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ScienceDirect
Journal of Magnetic Resonance 182 (2006) 308–314
JMR Journal of Magnetic Resonance
www.elsevier.com/locate/jmr

Field propagation phenomena in ultra high field NMR: A Maxwell–Bloch formulation

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Received 9 April 2006; revised 7 July 2006
Available online 1 August 2006

Abstract

The principal advantage of NMR at high field is the concomitant increase in signal-to-noise ratio (SNR). This can be traded for improved spatial resolution and combined with parallel imaging to achieve higher temporal resolution. At high field strength, the RF-wavelength and the dimension of the human body complicate the development of NMR coils. For example, at 7 T, the wavelength in free space corresponds to about 1 m. The dielectric constant in tissue with a high water content can be as high as 70 and at a larmor frequency of 300 MHz, this corresponds to a wavelength inside tissue of less than 15 cm. The operating wavelength is thus comparable to the diameter of most body parts. To this end, both temporal and spatial variations of the excitation field must be taken into account in addition to the expected increase in conductivity. For all these reasons, we find the propagation of radiation at ultra high fields (>4 T) new phenomena commonly observed in quantum optics but traditionally negligible in NMR such as phase modulation of the excitation field such that the identity between pulse area and flip angle is no longer valid. In this paper, the emergence of field propagation phenomena in NMR experiments is analytically and numerically demonstrated. It is shown that in addition to the well-studied dielectric resonance phenomena at high magnetic fields (>4 T), field propagation effects transform the excitation pulse into an adiabatic excitation. The high field strength also mean that nonlinear effects such as self-induced transparency are now possible in NMR experiments.

Keywords: Quantum optics; Photon echoes; Spin resonance; Dielectric resonance

1. Introduction

The NMR Bloch equations govern the effect that a coherent RF excitation has on a spin system in equilibrium under the influence of an applied main homogeneous field B_0. The RF field thus acts as a driving source for the spins perturbing this equilibrium situation. However, at ultra high magnetic fields strengths (>4 T), the wavelength of the propagating excitation field decreases. The wavelength decreases even further in biological tissues, since many biological samples have high relative dielectric constants (ε_r). For example, gray matter $\varepsilon_r = 56.2$, cerebrospinal fluid $\varepsilon_r = 70.3$, while the water/saline relative dielectric constant is 78 [1]. Hence the higher water content in tissue corresponds to a higher dielectric constant for that tissue. The high dielectric constant of tissue coupled with the reduced excitation pulse wavelength due to the high field strength lead to an even smaller wavelength that is on the order of the imaging field of view (FOV) such that field propagation effects become significant. For example, the electromagnetic wavelength at 7 T (300 MHz) is 1 m in free space, but only 14 cm in the head assuming an averaged relative dielectric constant of 49 for brain tissue. We thus find, where propagation of radiation is studied, new phenomena hitherto unknown in low field magnetic resonance experiments.

To this end, it is necessary to include Maxwell's wave equations where the spins in turn act as a source term for the propagating electromagnetic field. It is this coupled system of spins and electromagnetic fields that provide a full interaction picture in the NMR sample at high field strengths. To date, most research in this area has focused on the interaction between the RF pulse and the high

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doi:10.1016/j.jmr.2006.07.007

permittivity of the imaging sample whose dimension is comparable to the wavelength of electromagnetic fields at the resonant frequency for which B_1 inhomogeneity is significant. This B_1 inhomogeneity has to date been entirely attributed to the phenomena of dielectric resonance [2–4], a form of resonant cavity effect. It will be shown in detail in the next paper that the dielectric resonance arises from a resonant cavity set up by the index mismatch between the sample and air interfaces. It will be shown that such a formulation renders itself well to novel ways of mitigating this effect by dampening the resonance. Here we introduce another component of the phase modulation phenomena that arises entirely from the propagation of the excitation field across the sample in a single pass.

2. Excitation propagation effects

In general, the excitation RF field in an NMR medium is not affected by the transient response of the medium or is assumed negligible. This is a reasonable approximation if the medium is 'thin' such that no appreciable distortion of the exciting pulse can happen in propagating through the medium.

