NMR – Nuclear Magnetic Resonance

Atomic nuclei have an intrinsic $\underbrace{\text{magnetic moment}}_{}$ due to spin.

measure of "strength" of a magnetic dipole.

"Stern – Gerlach" Experiment
~ 1920

nr. of protons

$^{1}_{-}H$ Hydrogen

Proton – spin

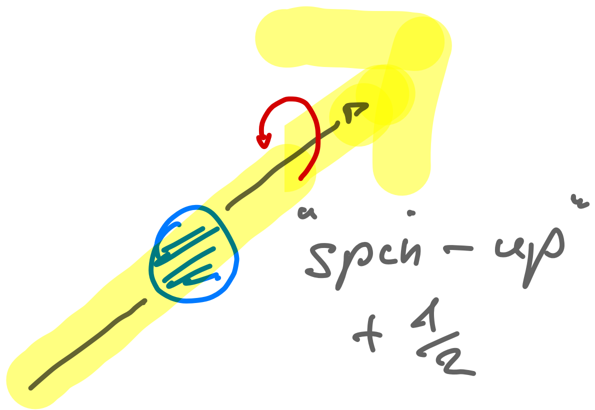
Spin is a quantum-mechanic property of elementary particles.

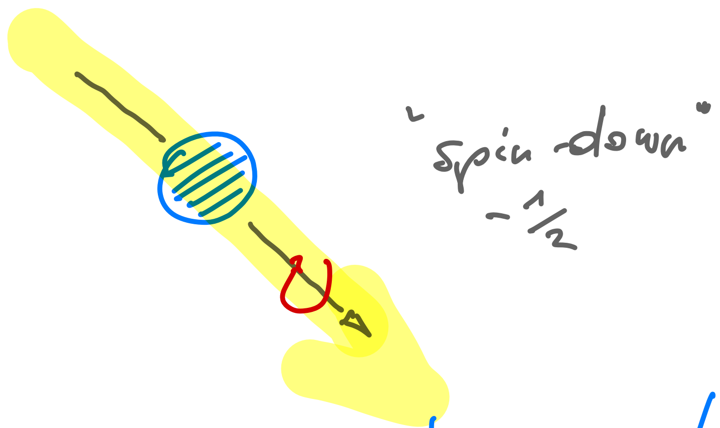
=> intrinsic motion of angular momentum.
(Drehimpuls)

As spin induces a magnetic moment, this allows particles to interact with an external magnetic field!

In case of an <u>odd</u> atomic number (e.g. ^1H), we have non-zero spin.

Quantum spin number of ^1H is $\pm 1/2$.





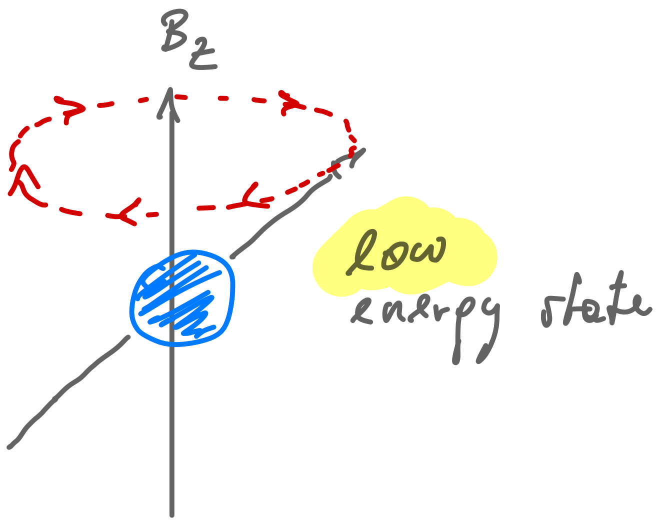
If placed in an external magnetic field, the protons experience <u>torque</u>.

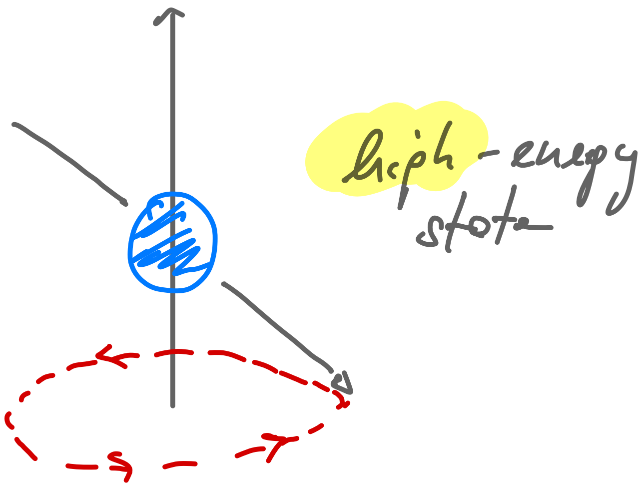
In general

$$D = m \times B$$

torque — magnetic moment — magnetic flux density

$\Rightarrow$ this induces an angular momentum!
The protons start to "precess" at a specific frequency, called the LAMOR FREQUENCY.





when considering more than one proton (i.e., a bulk of protons), there is a slight surplus of those in low energy state.

⇒ This gives a slight magnetization ("net" magnetization) in the direction of the magnetic field!

We can get a measurement of the proton density from this net magnetization – BUT, it's hard to measure, as it is tiny relative to the strength of the external magnetic field!

In MRI, we will perturb the net magnetization in a direction orthogonal to the magnetic field!

Q: How? By inducing electromagnetic waves at exactly the LARMOR FREQUENCY ⇒ this will induce a torque on the magnetic moments. The system will be in a state of excitation!

