

Nuclear Magnetic Resonance (NMR)

A Brief Introduction and Applications

Ali Ahmed Neil Mandar Zain Kamal

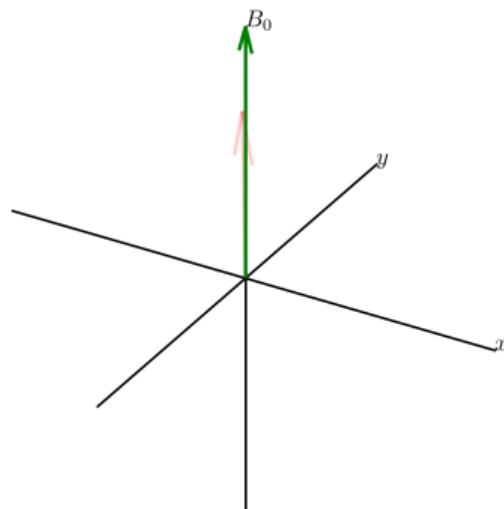
Department of Physics & Astronomy, Rutgers University

April 24, 2025

Overview

1. Principles of NMR
2. Apparatus and Experimental Procedures

Setup



- Spin 1/2 nuclei
- Strong magnetic field, denoted \vec{B}_0

Energy and Hamiltonian

Magnetic moment of nucleus

$$\vec{\mu} = \gamma \vec{S} \quad (1)$$

Yields energy and Hamiltonian of

$$E = -\vec{\mu} \cdot \vec{B}_0 \quad (2)$$

$$H = -\gamma \vec{B}_0 \cdot \vec{S} \quad (3)$$

Figure: Typical \vec{B}_0 and vector aligned with field

Larmor Precession

Evolving an arbitrary spin vector

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

yields, [1]

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

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

$$\langle S_z \rangle = \frac{\hbar}{2} \cos(\theta)$$

with the characteristic **Larmor frequency**

$$\omega_0 = \gamma B_0 \quad (4)$$

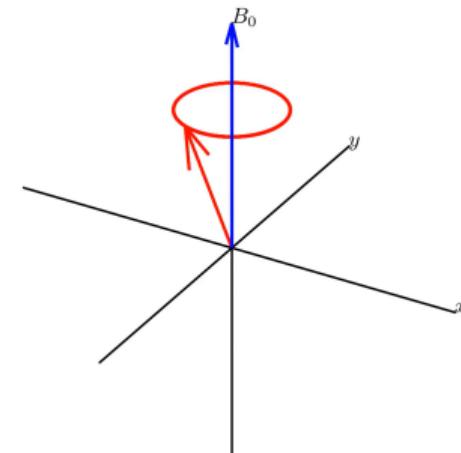


Figure: Larmor precession about \vec{B}_0

Net Magnetization and Relaxation

With many spins, any material can acquire a net magnetization.

Along \hat{z} , statistical mechanics tells us that

$$\frac{N_+}{N_-} = \exp\left(\frac{\gamma\hbar B_0}{kT}\right) \quad (5)$$

with total **net magnetization**

$$M_z = \sum_i \gamma\hbar m_i = \frac{\hbar}{2} \gamma (N_+ - N_-) \quad (6)$$

Expect spins to eventually re-align with \hat{z} direction.

Producing Transverse Magnetization

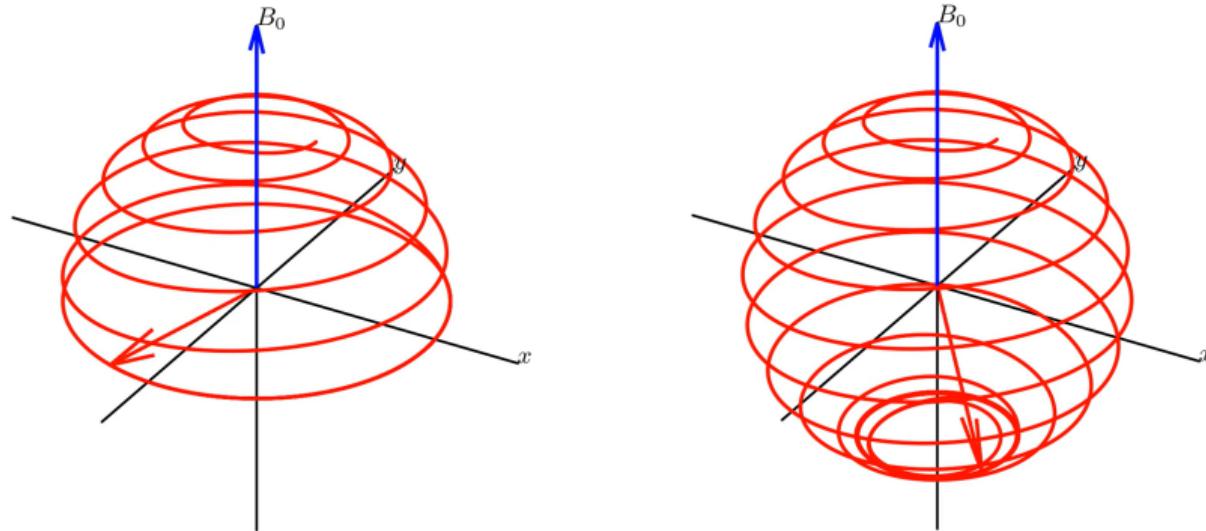
Circularly Polarized Field

$$\vec{B}_1(t) = B_1 \cos(\omega_0 t) \hat{x} \quad (7)$$

To “tip” magnetization into xy plane, apply a circularly polarized $\vec{B}_1(t)$. Classical torque result in a rotating frame yields,