We have previously shown that higher field NMR (>4 T) can be formulated as a diffraction off a spatial-spectral holographic grating [5,6]. The spectral component arises naturally from the imposed gradient fields or due to the intrinsic chemical anisotropy of the sample. We showed that the spatial holographic component arises from a high dielectric constant (>50) of the NMR medium at high field strength when the excitation wavelength is commensurate with the size of the NMR sample. This results in the emergence of the propagation wave vector $\vec{k}$ in NMR and its far reaching consequences to the phase dispersion of the excitation field as it propagates in the sample.

For an imaging FOV that is larger than the wavelength (thick material), it is necessary to account for the material's effect on the propagating field. In typical imaging applications, up to about 2 T, the solution to the Bloch equations can assume that the material does not act on the propagating field. This is only a good approximation when the absorption length of the material is small and it therefore has a minor effect on the propagating field. For thicker materials or equivalently for ultra high fields, this is not true and the effect of the material polarization on the field must be considered in order to take into account absorption and emission in the material. The medium's impact on the propagating field can be determined using Maxwell's wave equation. First, let us assume the following form for the propagating RF excitation field in the laboratory frame:

$$B_1'(t,\vec{r}) = B^{e}(t,\vec{r})e^{i[\vec{k}\cdot\vec{r}-\omega_0 t+\phi(t,\vec{r})]} + c.c, \tag{1}$$

where $\vec{r} = \hat{x} + i\hat{y}$ and with $B^{e}(t,\vec{r})$ as the excitation pulse envelope. The prime notation $B_1'(t,\vec{r})$ is used to distinguish it from the one in the rotating frame which we will adopt shortly throughout the rest of this paper. Note that both the propagation wave vector $\vec{k}$ and the spatially varying phase $\phi(t,\vec{r})$ of the excitation field are new to NMR. The transverse magnetic polarization vector arising from this excitation field is thus given by:

$$M_{x',y'}(t,\vec{r}) = \tfrac{1}{2}\{[M_{x'}(t,\vec{r}) + iM_{y'}(t,\vec{r})]e^{i[\vec{k}\cdot\vec{r}-\Delta\omega t+\phi(t,\vec{r})]} + c.c\}, \tag{2}$$

where $M_{x'}$ and $M_{y'}$ are the in phase and quadrature components of the magnetic polarization and where $\Delta\omega = \omega - \omega_0$ is the off-resonance component in a rotating frame at a rate $\omega_0 = \gamma B_0$. Plugging these last two equations into Maxwell's wave equation,

$$\nabla^2 B_1(t,\vec{r}) - \frac{n^2}{c^2}\frac{\partial^2 B_1(t,\vec{r})}{\partial t^2} = \frac{4\pi}{c^2}\frac{\partial^2 M}{\partial t^2} \tag{3}$$

and equating real (in-phase) and imaginary (quadrature) components, one gets

$$(K^2 - K^2)B^{e}(t,\vec{r}) = 2\pi k^2 Dp \times \int_{-\infty}^{\infty} M_{x'}(t,\vec{r};\Delta\omega)g(\Delta\omega)\,d\Delta\omega, \tag{4}$$

$$2\left[\vec{K}\cdot\frac{\partial B^{e}(t,\vec{r})}{\partial\vec{r}} + \frac{k}{c}\frac{\partial B^{e}(t,\vec{r})}{\partial t}\right] = -2\pi k^2 Dp\int_{-\infty}^{\infty} M_{y'}(t,\vec{r};\Delta\omega)g(\Delta\omega)\,d\Delta\omega, \tag{5}$$

where $g(\Delta\omega)$ is the normalized inhomogeneous broadening linewidth function (usually a Gaussian distribution), D is the spin density, p is the spin matrix element of a two-level transition (for example proton spectroscopy) and $\Delta\omega$ is the detuning or off-resonance frequency component. The use of the slowly varying envelope approximation is liberally applied as

$$\nabla^2 B^{e}(t,\vec{r}) \ll |K|^2\frac{\partial^2 B^{e}(t,\vec{r})}{\partial t^2} \ll \omega^2 B^{e}(t,\vec{r}) \tag{6}$$

and

$$\frac{\partial M_{x'}(t,\vec{r})}{\partial t} \ll 2\pi k^2 M_{y'}(t,\vec{r}), \quad \frac{\partial^2 M_{y'}(t,\vec{r})}{\partial t} \ll 2\pi k^2 M_{x'}(t,\vec{r}). \tag{7}$$

Here $k \equiv 2\pi/\lambda$ is the vacuum wave vector and $|K|^2 = k_x^2 + k_y^2 + k_z^2$ is the square of the material wave vector. Inhomogeneous linewidth broadening whether due to intrinsic chemical shift anisotropy or due to imposed gradient fields leads to a degeneration of the two-level spin system corresponding to a range of resonant frequencies as shown in Fig. 1.