Spin angular momentum (S)

$$\left(\hbar = \frac{h}{2\pi}\right)$$

$$|S| = \hbar \sqrt{I \cdot (I+1)} \qquad I = \frac{n}{2} \quad (n \in \mathbb{N})$$

(for ^1H we have $n = 1 \Rightarrow I = \frac{1}{2}$)

Associated magnetic moment (μ)

$$\mu = \gamma \cdot S$$

γ → gyromagnetic ratio

In principle, we have $(2I+1)$ energy sublevels, i.e. for ^1H

$$2 \cdot \frac{1}{2} + 1 = 2$$

(Zeeman splitting)

Energy of nucleus:

$$\begin{pmatrix} 0 \\ 0 \\ B_0 \end{pmatrix}$$

$$E = -\langle \mu, B_0 \rangle$$

$\hookrightarrow$ magnetic moment

By convention, B_0 points along the z-direction and the z-component of μ is

$$\mu_z = \gamma \cdot (\pm 1/2) \cdot \hbar$$

$$E_z = -\mu_z \cdot B_0 = -\gamma \cdot \left(\pm \tfrac{1}{2}\right) \hbar B_0$$

The two energy sublevels are

$$\boxed{1} \quad E_z^{(+\frac{1}{2})} = -\gamma \cdot \tfrac{1}{2} \cdot \hbar B_0$$

$$\boxed{2} \quad E_z^{(-\frac{1}{2})} = +\gamma \cdot \tfrac{1}{2} \hbar B_0$$

Diff. between energy sublevels is

$$\Delta E = \gamma \cdot \hbar B_0$$
$$= \gamma \cdot \frac{h}{2\pi} B_0$$

For the torque that the magnetic moment (μ) experiences, we have

$$t = \mu \times B_0 \qquad (\mu = \gamma \cdot s)$$

Also,

$$t = \frac{d}{dt} \underbrace{s}_{\text{spin angular momentum}} = \frac{1}{\gamma} \cdot \frac{d}{dt} \mu$$

$$\Rightarrow \frac{1}{\gamma} \cdot \frac{d}{dt} \mu = \mu \times B_0$$
$$\frac{d}{dt} \mu = \gamma \mu \times B_0$$

If we focus on the net magnetization (M), we have

$$\frac{d}{dt}M = \frac{d}{dt}\sum_i \mu_i$$

$$= \sum_i \frac{d\mu_i}{dt} \qquad \left(\text{using } \frac{d}{dt}\mu = \gamma\mu \times B_0\right)$$

$$= \sum_i \gamma \cdot \mu_i \times B_0$$

$$= \gamma \cdot (M \times B_0)$$

$$\Rightarrow \frac{d}{dt}M = \gamma \cdot (M \times B_0)$$

$$\boxed{\dot{M} = \gamma \cdot (M \times B_0)}$$

Solving $\dot{M} = \gamma \cdot (M \times B_0)$, will give us the motion eq. of the net magnetization vector M.

First, we set up a (time-dependent) rotation around the z-axis:

rotation angle

$$P_\omega(t) = \begin{pmatrix} \cos(\omega t) & \sin(\omega t) & 0 \\ -\sin(\omega t) & \cos(\omega t) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

3x3 rotation matrix

Let $M_0 = M(0)$ be the initial state at time $t = 0$, and

$B_0 = P_\omega(t) \cdot B_0$.

So, we have

$$M(t) = P_\omega(t) \cdot M_p$$

$$\dot{M} = \mu \cdot (M \times B_0)$$

$$\Rightarrow \dot{M} = \mu \cdot (M \times B_0) = \dot{P}_\omega M_p = \mu \cdot (P_\omega M_p) \times (P_\omega B_0)$$

Remark: $P_\omega^T P_\omega = I$

$$\Rightarrow \dot{M} = \mu \cdot (M \times B_0) = P_\omega \cdot \left(P_\omega^T \dot{P}_\omega M_p = \mu \underbrace{M_p}_{M(0)} \times B_0 \right)$$

What is $P_\omega^T \dot{P}_\omega$?

$$-\omega \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = A \qquad \left(A^T = -\omega \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right)$$

So $A^T = -A \Rightarrow$ skew-symmetric matrix

So $(P_w^T \dot{P}_w) M_p$ is a matrix-vector product with $(P_w^T \dot{P}_w)$ skew-symmetric, hence we can write

$$P_w^T \dot{P}_w M_p = -\omega e_z \times M_p \qquad e_z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$= \omega M_p \times e_z \qquad \text{(by anti-commutative?)}$$

$$= \frac{\omega M_p}{\|B_0\|} \times B_0$$

$$= \frac{\omega}{\|B_0\|} M_p \times B_0$$

Overall, we get

$$\dot{M} - \mu \cdot (M \times B_0) = P_w \cdot \left(\frac{\omega}{\|B_0\|} M_p \times B_0 - \mu \cdot M_p \times B_0 \right)$$

$$= \left(\frac{\omega}{\|B_0\|} - \mu \right) \cdot P_w \cdot (M_p \times B_0)$$

$$\underbrace{M(t) = P_\omega(t)\, M_p}_{\text{our model}}$$ is a solution to $\dot{M} = \gamma\, M \times B_0$ if

$$\boxed{\omega = \gamma \cdot \|B_0\|}$$ (i.e., LARMOR FREQUENCY)

Hence, we have shown that the net magnetization vector (M) precesses around the axis (z-axis) of the B_0 field at frequency of $\gamma \cdot \|B_0\|$