CHAPTER 3

Magnetic resonances in nuclei

Charge particles in a magnetic field. Time dependent magnetic fields. Time-dependent perturbation treatment. Rabi formula. Magnetic Resonance Imaging (MRI)

Charge particles in a magnetic field

Assume a nucleon in the presence of a magnetic field carrying only its intrinsic angular momentum, i. e. its 1/2-spin. This would happen is the nucleon is trapped within the region where the experiment is performed. For instance, a proton in some molecules forming a cristal, or a proton in a molecule of human tissue, which is largerly composed of water with two hydrogen atoms (where the nucleus is the proton itself) in each H_2O (water) molecule.

Assuming also that the magnetic field applied externally has the form

$$\boldsymbol{B} = B_0\boldsymbol{k}$$

where B_0 is constant and $\boldsymbol{k}$ is the unit vector in the z-direction, the Hamiltonian is

$$H = -\boldsymbol{\mu}\cdot\boldsymbol{B} = -\mu_z B_0 \tag{1}$$

where the magnetic moment is defined by,

$$\boldsymbol{\mu} = \frac{gq}{2mc}\boldsymbol{s} \tag{2}$$

In contrast to what we presented above, the magnetic moment is now defined with dimensions. This is an unfortunate change of notation. We keep the notation used in each field. In Nuclear Physics the Hamiltonian is as in Eq. (2), while in the applications of magnetic resonances to be analyzed here we will use the Hamiltonian (1).

Since only the intrinsic spin of the particle is considered, the g-factor in Eq. (2) is as the g_s factor above, but for clarity of presentation we give them again here. In the cases of interest in the applications the g-factors are

$$g = \begin{cases} 2.00 & \text{electron} \\ 5.58 & \text{proton} \\ -3.82 & \text{neutron} \end{cases}$$

As before, q is the charge of the particle ($q = -e$ for electron) and $\boldsymbol{s} = (s_x, s_y, s_z)$ are the Pauli matrices given by,

$$s_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad s_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}; \quad s_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The Hamiltonian becomes,

$$H = -\boldsymbol{\mu}\cdot\boldsymbol{B} = -\frac{gq}{2mc}B_0\boldsymbol{s}\cdot\boldsymbol{k} = \omega_0 s_z = \frac{\omega_0\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where

$$\omega_0 = -\frac{gq}{2mc}B_0$$

and the eigenvalues are,

$$H\begin{pmatrix}1\\0\end{pmatrix} = \frac{\omega_0\hbar}{2}\begin{pmatrix}1\\0\end{pmatrix}; \quad H\begin{pmatrix}0\\1\end{pmatrix} = -\frac{\omega_0\hbar}{2}\begin{pmatrix}0\\1\end{pmatrix}$$

There are two stationary (i.e. time independent) states with energies

$$E_\pm = \pm\frac{\omega_0\hbar}{2}$$

If the particle is in the state $+$, it will not decay unless a perturbation disturbs it. When it decays a photon with energy $E_+ - E_- = \hbar\omega_0$ will be emitted which can be measured with great precision, thus allowing one to determine precisely quantities like the g-factor.

Time dependent magnetic fields

A convenient way to perturb the system is by applying a weak and time-dependent magnetic field in the x-direction. Rabi chose for this purpose the form $B_1 \cos\omega t\, \boldsymbol{i}_x$. The perturbation will then vary from $-B_1$ to $+B_1$ as the time increases. The hope is that at a certain value of ω the transition will take place. Notice that B_1 has to be very small in comparison to B_0 in order not to destroy the spectrum determined by B_0 (i.e. the levels $E_\pm$). The problem is then to solve the Hamiltonian

$$H = \omega_0 s_z - \frac{gqB_1}{2mc}\cos\omega t s_x$$

with $\omega_1 = -\dfrac{gqB_1}{2mc}$, one gets

$$H = \frac{\omega_0\hbar}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} + \frac{\omega_1\hbar}{2}\cos\omega t\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}\omega_0 & \omega_1\cos\omega t\\ \omega_1\cos\omega t & -\omega_0\end{pmatrix}$$

where $|\omega_1| \ll |\omega_0|$. One has to use the time-dependent Schrödinger equation, i.e.

