Nuclear Magnetic Resonance – An Overview

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(Dated: April 10, 2025)

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I. INTRODUCTION

The study of nuclear magnetic resonance (NMR) utilizes weak magnetic fields to affect the nuclei of atoms in a strong magnetic field. Under certain conditions, atoms will exhibit "resonance," causing the observation of a transient magnetic field as nuclei relax back to their equillibrium state.

II. THEORETICAL DESCRIPTION

A. Larmor Precession

We will start with the phenomena of Larmor precession, occuring when atoms are placed in a strong magnetic field. Larmor precession most readily occurs when the nucleus has a net magnetic moment i.e. there is an odd number of protons, producing a spin $1/2$ system. In this case, the magnetic dipole moment μ of the nucleus is described as

$$\vec{\mu} = \gamma \vec{S} \tag{1}$$

where $\vec{S}$ denotes the spin vector and γ is a constant known as the gyromagnetic ratio (which differs depending on the type of nucleus). Under a magnetic field, the energy of this system reads

$$E = -\vec{\mu} \cdot \vec{B_0} \tag{2}$$

where we denote B_0 the external magnetic field. This yields the Hamiltonian

$$H = -\gamma \vec{B_0} \cdot S \tag{3}$$

where S is the Pauli spin operator $S = (\sigma_x, \sigma_y, \sigma_z)$. Let us orient our magnetic field against the z-axis, such that

$$\vec{B_0} = B_0 \hat{z} \tag{4}$$

and the Hamiltonian now reads

$$H = -\frac{\hbar}{2} \gamma B_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{5}$$

The Hamiltonian has eigenstates

$$|\pm\rangle : E_\pm = \mp \frac{\hbar}{2} \gamma B_0 \tag{6}$$

These eigenstates correspond to nuclei aligned either parallel or antiparallel to the magnetic field B_0. We will use these vectors $|\pm\rangle$ as our basis. We can evolve these stationary states with the time-dependent Schrödinger equation and then calculate the expectation of each of our Pauli matrices to obtain

$$\langle S_x \rangle = \frac{\hbar}{2} \sin(\theta) \cos(\gamma B_0 t)$$
$$\langle S_y \rangle = \frac{\hbar}{2} \sin(\theta) \sin(\gamma B_0 t)$$
$$\langle S_z \rangle = \frac{\hbar}{2} \cos(\theta)$$

These equations are the classical precession equations; our spin vector will precess about the magnetic field at a constant frequency

$$\omega_0 = \gamma B_0 \tag{7}$$

This frequency is known as the **Larmor frequency**, and θ indicates the angle between $\vec{\mu}$ and $\vec{B_0}$.

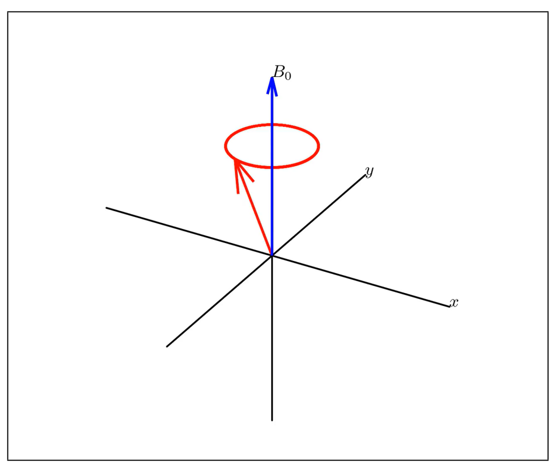


FIG. 1: Larmor precession about $\vec{B_0}$

θ characterizes the system, up to a phase,

$$|\psi\rangle = \cos(\theta/2)\,|+\rangle + e^{i\phi} \sin(\theta/2)\,|-\rangle \tag{8}$$

These equations above can also be derived from a classical viewpoint; we can calculate the torque $\vec{\tau} = \vec{\mu} \times \vec{B_0}$ on the nucleus by the magnetic moment and use Newton's second law to derive a similar precession.