Now, returning to the NMR torque equation in the rotating frame (at $\omega_0 = \gamma B_0$), and with the transformation of the circularly polarized excitation field into the rotating frame so that $B_1'(t,\vec{r}) = B_1(t,\vec{r})\hat{x}$ we have

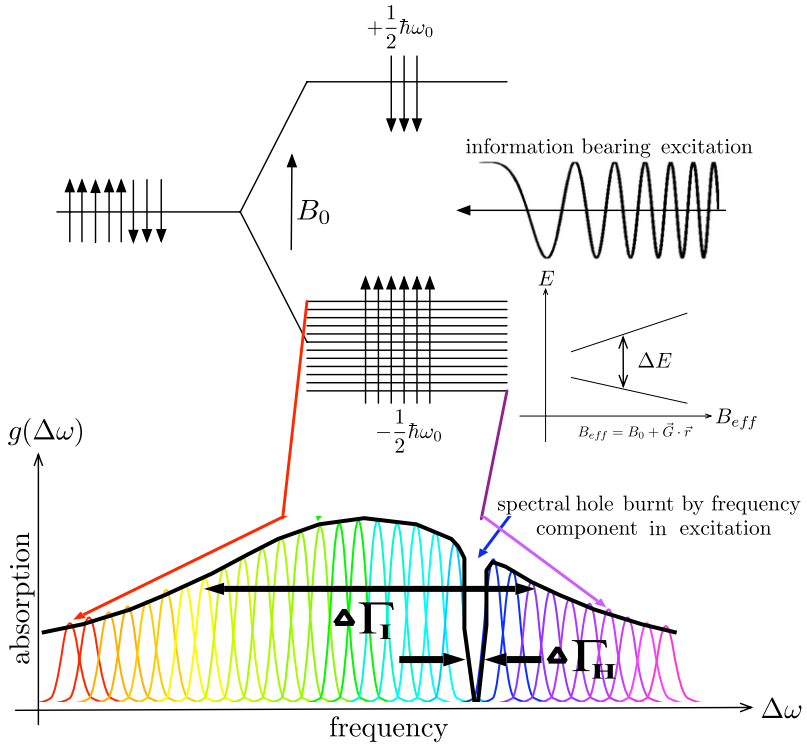

Fig. 1. Gradient induced inhomogeneous broadening of an NMR sample with an inhomogeneous bandwidth that is given by $\Gamma_I = \vec{G}\cdot\vec{r}$. An excitation pulse resonantly excites portions of the absorption spectrum coincident with its bandwidth. The spectral content of the excitation is thus stored in the absorption profile as an ensemble of spectral holes corresponding to the bandwidth of the excitation.

$$\frac{d\vec{M}}{dt} = \vec{M}\times\left[\gamma B_1(t,\vec{r})\hat{x}' + \overbrace{\left(\vec{k}\cdot\vec{r}+\Delta\omega+\frac{\partial\phi(t,\vec{r})}{\partial t}\right)}^{\Delta}\hat{z}\right] - \frac{(M_x\hat{x}'+M_y\hat{y}')}{T_2} - \frac{(M_z-M_0)\hat{z}}{T_1}, \tag{8}$$

where $\vec{M} = M_x\hat{x}' + M_y\hat{y}' + M_z\hat{z}'$ is the total macroscopic polarization vector and $(\hat{x}',\hat{y}',\hat{z})$ are the unit vector in the rotating frame pivoted on axis $\hat{z}$ and Δ is the total detuning parameter.

The effective off-resonance frequency and instantaneous propagation wave vector in this rotating frame are given by

$$\omega_e = \Delta\omega + \frac{\partial\phi(t,\vec{r})}{\partial t} \tag{9}$$

and

$$\vec{k}_e = \vec{k} + \frac{\partial\phi(t,\vec{r})}{\partial\vec{r}}, \tag{10}$$

respectively.

