excursion that returns it to the z-axis.

5. Conclusion

The differential equations (1) of Bloch [2] are integrated with a matrix diagonalization method to give the solution equation (3). It correctly describes a number of experimental situations including resonant nutation, free precession and relaxation, and spin-locked relaxation. Equation (3) is exact for the case of equal longitudinal and transverse relaxation rates and leads to the general equation (34) for a spin ensemble initially at equilibrium.

Data Availability

No data were used to support this study.

Conflicts of Interest

The author declares that there are no conflicts of interest.

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