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Rabi resonance in spin systems: Theory and experiment

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ABSTRACT

The response of a magnetic resonance spin system is predicted and experimentally verified for the particular case of a continuous wave amplitude modulated radiofrequency excitation. The experimental results demonstrate phenomena not previously observed in magnetic resonance systems, including a secondary resonance condition when the amplitude of the excitation equals the modulation frequency. This secondary resonance produces a relatively large steady state magnetisation with Fourier components at harmonics of the modulation frequency. Experiments are in excellent agreement with the theoretical prediction derived from the Bloch equations, which provides a sound theoretical framework for future developments in NMR spectroscopy and imaging.

1. Introduction

Excitation of magnetic resonance systems is typically achieved using short radiofrequency (RF) pulses with relatively high power in the order of kilowatts. Pulsed techniques predominantly replaced early continuous wave (CW) methods [1–3] due to their improved sensitivity and efficiency [4]. Recently, there has been renewed interest in CW techniques for magnetic resonance imaging (MRI) [5–7], largely motivated by the need to image samples with very short relaxation times. Continuous wave alternatives to the pulsed excitation paradigm are particularly advantageous for MRI, as opposed to spectroscopy, since the object is relatively large and thus high RF power is required to produce uniform flip angles using pulsed excitation methods.

In this work we demonstrate proof-of-concept measurements of the magnetisation during a CW excitation with an amplitude envelope modulated by a sinusoid. We measure the steady state magnetisation waveform and observe substantial frequency components at harmonics of the modulation frequency. Furthermore, we demonstrate that the steady state signal is maximum when the amplitude of the RF field equals the modulation frequency, establishing a secondary resonance condition that is analogous to resonance at the Larmor frequency.

Periodic modulation in NMR has been previously considered in numerous works. For example, Redfield observed a similar secondary resonance when the Rabi frequency of an RF field matched the frequency of an external magnetic field oscillating in the direction of the B_0 field [8]. Floquet theory was applied to systems consisting of an RF field with multiple frequencies in [9] and later generalised to solid-state NMR of rotating samples, where secondary resonances exist with respect to the sample spinning frequency, e.g. [10–12].

To our knowledge, the work presented here is the first experimental demonstration of such phenomena using an amplitude modulated RF field and provides a magnetic analogue of work in quantum optics. In the context of optics, Cappeller and Müller [13] considered a two-level atom excited with a sinusoidally varying phase and demonstrated a secondary resonance condition they termed 'Rabi resonance'. Specifically, they showed an increase in the atom's response when the rate of phase change is equal to the Rabi frequency. An amplitude modulated field was examined in [14] where the first six subharmonics of the Rabi frequency were observed experimentally. The second harmonic response to a phase modulated excitation has also been used as feedback to stabilise the intensity of an electromagnetic field [15,16].

The novel magnetisation behaviour we demonstrate here arises from the nonlinear interaction of the RF field with the bulk magnetisation, accentuated by the use of an amplitude modulated CW pulse. Traditionally, pulsed techniques as well as continuous wave techniques such as stochastic MRI [5] and 'sweep imaging with Fourier transformation' [7] have assumed that the spin system can be treated in a linear time invariant framework. Indeed a focus of early work in spectroscopy was to ensure the linearity assumption remained valid to avoid distortion in the spectra, e.g. [17]. Although the system is approximately linear under certain conditions [18], it is our goal to investigate and exploit the nonlinear interactions.

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The nonlinear features of the spin system are intrinsically interesting in their own right although we also envisage practical applications. For example, improved isolation between the transmitted and received signal can be achieved by transmitting at one frequency and receiving at a harmonic frequency. The two signals are separated in frequency, which allows digital or analog filters to extract only the signal of interest. This is particularly important in continuous wave NMR applications since the desired signal is orders of magnitude smaller than the transmitted RF signal [7].

A theoretical analysis and averaging solution of the Bloch equations were presented for a similar excitation in [19,20]. The contribution here is twofold. First, we obtain experimental magnetic resonance data verifying the theoretical results. Secondly, we extend the analytic results to more general excitation and provide an explicit solution in terms of Bessel functions.

2. Theory

We consider a radiofrequency field oscillating at the Larmor frequency with an amplitude modulated envelope given by

$$\omega_e(t) = \omega_1(1 + \alpha\cos(\omega_m t)), \tag{1}$$

where $\omega_1 = \gamma B_1$, γ is the gyromagnetic ratio, B_1 is the amplitude of the RF field without modulation, α is the modulation factor and ω_m is the modulation frequency. The frequencies ω_1 and ω_m defining the signal envelope are small compared to the Larmor frequency of the static field.

The starting point for the theoretical analysis of the response to amplitude modulated RF is the Bloch equation in the rotating frame of reference,

$$\begin{bmatrix} \dot{m}_x \\ \dot{m}_y \\ \dot{m}_z \end{bmatrix} = \begin{bmatrix} -R_2 & \Delta & 0 \\ -\Delta & -R_2 & \omega_e(t) \\ 0 & -\omega_e(t) & -R_1 \end{bmatrix} \begin{bmatrix} m_x \\ m_y \\ m_z \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ R_1 \end{bmatrix} \tag{2}$$

where R_1 and R_2 are the relaxation rates representing spin–lattice and spin–spin relaxation, respectively, and Δ is any deviation from the Larmor frequency including inhomogenities, gradients and off-resonant excitation. Without loss of generality, we have assumed an equilibrium magnetisation of unity and zero RF phase, equivalent to excitation along the x-axis in the rotating frame.