In the presence of damping, the modified Bloch equation in a rotating frame, is written out completely in component form as

$$\frac{dM_x'}{dt} = M_y'\left(\vec{k}\cdot\vec{r}+\Delta\omega+\frac{\partial\phi(t,\vec{r})}{\partial t}\right) - \frac{M_x'}{T_2}, \tag{11}$$

$$\frac{dM_y'}{dt} = -M_x'\left(\vec{k}\cdot\vec{r}+\Delta\omega+\frac{\partial\phi(t,\vec{r})}{\partial t}\right) + \gamma B_1(t,\vec{r})M_z - \frac{M_y'}{T_2}, \tag{12}$$

$$\frac{dM_z}{dt} = -\gamma B_1(t,\vec{r})M_y' + \frac{M_0-M_2}{T_1}, \tag{13}$$

and M_x', M_y', and M_z are strongly restricted by the probability

$$M_x'^2 + M_y'^2 + M_z^2 = \text{constant}, \tag{14}$$

which is valid over time intervals short compared to T_1 and T_2. If T_1 and T_2 are both much longer than the excitation pulse duration, damping may be ignored altogether and

$$M_x'^2 + M_y'^2 + M_z^2 = 1 \tag{15}$$

may be used for the conservation of probability. Combining Eqs. (4), (5), (7), and (11)–(13) yields

$$\vec{K}\cdot\nabla B^e(t,\vec{r}) + \frac{kn}{c}\frac{\partial B^e(t,\vec{r})}{\partial t} = -2\pi k^2 Dp \times\int_{-\infty}^{\infty} M_y(\Delta\omega,\vec{r},t)g(\Delta\omega)\,d\Delta\omega \tag{16}$$

and

$$\frac{\partial\phi(t,\vec{r})}{\partial x} = 2\pi k^2 Dp\int_{-\infty}^{\infty} M_x(t,\vec{r})g(\Delta\omega)\,d\Delta\omega. \tag{17}$$

Eqs. (16) and (17) along with the inhomogeneous Bloch equations (11)–(13) give us a complete system of equations for analyzing material responses due to a propagating field whose frequency bandwidth spans the larmor resonance. These modified equations are similar in general form to those in quantum optics where they are collectively known as the coupled Maxwell–Bloch equations [7].

The solution to these four-dimensional coupled equations is quite complex to unravel analytically, but in the small perturbation regime (small excitation pulse areas corresponding to small tip-angle regime), a good approximation to the solution can be found. A complete solution would involve determining the Bloch vector at each spatial location from the beginning of the imaging volume given the initial field and then using this information to determine the effect of the spins on this field. This field is then used as a driving term for the next set of spins for next successive thin slice in this volume. These spins produce a macroscopic polarization that is again used as a driving term in Maxwell's propagation equation for the next thin slice in the volume. In this iterative fashion throughout the imaging volume, one can determine the overall radiated field that is a result of initial material excitation. Let us begin by analyzing the impact of this spatial variation of the electromagnetic field on the Bloch solutions in both the on-resonance and off-resonance cases.

With the assumption that the duration of the RF excitation pulse is shorter than both T_1 and T_2, the dynamical evolution of the spin variables can thus be studied as if the damping terms were not present. In the absence of damping, the Bloch equation reduces to

$$\frac{dM_x}{dt} = M_y \underbrace{\left(\vec{k}\cdot\vec{r} + \Delta\omega + \frac{\partial\phi(t,\vec{r})}{\partial t}\right)}_{\Delta}, \tag{18}$$

$$\frac{dM_y}{dt} = -M_x(\vec{k}\cdot\vec{r} + \Delta\omega + \frac{\partial\phi(t,\vec{r})}{\partial t}) + \gamma B_1(t,\vec{r})M_z, \tag{19}$$

$$\frac{dM_z}{dt} = -\gamma B_1(t,\vec{r})M_y, \tag{20}$$

and the conservation law hold exactly. Note that we have dropped the prime notation for brevity with the understanding that all subsequent analysis is done in the rotating coordinate frame.

