Field Propagation Phenomena in Ultra High Field NMR: A Maxwell-Bloch Formulation

A. J. Kiruluta[1]

[1]Physics, Harvard University, Cambridge, MA, United States

Abstract: At ultra high field strength (>4T), the excitation wavelength relative to the dimension of the human body lead to significant B_1 inhomogeneity. The dielectric constant of tissue with a high water content can be as high as 70 leading to a wavelength inside tissue of less than 15 cm at 7T, which is commensurate or less than most body parts. The excitation field is thus spatio-temporal and in conjunction with the increase in tissue conductivity, we find that in the propagation of radiation at ultra high fields, new phenomena commonly observed in quantum optics but traditionally negligible in NMR such as spatio-temporal phase modulation of the excitation field such that the identity between pulse area and flip angle is no longer valid. It is shown that in addition to the well studied dielectric resonance phenomena at high magnetic fields, field propagation effects transform the excitation pulse into an adiabatic excitation. The high field strength also mean that nonlinear effects such as transient four wave mixing, are now possible in NMR experiments. Additional constraints due to phase matching considerations are imposed on the formalism of echo formation in high field NMR, due to momentum matching considerations.

Methods: Under quasi-static conditions of low field NMR (<4T), the excitation field is not affected by the transient response of the medium or is assumed negligible for 'thin' medium. However, for high fields NMR, a complete analysis requires consideration of the excitation field propagation wave vector. The NMR torque equation in the rotating frame including field propagation phenomena is then expressed as[1]:

$$\frac{d\vec{M}}{dt} = \vec{M}\times\left[\gamma B_1(t,\vec{r})\hat{x}' + \overbrace{\left(\vec{k}\cdot\frac{d\vec{r}}{dt} + \Delta\omega + \frac{\partial\phi(t,\vec{r})}{\partial t}\right)}^{\Delta}\hat{z}\right] - \frac{(M_x\hat{x}' + M_y\hat{y}')}{T_2} - \frac{(M_z - M_0)\hat{z}}{T_1} \qquad (1)$$

where Δ is the total detuning parameter. This detuning parameter consists of two distinct components: the instantaneous propagation wave vector and a spectral off-resonance component respectively. Not surprisingly, the 'natural' solution to this equation, in the absence of damping constraints, is the well known approximate result in the context of adiabatic inversion.

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

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 Equation 2 is given by

$$A = \int \gamma B(t,\vec{r})dt = \pi\sqrt{1+(\delta\omega)^2} \qquad (3)$$

which reduces to $A=\pi$ as $\delta \to 0$. 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 for FOVs larger than the RF wavelength. Adiabatic changes implied by the solutions given in Eq. 2 were simulated in Mathematica (Wolfram, Champagne, IL) and are plotted in Fig. 1. Low field NMR is in the linear regime in the interval (-0.5, 0.5) τ beyond which the area relationship between the excitation field and the flip angle is not valid.

Results:

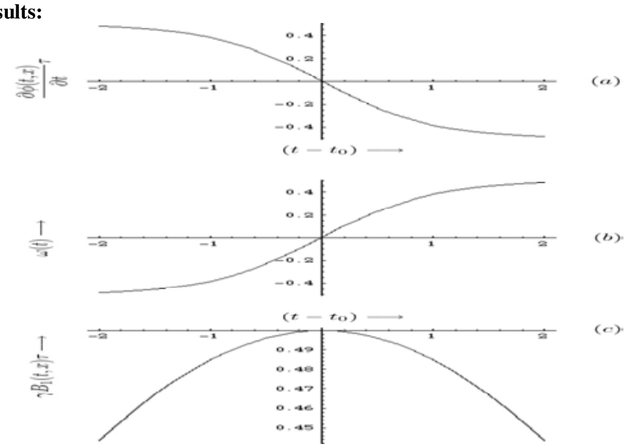

Figure 3: Graph of solutions in Equation 1. All horizontal scale are in multiples of τ. The spin inversion M_z is shown on the same time axis with the excitation field and the instantaneous frequency shift $\partial\phi(t,\vec{r})/\partial t$. In conventional NMR where propagation effects are negligible, the constant-amplitude field and linear frequency sweep are usually assumed in approximate treatments in the interval (-0.5, 0.5) τ in the quasi-static regime. Beyond this linear regime (>4T), propagation effects become significant and must be taken into consideration.

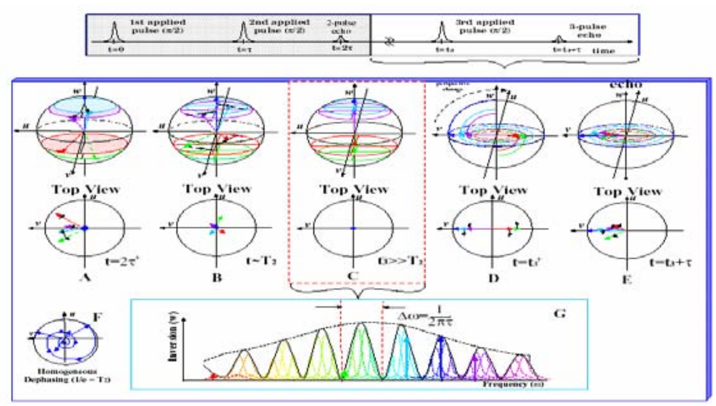

Figure 2: Application of the 3rd pulse in a STE sequence. Figure A-F illustrate the effect on the Bloch vectors for different resonance detunings as a function of time just after the two pulse echo at $t = 2\tau$ and up until the STE. The inset (G) shows a simulation of the spatial-spectral holographic grating after the second pulse stored as an inversion of the spin population. The echo signal is given by:

$$M_{xy}(\vec{r},t) = M_0 e^{-i(\vec{k}_3+\vec{k}_2-\vec{k}_1)}\int B_1^*(\omega)B_2(\omega)e^{-i\omega(t-t_3+t_2-t_1)}d\omega$$

so that the phase matching condition in this case is $\vec{k}_4 = \vec{k}_3 + \vec{k}_2 - \vec{k}_1$.

Conclusions:

The current trend towards high field NMR systems both for the improvement in SNR and hence improved 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 NMR when the imaging FOV is larger than the excitation wavelengths. Field propagation phenomena transforms excitation pulses adiabatic ones. As well, we showed that phase matching is required for the formation of echoes at higher field strength in addition to the usual timing constraints. This is due to the requirement for both the excitation and echo wave vectors to phase match-Fig. 2.

References: [1] AJM Kiruluta, JMR, 182 (2), pp. 308-314 (2006).