$$H\Psi(t) = \mathrm{i}\hbar\frac{\mathrm{d}\Psi(t)}{\mathrm{d}t}$$

Time-dependent perturbation treatment

Since B_1 is very small the solution $\Psi(t)$ should not be very different from the solution corresponding to $B_1 = 0$. We will therefore solve first the case $B_1 = 0$, i. e.

$$\frac{\hbar}{2}\begin{pmatrix}\omega_0 & 0\\0 & -\omega_0\end{pmatrix}\begin{pmatrix}a(t)\\b(t)\end{pmatrix} = \mathrm{i}\hbar\begin{pmatrix}\dot a(t)\\ \dot b(t)\end{pmatrix}$$

where $\dot{a}(t) = \dfrac{\mathrm{d}a(t)}{\mathrm{d}t}$. One thus has

$$\left\{ \begin{array}{rcl} \dfrac{\hbar}{2}\,\omega_0 a(t) & = & \mathrm{i}\hbar\dfrac{\mathrm{d}a(t)}{\mathrm{d}t} \\ -\dfrac{\hbar}{2}\,\omega_0 b(t) & = & \mathrm{i}\hbar\dfrac{\mathrm{d}b(t)}{\mathrm{d}t} \end{array} \right. \quad \Longrightarrow \quad \left\{ \begin{array}{rcl} a(t) & = & a(0)\,\mathrm{e}^{-\mathrm{i}\omega_0 t/2} \\ b(t) & = & b(0)\,\mathrm{e}^{\mathrm{i}\omega_0 t/2} \end{array} \right.$$

The general case is

$$\frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1\cos\omega t \\ \omega_1\cos\omega t & -\omega_0 \end{pmatrix}\begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \mathrm{i}\hbar\begin{pmatrix} \dot{a}(t) \\ \dot{b}(t) \end{pmatrix}$$

since $|\omega_1| \ll |\omega_0|$, one proposes as solution

$$\begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\omega_0 t/2}\,c(t) \\ \mathrm{e}^{\mathrm{i}\omega_0 t/2}\,d(t) \end{pmatrix}$$

which contains the main term explicitly.

The Schrödinger equation becomes

$$\frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1\cos\omega t \\ \omega_1\cos\omega t & -\omega_0 \end{pmatrix}\begin{pmatrix} \mathrm{e}^{-\mathrm{i}\omega_0 t/2}\,c(t) \\ \mathrm{e}^{\mathrm{i}\omega_0 t/2}\,d(t) \end{pmatrix}$$
$$= \mathrm{i}\hbar\begin{pmatrix} -\mathrm{i}\frac{\omega_0}{2}\mathrm{e}^{-\mathrm{i}\omega_0 t/2}c(t) + \mathrm{e}^{-\mathrm{i}\omega_0 t/2}\dot{c}(t) \\ \mathrm{i}\frac{\omega_0}{2}\mathrm{e}^{\mathrm{i}\omega_0 t/2}d(t) + \mathrm{e}^{\mathrm{i}\omega_0 t/2}\dot{d}(t) \end{pmatrix} \qquad (3)$$

with $\cos\omega t = \left(\mathrm{e}^{\mathrm{i}\omega t/2} + \mathrm{e}^{-\mathrm{i}\omega t/2}\right)/2$,

$$\mathrm{i}\begin{pmatrix} \dot{c}(t) \\ \dot{d}(t) \end{pmatrix} = \frac{\omega_1}{4}\begin{pmatrix} \left[\mathrm{e}^{\mathrm{i}(\omega_0+\omega)t} + \mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}\right] d(t) \\ \left[\mathrm{e}^{-\mathrm{i}(\omega_0-\omega)t} + \mathrm{e}^{-\mathrm{i}(\omega_0+\omega)t}\right] c(t) \end{pmatrix}$$