First we look at the Bloch equations exactly on-resonance ($\Delta = 0$), remembering that $B_1(t,\vec{r})$, is now a spatial-temporal field. The most common initial condition, in which all the spin bulk magnetization is along the longitudinal axis, leads to $M_x(t,\vec{r};\Delta = 0) = 0$ for the duration of the RF excitation pulse and $M_z = M_0$. In that case, the Bloch equations reduce to a pair

$$\frac{dM_y}{dt} = \gamma B_1(t,\vec{r})M_z, \tag{21}$$

$$\frac{dM_z}{dt} = -\gamma B_1(t,\vec{r})M_y \tag{22}$$

with solutions

$$M_{x'}(t,\vec{r};0) = 0, \tag{23}$$

$$M_{y'}(t,\vec{r};0) = \sin\theta(t,\vec{r}) \quad 0 \leqslant t \leqslant \tau_p, \tag{24}$$

$$M_z(t,\vec{r}) = \cos\theta(t,\vec{r}), \tag{25}$$

where we have normalized the initial longitudinal magnetization magnitude such that $M_0 = 1$ for notational simplicity, τ_p is the duration of the RF pulse and with the Bloch tipping angle identical to the pulse area in the usual way

$$\theta(t,\vec{r}) = \gamma\int_{-\infty}^{t} B_1(t',\vec{r})\,dt' \tag{26}$$

except that now the dependence on position is allowed for so that the spin flip angle is not just determined by the area of the pulse but also by the propagation distance of the RF pulse from the excitation coil to the spin location.

Now consider the case of an off-resonance excitation with an arbitrary RF envelope. Because the RF field is spatially varying, the usual Rabi solutions for spin population inversion in the presence of detuning [8] cannot be expected to be relevant here in solving the Bloch equation (18)–(20). Here we present an extension of Eberly [9] original approach for solving a related optical Bloch equation problem in quantum optics. It is reasonable to expect that the off-resonance spins respond to the RF pulse in the same way as the resonant spins, but perhaps with a detuning-dependent reduction in amplitude. Thus we assume the validity of the simple factorization into a product of on- and off-resonance components.

$$M_y(t,\vec{r};\Delta) = M_y(t,\vec{r};0)F(\Delta), \tag{27}$$

where $F(\Delta)$ is the spin 'spectral response' function. Eq. (20) is integrable if $\dot{\theta} = \partial\theta(t,\vec{r})/\partial t$ is substituted for $\gamma B_1(t,\vec{r})$ and $M_{y'}$ is expressed in terms of θ by using Eqs. (23), (25), (26), and (27), the z-component of magnetization in Eqs. (18)–(20) is then expressed as

$$M_z(t,\vec{r};\Delta) = -F(\Delta)\cos\theta + F(\Delta) - 1. \tag{28}$$

We now have both M_y and M_z as functions of θ. We proceed to also express M_x as a function of θ. Eqs. (18) and (20) can then be solved for $\frac{dM_{x'}}{dt}\Delta$, where $\Delta = \omega - \omega_0$ is the usual detuning operator.

When these two equations are equated for $\frac{dM'_x}{dt}\Delta$, they yield an equation for θ alone

$$\ddot{\theta} = \frac{\Delta^2 F(\Delta)}{1 - F(\Delta)}\sin\theta. \tag{29}$$

This equation can be formulated into the well-known pendulum problem

$$\ddot{\theta} - \frac{1}{\tau^2}\sin\theta = 0, \tag{30}$$

where $\tau^2 = 1 - F(\Delta)$. Only one solution out of a full range of elliptic functions can be made to fit the boundary conditions relevant to a single RF pulse. Both $B_1(t,\vec{r})$ and $\partial B_1(t,\vec{r})/\partial t$ must vanish at $t = \pm\infty$, so that $\dot{\theta}$ and $\ddot{\theta}$ must satisfy the same conditions. The solution for θ is

$$\theta(t,\vec{r}) = 4\tan^{-1}\left[\exp\left(\frac{t-t_0}{\tau}\right)\right] \tag{31}$$

and the RF field envelope corresponding to such θ behavior is the famous hyperbolic secant pulse of McCall and Hahn [10].

$$B_1(t,\vec{r}) = \frac{2}{\gamma\tau}\operatorname{sech}\left(\frac{t-t_0}{\tau}\right). \tag{32}$$

