Frequency Sweep NMR

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1 Introduction

Thus far, we've been successfully employing Field Sweep AFP NMR on the polarized target system. But for the G_E^n experiment, this is not feasible. Since the target system is enclosed in a metal box (to mask it from the powerful BigBite magnet), the eddy currents produced in it, and the magnetic hysteresis effect prevent reliable measurements using field sweep. We, hence, employ the frequency sweep technique.

2 Classical Treatment[1]

According to the classical theory of electromagnetism, a magnetic moment $\vec{M}$ in a field $\vec{H}$ experiences a torque $\vec{T} = \vec{M} \times \vec{H}$, equal to the rate of change of angular momentum of the magnetic moment, $\hbar(\mathrm{d}\vec{I}/\mathrm{d}t)$. Since $\vec{M} = \gamma\hbar\vec{I}$, we get

$$\frac{\mathrm{d}\vec{M}}{\mathrm{d}t} = \gamma\vec{M} \times \vec{H} \tag{1}$$

Now, let us consider a frame S' rotating with respect to the laboratory frame with an angular velocity $\vec{\omega}$. From the general law of relative motion, we can relate the time derivatives of $\vec{M}$ in the two reference frames as

$$\frac{\mathrm{d}\vec{M}}{\mathrm{d}t} = \frac{\partial\vec{M}}{\partial t} + \vec{\omega} \times \vec{M} \tag{2}$$

Combining (1) and (2), the motion of the magnetic moment in the rotating frame is given by

$$\frac{\partial\vec{M}}{\partial t} = \gamma\vec{M} \times (\vec{H} + \frac{\vec{\omega}}{\gamma}) \tag{3}$$

This has the same form as equation (1) provided we replace the magnetic field $\vec{H}$ by an effective field $\vec{H}_e = \vec{H} + (\vec{\omega}/\gamma)$, the sum of the laboratory field $\vec{H}$ and a fictitious field $\vec{H}_f = +(\vec{\omega}/\gamma)$.

Let $\vec{H} = \vec{H}_0$, the holding field in the lab frame directed along the z-axis. By choosing a rotating frame with $\vec{\omega} = -\gamma\vec{H}_0$, the effective field $\vec{H}_e$ vanishes. This is the Larmor frequency,

[1] cf. A. Abragam, *Principles of Nuclear Magnetism*

$\omega_0 = \gamma H_0$, with which the magnetic moment precesses in the laboratory frame. Now suppose we turn on a field $\vec{H}_1$ perpendicular to $\vec{H}_0$ and rotating about it with angular velocity ω. The unit vector $\hat{\imath}$ of the x-axis in the rotating frame S' being taken along the field $\vec{H}_1$, the effective field $\vec{H}_e$ is static in S' and is given by

$$\vec{H}_e = (H_0 + \frac{\omega}{\gamma})\hat{k} + H_1\hat{\imath} \tag{4}$$

3 The Adiabatic Condition

Here, we derive the adiabatic fast passage condition for the RF Sweep rate. From the equation of motion (1), we can deduce that

$$\frac{\mathrm{d}}{\mathrm{d}t}(M^2) = 2\vec{M} \cdot \frac{\mathrm{d}\vec{M}}{\mathrm{d}t} = 0 \tag{5}$$

that is, the magnitude of the magnetization M is a constant of the motion, whatever the variation of H with time. If this variation is sufficiently slow, the angle of the magnetization with the instantaneous direction of the field is also a constant of the motion, as we shall now show.
The variation of the vector $\vec{H}$ with time can be described generally by

$$\frac{\mathrm{d}\vec{H}}{\mathrm{d}t} = \vec{\Omega} \times \vec{H} + \Omega_1 \vec{H} \tag{6}$$

where the vector $\vec{\Omega}$ and the scalar Ω_1 have the dimensions of frequency.