An approximate analytical solution can be found for the case of on-resonance excitation, $\Delta = 0$. First, we consider the Bloch equation in an excitation dependent reference frame given by the transformation,

$$\begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos s(t) & -\sin s(t) \\ 0 & \sin s(t) & \cos s(t) \end{bmatrix} \begin{bmatrix} m_x \\ m_y \\ m_z \end{bmatrix} \tag{3}$$

where

$$s(t) = \omega_m t + \alpha\frac{\omega_1}{\omega_m}\sin(\omega_m t). \tag{4}$$

The form of $s(t)$ in Eq. (4) is chosen such that $\omega_e(t) - \dot{s}(t) = \omega_1 - \omega_m$, which removes the time dependence of the excitation and leads to an analytical solution. Other rotating coordinate systems have been used in previous NMR studies to simplify mathematical analyses, e.g. [8,21,22]. The transformed equation, derived in Appendix A, is

$$\begin{bmatrix} \dot{n}_x \\ \dot{n}_y \\ \dot{n}_z \end{bmatrix} = \begin{bmatrix} -R_2 & 0 & 0 \\ 0 & f_a(t) & f_c(t) \\ 0 & f_d(t) & f_b(t) \end{bmatrix} \begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix} + \begin{bmatrix} 0 \\ -R_1\sin s(t) \\ R_1\cos s(t) \end{bmatrix} \tag{5}$$

where

$$f_a(t) = -R_2\cos^2 s(t) - R_1\sin^2 s(t) \tag{6}$$

$$f_b(t) = -R_1\cos^2 s(t) - R_2\sin^2 s(t) \tag{7}$$

$$f_c(t) = \frac{R_1 - R_2}{2}\sin(2s(t)) + \omega_1 - \omega_m \tag{8}$$

$$f_d(t) = \frac{R_1 - R_2}{2}\sin(2s(t)) - (\omega_1 - \omega_m). \tag{9}$$

The Bloch equation in this reference frame, while appearing more complicated, represents a slowly varying signal and is therefore amenable to periodic averaging techniques from nonlinear systems theory [23]. This requires calculating the averages of the sinusoid terms in Eqs. (5)–(9). As calculated in Appendix B, the average of $\sin s(t)$ and $\sin(2s(t))$ are zero and the remaining averages are

$$\overline{\cos s(t)} = -J_1\left(\frac{\alpha\omega_1}{\omega_m}\right) \tag{10}$$

$$\overline{\cos^2 s(t)} = \frac{1}{2}\left(1 + J_2\left(\frac{2\alpha\omega_1}{\omega_m}\right)\right) \tag{11}$$

$$\overline{\sin^2 s(t)} = \frac{1}{2}\left(1 - J_2\left(\frac{2\alpha\omega_1}{\omega_m}\right)\right) \tag{12}$$

where $\overline{}$ represents the average and J_k denotes the Bessel function of the first kind of order k. The averaged equation can be written concisely as

$$\begin{bmatrix} \dot{n}_x \\ \dot{n}_y \\ \dot{n}_z \end{bmatrix} = \begin{bmatrix} -R_2 & 0 & 0 \\ 0 & -R_a & \omega_1 - \omega_m \\ 0 & -(\omega_1 - \omega_m) & -R_b \end{bmatrix} \begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ R_c \end{bmatrix} \tag{13}$$

where

$$R_a = R_2\,\overline{\cos^2 s(t)} + R_1\,\overline{\sin^2 s(t)} \tag{14}$$

$$R_b = R_1\,\overline{\cos^2 s(t)} + R_2\,\overline{\sin^2 s(t)} \tag{15}$$

$$R_c = R_1\,\overline{\cos s(t)}. \tag{16}$$

The average solution in this reference frame is denoted $\boldsymbol{n}(t) = [n_x(t),\ n_y(t),\ n_z(t)]^T$ and consists of a steady state component, $\boldsymbol{n}_{ss}$, and a transient component, $\boldsymbol{n}_t$, such that

$$\boldsymbol{n}(t) = \boldsymbol{n}_{ss} + \boldsymbol{n}_t(t). \tag{17}$$

The steady state solution is found by assigning the lefthand side of Eq. (13) to zero and solving the resulting linear matrix equation. This gives

$$\boldsymbol{n}_{ss} = \frac{R_c}{R_aR_b + (\omega_1 - \omega_m)^2}\begin{bmatrix} 0 \\ \omega_1 - \omega_m \\ R_a \end{bmatrix}. \tag{18}$$

The magnitude of $\boldsymbol{n}_{ss}$ is maximum when the RF amplitude equals the modulation frequency, i.e. $\omega_1 = \omega_m$. Furthermore, a transformation of Eq. (18) back to the traditional rotating frame of reference does not change the signal amplitude. Therefore, the measured steady state response will also be maximum when $\omega_1 = \omega_m$, defining a secondary resonance condition referred to as Rabi resonance, as has previously been demonstrated in optical systems [14].

The transient response, $\boldsymbol{n}_t(t)$, is found by directly solving the coupled differential equations in Eq. (13) with an initial magnetisation of unity along the z-axis. The three elements of $\boldsymbol{n}_t$ are

$$n_{t,x}(t) = 0 \tag{19a}$$

$$n_{t,y}(t) = \frac{e^{-R_p t}}{\xi}(\omega_1 - \omega_m)\left[(1 - CR_p)\sinh(\xi t) - C\xi\cosh(\xi t)\right] \tag{19b}$$