The $\vec{r}$ dependence of θ and B_1 are hidden in t_0. The parameter τ is clearly the pulse length. The dipole spectral response function can be found in terms of the pulse length and the Lorentzian detuning term,

$$F(\Delta) = \frac{1}{1+(\Delta)^2}. \tag{33}$$

What then is the relationship between Maxwell's equations and the solution given in Eq. (31)? Consider for example, the area under the envelope of the RF pulse as given by

$$A(t,\vec{r}) = \int_{-\infty}^{t} B^{e}(t,\vec{r})\,dt'. \tag{34}$$

The first step is the integration of the quadrature Maxwell equation (5) from $t=-\infty$ up to time t'' that occurs after the pulse has passed the point of observation $\vec{r}$. The quantum mechanical result is

$$\frac{\partial A(t'',\vec{r})}{\partial\vec{r}} = \frac{\pi Dp}{2K}k^2\int d\Delta\omega g(\Delta\omega)\int_{-\infty}^{t''} M_y(t,\vec{r};\Delta\omega)\,dt. \tag{35}$$

This equation integrates to

$$\frac{\partial A(t'',\vec{r})}{\partial\vec{r}} = \frac{\pi Dp}{2K}k^2\pi g(0)M_y(t_0,\vec{r};0). \tag{36}$$

Now, the absorptive part of the on-resonance spin amplitude is a nonlinear function of θ, and thus of area:

$$M_y(t_0,\vec{r};0) = -\sin A(t_0,\vec{r}). \tag{37}$$

Because $B^{e}(t,\vec{r}) = 0$ for all $t > t_0$, $A(t'',\vec{r})$ is exactly as $A(t_0,\vec{r})$. The area theorem first derived by McCall and Hahn [10,11], and now extended here to high field NMR, is thus given by

$$\frac{\partial}{\partial\vec{r}}A(t'',\vec{r}) = -\tfrac{1}{2}\alpha\sin A(t'',\vec{r}). \tag{38}$$

The absorption coefficient α is then defined

$$\alpha = \frac{4\pi^2 Dp\omega}{\hbar c}g(0). \tag{39}$$

In the limit of the weak excitation fields, the area is small and $\sin A \approx A$ so that in this limit the quantum area theorem becomes a linear relation

$$\frac{\partial}{\partial\vec{r}}A(t,\vec{r}) = -\tfrac{1}{2}\alpha A(t,\vec{r}). \tag{40}$$

It is apparent that when $A \geqslant \pi$, there are significant new features in the quantum expression. Most notably, if $A = n\pi$, for any n, the pulse envelope area suffers no attenuation in propagation since $\frac{\partial A}{\partial\vec{r}} = 0$. The areas that are even multiples of π are more stable than those that are odd multiples. Hence, with increasing penetration of the RF excitation pulse into the NMR medium, the area tends towards even multiples of π pointing a way to optimizing pulses via Eq. (38) a subject of a subsequent paper. This is the NMR equivalent of the quantum optics self-induced transparency result of McCall and Hahn [10] which states that if the pulse has an area $\theta = \int_{-\infty}^{\infty}\gamma B(t)\,dt$ equal to $2n\pi$ with n as an integer, and has a certain definite pulse shape, then it can propagate through the resonant (ordinarily absorbing) medium without attenuation and change in pulse shape, as long as the T_1 and T_2 relaxations are much longer than the transit time of the pulse through the material.

The basic idea of self-induced transparency can be seen from the Bloch vector picture. Normally, the excitation pulse would spread out in space and time as a result of diffraction and dispersion. However when the pulse is very intense, nonlinear effects can exactly cancel this spreading, and the excitation pulse will propagate without any change in shape.

Consider a $2n\pi$ pulse excitation field, with n as an integer, such that the magnetization vector $\vec{M}$ precesses about B_0 over full circles and ending up in its original position. Therefore, since the spin energy population distribution is the same before and after the pulse, it absorbs no net energy from the pulse. However, during the pulse propagation, it does absorb and emit photons while redistributing energy in the pulse. Consequently, the transmitted pulse appears to be altered in shape unless it already has the proper shape. As we showed, the proper field envelope for a 2π pulse is of a hyperbolic secant form. In propagating through the medium, the pulse is apparently delayed because the medium absorbs energy from the leading part of the pulse and deposits it back to its tail end.

