Nuclear Magnetic Resonance (NMR)

A Brief Introduction and Applications

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Overview

1. Principles of NMR

Setup

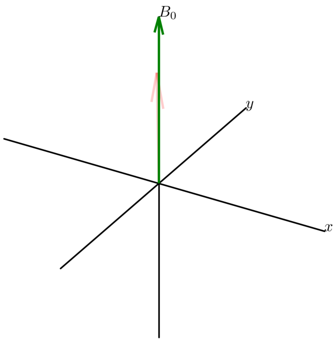


Figure: Typical $\vec{B}_0$ and vector aligned with field

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

Energy and Hamiltonian

Magnetic moment of nucleus

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

Yields energy and Hamiltonian of

$$E = -\vec{\mu} \cdot \vec{B}_0 \tag{2}$$

$$H = -\gamma \vec{B}_0 \cdot S \tag{3}$$

Larmor Precession

Evolving an arbitrary spin vector

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

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**

$$\omega_0 = \gamma B_0 \tag{4}$$

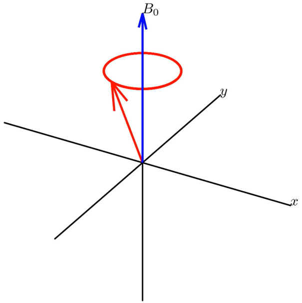


Figure: Larmor precession about $\vec{B}_0$

Net Magnetization and Relaxation

With many spins, any material can acquire a net magentization.
Along $\hat{z}$, statistical mechanics tells us that

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

with total **net magnetization**

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

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

Producing Transverse Magnetization

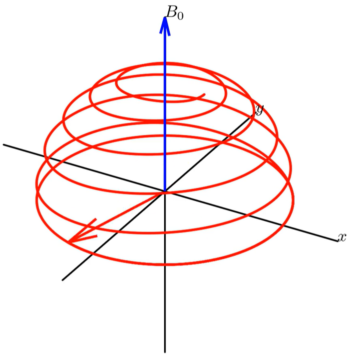
Circularly Polarized Field

$$\vec{B}_1(t) = B_1 \left[\cos(\omega_0 t)\hat{x} + \sin(\omega_0 t)\hat{y}\right] \tag{7}$$

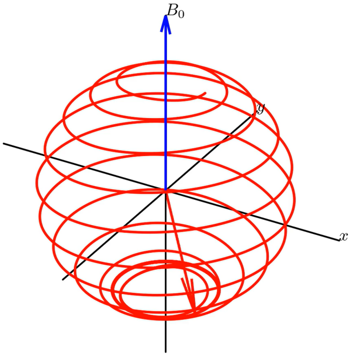
To "tip" magnetization into xy plane, apply a circularly polarized $\vec{B}_1(t)$. Classical torque result in a rotating frame yields,

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

$\frac{\pi}{2}$ and π pusles



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



(b) π pulse flips magentization 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 $+\hat{z}$.

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

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,

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

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]

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

References

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Cambridge ; New York, NY: Cambridge University Press, 3 ed., 2018.

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USA: Springer Science, 3 ed., 1990.