$$\vec{B}^* = \left(\left[\vec{B}_0 - \frac{\omega_0}{\gamma} \right] \hat{z}^* + B_1 \hat{x}^* \right) \quad (8)$$

$\frac{\pi}{2}$ and π pulses



- (a) $\frac{\pi}{2}$ pulse produces transverse magnetization (b) π pulse flips magnetization from $+\hat{z}$ to $-\hat{z}$

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

Spin-Lattice Relaxation (T_1)

Time constant associated with decay of net magnetization back towards $+\hat{z}$.

$$\frac{d\vec{M}(t)}{dt} = \frac{\vec{M}(t) - \vec{M}_0}{T_1} \quad (9)$$

Referred to as the **Bloch equations**.

Spin-Spin Relaxation (T_2)

Time constant associated with the decay of the relative “coherence” of spins in xy plane, with associated Bloch equation [2],

$$\frac{d\vec{M}_{x,y}}{dt} = \frac{\vec{M}_{x,y}}{T_2} \quad (10)$$

Free Induction Decay and T_2^*

- Observations performed with a pickup coil detecting flux in transverse direction
- Magnetization becomes increasingly decoherent; produces **free induction decay (FID)** signal
- Combined effects of spin-lattice, spin-spin, and field inhomogeneities [2]

$$\frac{1}{T_2^*} = \frac{1}{T_1} + \frac{1}{T_2} + \gamma \Delta B_0 \quad (11)$$

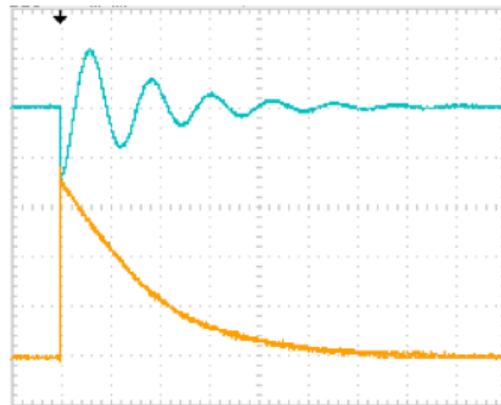


Figure: Basic FID signal of mineral oil [3]

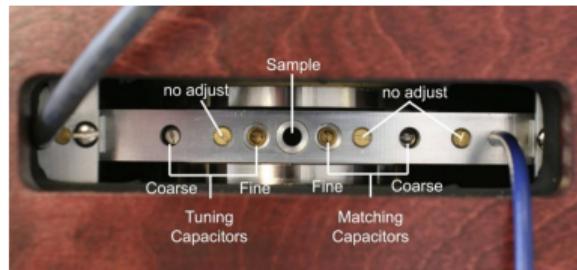
Apparatus: TeachSpin NMR Set



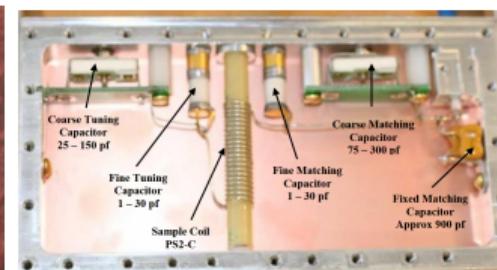
Figure: Pulsed/CW NMR Spectrometer, PS2-B

Permanent Magnet

- .5 T magnetic field
- RF sample measurement coil
- Tuning capacitors (find resonance with RF coil)
- Thermal servo units/Field gradient coils



(a) Capacitors



(b) RF Coil

Figure: Diagrams of RF coil and capacitors

PS2 Controller

- Field gradient coil control → Maximize homogeneity
- Magnet temperature control → Indicate reference temperature