Self-induced transparency is characterized by reduced absorption, pulse delay, pulse deformation and pulse splitting. It is however a much harder experiment to devise due to inherent losses in the system and especially in an inhomogeneous media like tissue. For example, when an excitation pulse propagates in a non-uniform resonant medium, such as a periodic array of resonant absorbers or through a heterogeneous dielectric medium such as tissue, such structures can destroy self-induced transparency , because the pulse area is then split between the forward and backward (reflected) coupled waves, and the phase coherence of the pulse is no longer conserved. This is exactly what happens in the presence of dielectric resonance effect in NMR.

The pulse delay and pulse breakup are the more convincing evidence of the presence of self-induced transparency and those are predicted in homogeneous medium with a high dielectric constant at pulse energies capable of multiple rotations ($2n\pi$).

3. Phase modulation effects

Let us take a closer look at the impact of the detuning parameter Δ. A more general expression for the excitation

field, in the rotating frame, is given in Eq. (2) and is repeated here for brevity

$$M_{xy}(t,\vec{r}) = \frac{1}{2}\left\{[M_{x'}(t,\vec{r}) + \mathrm{i}M_{y'}(t,\vec{r})]\mathrm{e}^{\mathrm{i}[k\cdot\vec{r}-\Delta\omega\vec{t}+\phi(t,\vec{r})]} + c.c\right\}. \tag{41}$$

The instantaneous wave vector can now be identified as $k - \frac{\partial\phi}{\partial z}$ and is not necessarily a constant. The field frequency is no longer constant and can be denoted as

$$\omega(t) = -\Delta\omega + \frac{\partial\phi(t,\vec{r})}{\partial t} \tag{42}$$

leading to frequency modulation phenomena similar to adiabatic excitations.

We are interested in the response of the spins to an applied field and not the radiation emitted by the material. We thus set $\Delta\omega = 0$ and ignore Maxwell's equation to solve the Eqs. (11)–(13). Not surprisingly, the 'natural' solutions to these equations under these conditions are the well-known approximate results in the context of adiabatic inversion. If the magnitude of the frequency sweep is denoted by $2\delta\omega$, then

$$\frac{\partial\phi(t,\vec{r})}{\mathrm{d}t} = -\delta\omega\ \tanh\left(\frac{t-t_0}{\tau}\right), \tag{43}$$

$$M_x = \frac{-\delta\omega\tau}{\sqrt{1+(\delta\omega\tau)^2}}\,\mathrm{sech}\left(\frac{t-t_0}{\tau}\right), \tag{44}$$

$$M_y = \frac{-1}{\sqrt{1+(\delta\omega\tau)^2}}\,\mathrm{sech}\left(\frac{t-t_0}{\tau}\right), \tag{45}$$

$$M_z = \tanh\left(\frac{t-t_0}{\tau}\right). \tag{46}$$

Hence

$$B_1(t,\vec{r}) = \frac{1}{\gamma\tau}\sqrt{1+(\delta\omega\tau)^2}\,\mathrm{sech}\left(\frac{t-t_0}{\tau}\right). \tag{47}$$

The similarity of the solution with adiabatic inversion is not a coincidence. Adiabatic inversion is achieved by slowly changing the magnitude of the longitudinal component of the magnetic field so that the effective field changes sign, thus inverting all of the spins that are following the effective field.

It is just as effective to frequency modulate the driving field, that is, put time dependence into ω, as it is to vary ω_0. Note that if $\delta\omega \to 0$, then $B(t,\vec{r})$ becomes a standard π pulse. That is the area of the envelope in Eq. (47) is

$$A = \int \gamma B(t,\vec{r})\mathrm{d}t = \pi\sqrt{1+(\delta\omega)^2}, \tag{48}$$

which reduces to $A = \pi$ as $\delta \to 0$. A π pulse naturally inverts the spins. However, if the frequency modulation is substantial such that $\delta\omega\tau = \sqrt{3}$, then $A = 2\pi$. Unusual phenomena such as a 2π pulse that acts as an inversion pulse become apparent! The reason for this is that in the presence of frequency modulation, the identity between pulse area and spin flip angle is no longer valid. As soon as frequency modulation of the driving field is present, the area theorem cannot be derived and hence the concept of flip angle in high field NMR is problematic.