The idea is to change ω in the perturbation term $B_1\cos\omega t$ such that $\hbar\omega_0 \approx \hbar\omega$. Since ω_0 is large, the highly oscillating functions $\mathrm{e}^{\pm\mathrm{i}(\omega_0+\omega)t}$ can be neglected. One thus gets

$$\left\{ \begin{array}{l} \mathrm{i}\dot{c}(t) = \dfrac{\omega_1}{4}\,\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}d(t) \\ \mathrm{i}\dot{d}(t) = \dfrac{\omega_1}{4}\,\mathrm{e}^{-\mathrm{i}(\omega_0-\omega)t}c(t) \end{array} \right. \qquad (4)$$

which is a coupled set of two first order differential equations. To solve it one transforms it in a second order differential equation as follows.

$$\left\{ \begin{array}{l} \mathrm{i}\ddot{c}(t) = \dfrac{\omega_1}{4}\,\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}\Big[\mathrm{i}(\omega_0-\omega)d(t) + \dot{d}(t)\Big] \\ \mathrm{i}\ddot{d}(t) = \dfrac{\omega_1}{4}\,\mathrm{e}^{-\mathrm{i}(\omega_0-\omega)t}\Big[-\mathrm{i}(\omega_0-\omega)c(t) + \dot{c}(t)\Big] \end{array} \right.$$

and replacing $c(t)$ and $\dot{c}(t)$ from Eq. (4)

$$\begin{array}{rcl} \mathrm{i}\ddot{d}(t) & = & \dfrac{\omega_1}{4}\,\mathrm{e}^{-\mathrm{i}(\omega_0-\omega)t}\Big[-\mathrm{i}(\omega_0-\omega)\,\dfrac{4\mathrm{i}}{\omega_1}\,\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}\dot{d}(t) + \dfrac{\omega_1}{4\mathrm{i}}\,\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}d(t)\Big] \\ & = & (\omega_0-\omega)\dot{d}(t) - \mathrm{i}\left(\dfrac{\omega_1}{4}\right)^2 d(t) \end{array}$$

$$\ddot{d}(t) + \mathrm{i}(\omega_0 - \omega)\dot{d}(t) + \left(\frac{\omega_1}{4}\right)^2 d(t) = 0 \tag{5}$$

which has the solution

$$d(t) = A\mathrm{e}^{-\mathrm{i}(\omega_0-\omega)t/2} \sin\Omega t, \quad \Omega = \frac{1}{2}\sqrt{(\omega_0-\omega)^2 + (\omega_1/2)^2} \tag{6}$$

where A is a constant which is determined by the normalization condition, i.e.

$$\left(c^*(t), d^*(t)\right)\begin{pmatrix} c(t) \\ d(t) \end{pmatrix} = \left|c(t)\right|^2 + \left|d(t)\right|^2 = 1$$

One proceeds in the same fashion with $c(t)$ to obtain

$$c(t) = 2A\,\frac{\omega_0 - \omega_1}{\omega_1}\,\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t/2}\left(-\sin\Omega t - \mathrm{i}\sqrt{1 + \frac{\omega_1^2}{4(\omega_0-\omega)^2}}\cos\Omega t\right)$$

Rabi formula

We have assumed that before the perturbation the system is in the state $(+)$, i.e.

$$c(0) = 1; \quad d(0) = 0$$

$$\left|c(0)\right|^2 + \left|d(0)\right|^2 = \left|c(0)\right|^2 = 1$$

From $\left|c(0)\right|^2 = 1$, and after some algebra, one gets,

$$\left|A\right|^2 = \frac{(\omega_1/2)^2}{(\omega_0-\omega)^2 + (\omega_1/2)^2}$$

and the probability that the transition takes place, i.e. that the system is in the state $(-)$ is

$$\left|d(t)\right|^2 = \frac{(\omega_1/2)^2}{(\omega_0-\omega)^2 + (\omega_1/2)^2}\,\sin^2\Omega t \tag{7}$$

and a resonance occurs when $\omega = \omega_0$

Eq. (7) is the Rabi's formula

Magnetic Resonance Imaging (MRI)

One sees that

$$\frac{(\omega_1/2)^2}{(\omega_0-\omega)^2 + (\omega_1/2)^2}\,\frac{\hbar^2}{\hbar^2} = \frac{(\Gamma_1/2)^2}{(E_0-E)^2 + (\Gamma_1/2)^2}$$

where $E = \hbar\omega_0$ is the resonance energy and $\Gamma_1 = \hbar\omega_1$ the width.