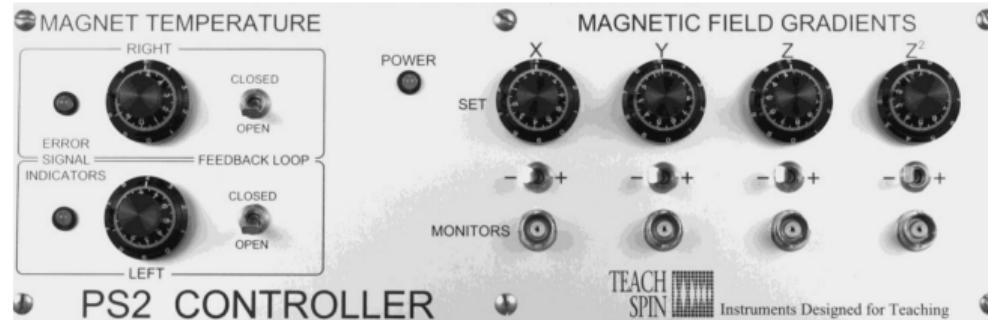


Figure: Temperature controller

Mainframe

- Receiver
 - Process RF sample signal
 - Tunable gain and filter
- Synthesizer
 - Generates RF excitation signal
- Pulse Programmer → Some Controls:
 - A and B length
 - A and B delay time

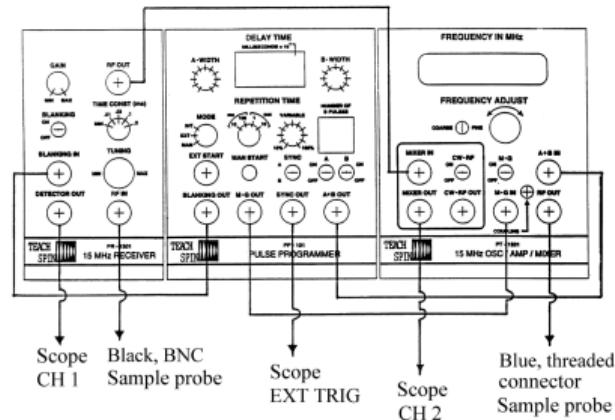


Figure: Mainframe (deprecated)

Some Notes on Pulse Sequencing

Recall,

$\frac{\pi}{2}$ pulse

- Flips net magnetization into xy plane
- Generates FID signal

π pulse

- Flips net magnetization along $-\hat{z}$ axis
- No FID signal

What happens after a $\frac{\pi}{2}$ pulse?

- FID signal decays primarily due to spin dephasing from field inhomogeneities*
- Spins decay back to the $+\hat{z}$ -axis (even after FID signal disappears)

Dephasing due to field inhomogeneities

- Static magnetic field pointing in z produces a torque that causes the spin to rotate in the xy plane
- Different field magnitudes cause different rotation speeds
- If all the spins are aligned in the xy plane, FID signal is strong
- If they are misaligned (out of phase), FID signal is weak
- This makes it hard to measure T_2

What happens after a π pulse?

- FID does not form since spins are not in xy plane
- Spins decay back to the $+z$ -axis (no FID signal forms)

T_1 Measurement Sequence: $\frac{\pi}{2} - \pi$

- Apply a $\frac{\pi}{2}$ pulse.
 - Magnetization enters xy plane and dephases Spins slowly decay to $+\hat{z}$
- Apply another $\frac{\pi}{2}$ pulse a little later
 - xy spins kicked to the $-\hat{z}$ -axis (no FID signal)
 - $+\hat{z}$ spins kicked to the xy (FID signal)
- Gives an idea of how fast longitudinal spins decay

T_1 Measurement Sequence: $\pi - \frac{\pi}{2}$

- Apply a π pulse.
 - Net magnetization jumps to $-\hat{z}$ (no signal)
 - Spins slowly decay to $+\hat{z}$
- Apply a $\frac{\pi}{2}$ pulse a little later
 - Spins along $-\hat{z}$ are kicked to $-\hat{x}$
 - Spins along $+z$ are kicked to $+\hat{x}$
 - If no FID signal is produced (half life)
- Much more elegant

T_2 Measurement Sequence: $\frac{\pi}{2} - \pi$

- Apply a $\frac{\pi}{2}$ pulse → Net magnetization enters the xy plane and dephases
- Apply a π pulse a little later
 - Spins remain in xy plane, but ‘reverse’ rotation direction
 - Spins rephase a little later
- The decay in rephasing signal follows T_2

Using More Pulses

- To better characterize the decay multiple π pulses are applied
- Must be close together to mitigate molecular diffusion
 - Spin dephases at one speed and returns at another
 - Will not rephase with the rest

Experimental Procedure: Resonance

- Tune RF frequency to proton resonance (21 MHz) → Minimize beats
- Use tuning capacitor to maximize FID signal

$\frac{\pi}{2}$ and π pulses

- Apply a single RF pulse and vary its length
- Find the length with maximum FID signal
- This is a $\frac{\pi}{2}$ pulse
- Double the length to find π pulse length

Sequencing

- Use adequate pulse sequences to measure decay times
- Record data for processing to calculate characteristic times T_1 and T_2

References

-  D. J. Griffiths and D. F. Schroeter, *Introduction to Quantum Mechanics*.
Cambridge ; New York, NY: Cambridge University Press, 3 ed., 2018.
-  C. P. Slichter, *Principles of Magnetic Resonance*.
USA: Springer Science, 3 ed., 1990.
-  *Pulsed Nuclear Magnetic Resonance*.