Adiabatic changes implied by the solutions given in Eqs. (43)–(46) were simulated in matlab and are plotted in Fig. 2. The spin inversion M_z is shown on the same time axis with the excitation field $B_1(t,\vec{r})$ and the instantaneous frequency shift $\frac{\partial\phi(t,\vec{r})}{\partial t}$. In conventional NMR where propagation effects are negligible, the constant-amplitude field $B1(t,x)$and linear frequency sweep $\frac{\partial\phi(t,\vec{r})}{\partial t}$ are usually assumed in approximate treatments in the interval $(-0.5\tau\ 0.5\tau)$. Beyond this

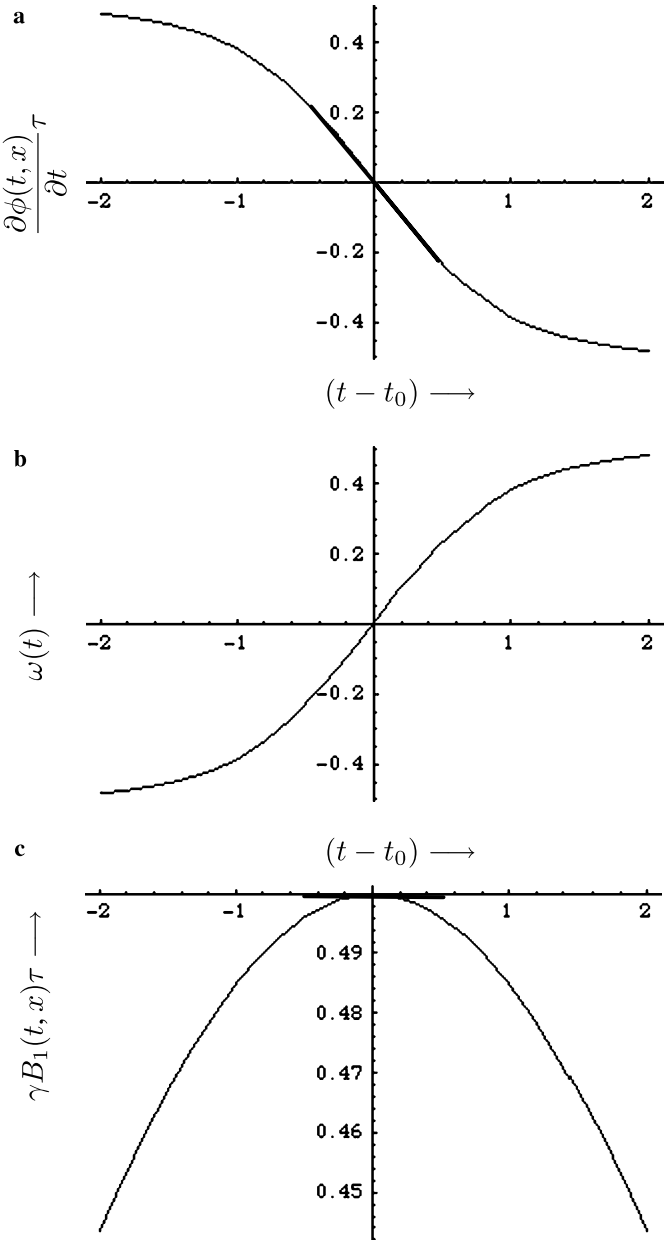

Fig. 2. Graph of solutions in Eqs. (43)–(46). All horizontal scale are in multiples of τ.

linear regime (>4 T), propagation effects become significant and must be taken into consideration.

4. Discussion

The current trend towards high field NMR systems both for the improvement in SNR and hence resolution as well as more spectral dispersion in spectroscopy studies, is complicated by the emergence of field propagation phenomena due to the small wavelength compared to the FOV. In this paper, an analysis of field propagation phenomena has been presented by deriving an NMR equivalent set of coupled Bloch–Maxwell equations. Solutions to this set of equations yielded an extension of the well-known adiabatic inversion problem. The traditional link between pulse area and flip angle in low field NMR is also shown to be invalid in high field strength NMR when the imaging FOV is larger than the excitation wavelengths.

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