In Fig. 1 the form of the signal resulting from this expression is shown.

According to the energy-time relation one has

$$\Gamma_1 T = \hbar$$

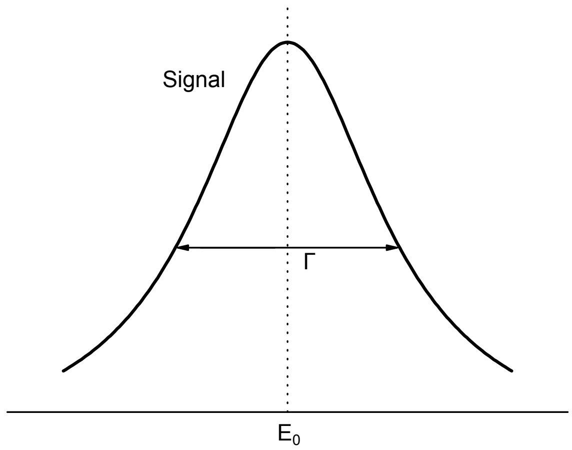

Figure 1: The resonant form of the signal as the energy E, corresponding to the weak magnetic field $\mathbf{B}_1$, approaches the energy E_0 induced by $\mathbf{B}_0$. The width of the resonance is Γ.

where T is the mean life of the initial state (+), i.e.

$$T_{(+)} = \frac{\hbar}{\Gamma_1} = \frac{1}{|\omega_1|} = \frac{2mc}{g|q|B_1}$$

if $B_1 = 0$, $T_{(+)} = \infty$, i.e. the state does not decay

Magnetic Resonance Imaging (MRI)

The signal-energy plot shown in Fig. 1 has been used to investigate the inner structure of materials. In particular, it is used in Medicine to image nuclei of atoms inside the body. Quoting the Wikipedia site

http://en.wikipedia.org/wiki/Magnetic_resonance_imaging
(where some details and farther references can be found)

An MRI machine uses a powerful magnetic field to align the magnetization of some atoms in the body, and radio frequency fields to systematically alter the alignment of this magnetization. This causes the nuclei to produce a rotating magnetic field detectable by the scanner and this information is recorded to construct an image of the scanned area of the body. Strong magnetic field gradients cause nuclei at different locations to rotate at different speeds. 3-D spatial information can be obtained by providing gradients in each direction.

MRI provides good contrast between the different soft tissues of the body, which make it especially useful in imaging the brain, muscles, the heart, and cancers compared with other medical imaging techniques such as computed tomography (CT) or X-rays. Unlike CT scans or traditional X-rays, MRI uses no ionizing radiation.

This last is a very important point, since it implies that no damage of the human tissue is associated with MRI.

In all applications of Magnetic Resonance Imaging one uses SI units and introduces the Bohr magneton

$$\mu_B = \frac{q\hbar}{2mc} \tag{8}$$

In these units the frequency becomes

$$\omega_0 = \frac{gqB_0}{2mc} = \frac{g\mu_B B_0}{\hbar} \tag{9}$$

As already mentioned, for electrons it is $g = 2.00$ and $\mu_B = 5.79 \times 10^{-5}$eV/T, where the unit Tesla is $1\mathrm{T} = 10^4$gauss.

For protons $g = 5.58$ (as also already mentioned) and $\mu_B = 3.15 \times 10^{-8}$eV/T. Remember $\hbar c \approx 200$MeVfm. The precise value of $\hbar$ is $\hbar = 6.58 \times 10^{-22}$MeVsec