B. Net Magnetization and Relaxation

The lower energy E_+ is the favored energy state; slightly more spins will align parallel to $\vec{B_0}$ as opposed to antiparallel. Using statistical mechanics, we can derive the expected number of $|+\rangle$ vs $|-\rangle$. Since this is a canonical two-state system, the ratio $\frac{N_+}{N_-}$ is equal to the ratio of the Boltzmann factors, yielding

$$\frac{N_+}{N_-} = \exp\left(\frac{\gamma\hbar B_0}{kT}\right) \tag{9}$$

This small difference produces a net longitudinal magnetization (in this context, "longitudinal" refers "along the B_0 field"), which is the sum of the individual quantized spins of the sytem.

$$M_z = \sum_i \gamma\hbar m_i = \frac{\hbar}{2}\gamma(N_+ - N_-) \tag{10}$$

In equillibrium with our original magnetic field B_0, we expect a slight magnetization in the $+\hat{z}$ direction. However, if we were to apply another magnetic field briefly to this system, we would see a change in the net magnetization $\vec{M}(t)$. Eventually, the system will return back to its equillibrium state. In order to reach equillibrium, the system must give back energy to the surrounding lattice.

We are interested in understanding how long it takes for our system to reach equillibrium. In general, after a disturbance, the magnetization follows the Bloch equation, reproduced in Equation 11

$$\frac{d\vec{M}(t)}{dt} = \frac{\vec{M}(t) - \vec{M}_0}{T_1} \tag{11}$$

where $\vec{M}_0$ denotes the equillibrium magnetization. We refer to T_1 as the **spin-lattice relaxation time**.

C. Producing Transverse Magnetizations

1. *Apply a Circularly Polarized Field*

So far, we have discussed the uniform $\vec{B_0}$ field. However, to produce a transverse magnetization (i.e. a magnetization in the x-y plane) we need to get creative. We will use a circularly polarized field,

$$\vec{B_1}(t) = B_1\left[\cos(\omega_0 t)\hat{x} + \sin(\omega_0 t)\hat{y}\right] \tag{12}$$

Note that $\vec{B_1}(t)$ oscillates at the Larmor frequency. Thus, the new Hamiltonian has an extra time-dependant term, still in the form of Equation 3. Solving this Hamiltonian is beyond the scope of this lab report; however, can still apply the classical torque result

$$\vec{\tau} = \vec{\mu} \times \gamma\left[\vec{B_0} + \vec{B_1}(t)\right] \tag{13}$$

by transforming into a rotating reference frame (rotating at the Larmor frequency), we find that the effective field becomes

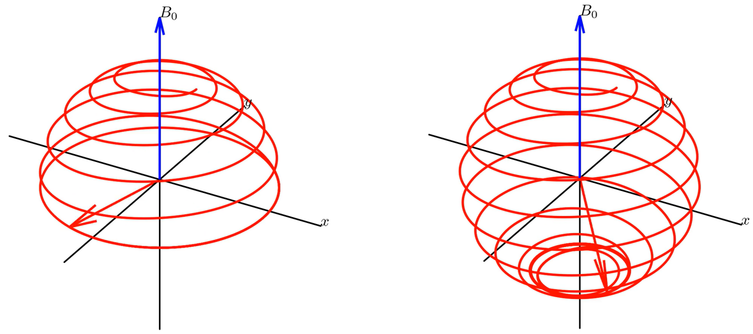
$$\vec{\tau}^* = (B_0 - {}^{\mu}/_{\gamma})\hat{z} + B_1\hat{x} \tag{14}$$

In this rotating frame, applying a circularly polarized magnetic field has the effect of "tipping" the magnetization into a transverse plane. Transforming back into the lab frame, we will observe the magnetization in the x-y plane still precessing about the z-axis.

2. *$\frac{\pi}{2}$ and π pulses*

Doing this, we will create two types of pulses. We will first define a $\frac{\pi}{2}$ **pulse**, a pulse of $B_1(t)$ that will be applied for exactly long enough such that the magnetization is entirely in the $x-y$ plane. We will also define a π **pulse**, a pulse that flips the magnetization from $+\hat{z}$ to $-\hat{z}$.

During a $\frac{\pi}{2}$ or π pulse, we can plot the expectation $\langle\vec{S}\rangle = (\langle S_x\rangle, \langle S_y\rangle, \langle S_z\rangle)$ over time, as shown in Figure 2.



(a) $\frac{\pi}{2}$ pulse produces transverse magentization

(b) π pulse flips magentization from $+\hat{z}$ to $-\hat{z}$

FIG. 2: $\langle \vec{S} \rangle$ over time during a $\frac{\pi}{2}$ and π pulse