Consider a frame S' where the z-axis is continuously aligned along the instantaneous direction of the field $\vec{H}$. According to (6) the relative motion of S' with respect to the laboratory will be a rotation about the instantaneous axis $\vec{\Omega}$. In that frame the magnetization will change in time according to

$$\frac{\partial \vec{M}}{\partial t} = \gamma \vec{M} \times (\vec{H} + \frac{\vec{\Omega}}{\gamma}) \tag{7}$$

By definition, in this frame $H_x = H_y = 0$ and

$$\frac{\partial M_z}{\partial t} = M_x \Omega_y - M_y \Omega_x \tag{8}$$

If $|\Omega| \ll |\gamma H|$ then, approximately,

$$\frac{\partial M_x}{\partial t} \cong \gamma H M_y, \qquad \frac{\partial M_y}{\partial t} \cong -\gamma H M_x.$$

M_x and M_y are approximately sinusoidal functions with instantaneous frequency $\omega_0(t) = -\gamma H(t)$.

After a long time t, the change in M_z would be

$$\Delta M_z = M_z(t) - M_z(0) = \int_0^t [M_x(t')\Omega_y(t') - M_y(t')\Omega_x(t')]\,\mathrm{d}t.$$

If the variation of $\vec{\Omega}$ with time is sufficiently slow, or to be precise, if its Fourier expansion has negligible components at frequencies of the order of $|\gamma H(t)|$, then, for any t,

$$|\Delta M_z| \sim \left|\frac{M\Omega}{\gamma H}\right| \ll M$$

and M_z, that is, the component of $\vec{M}$ along the field, will remain constant. This is the adiabatic theorem.

We apply this result to our system of magnetic moments. For the RF sweep, we have,

$$\frac{\mathrm{d}\vec{H}_e}{\mathrm{d}t} = \frac{\dot{\omega}}{\gamma}\hat{k} + \dot{H}_1\vec{\imath} \tag{9}$$

where the dot represents the derivative with respect to time. Substituting for $\hat{k}$ and $\hat{\imath}$ to transform into a frame defined by $\vec{H}_e$ and $\hat{n} \times \vec{H}_e$, we get

$$\frac{\mathrm{d}\vec{H}_e}{\mathrm{d}t} = (\cos\theta\frac{\dot{\omega}}{\gamma} + \sin\theta\,\dot{H}_1)\hat{H}_e + (\sin\theta\frac{\dot{\omega}}{\gamma} - \cos\theta\,\dot{H}_1)(\hat{n} \times \hat{H}_e) \tag{10}$$

where $\hat{H}_e = \vec{H}_e/|\vec{H}_e|$, and $\hat{n}$ is a unit vector orthogonal to $\vec{H}_0$ and $\vec{H}_1$. Comparing this with equation (6) gives

$$\Omega = \sin\theta\frac{\dot{\omega}}{\gamma H_e} - \cos\theta\frac{\dot{H}_1}{H_e} = \frac{H_1}{\gamma H_e^2}\dot{\omega} - \frac{H_0}{H_e^2}\dot{H}_1 \tag{11}$$

The quantity Ω is the smaller, the farther from resonance. We assume that the variation of H_1 with respect to time (due the different frequency response of the electronics at different frequencies), over the range of frequency swept, is small compared to the sweep rate. It is observed that H_1 changes about 2 to 5% over the entire range. Now, applying the adiabatic condition $|\Omega| \ll |\gamma H_e|$, we get

$$\dot{\omega} \ll \frac{\gamma^2 H_e^2}{\sin\theta} \tag{12}$$

This condition is strongest at resonance ($\theta = 90°$) and gives

$$\dot{\omega} \ll \gamma^2 H_1^2 \tag{13}$$

Note that, at resonance, $H_e = H_1$ and that the $\cos\theta$ term in equation (11) vanishes. This is the AFP condition for frequency sweep NMR.

I'll soon put up the lower inequality analysis. Both these results finally give us the Adiabatic Fast Passage condition for Frequency Sweep NMR as

$$\boxed{\frac{\gamma H_1}{T_2} \ll \dot{\omega} \ll \gamma^2 H_1^2} \tag{14}$$

Reference

A. Abragam, *The Principles of Nuclear Magnetism*, Chapter 2.