FYS-KJM4740
MR Spectroscopy and Tomography – Part I
Solutions Manual to Exercises presented in the Lecture

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The new solid-state NMR spectrometer (located at SINTEF Oslo) which is available for researchers at KI/UiO/Sintef.

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Preface

This booklet is designed to serve as a Solutions Manual to the exercises presented in the NMR course FYS-KJM4740, Part I in “MR Spectroscopy and Tomography”. The major reason for preparing such a booklet was a sincere request from the students. Also, such an extensive and detailed collection of solved problems is believed to be of help to students who meet the challenging world of MR for the first time.

During this first part of this course (Part I) Hansen will (for the first time) arrange a “colloquium” each week (2 hours) in which solution to the exercises will be discussed. A tentative solution of the problems will be submitted to the students after each colloquium. I have no doubt, that in spite of strenuous efforts, there remain errors of one sort or another. I will therefore appreciate any feedback from student who discovers errors in this solution manual (eddÿwh@kjemi.uio.no).

Eddy W. Hansen
UiO January 2015

Exercise 1.1

A charge q moves in a circular loop with frequency ν. According to classical electromagnetic theory, a magnetic dipole moment **μ** is generated, given by;

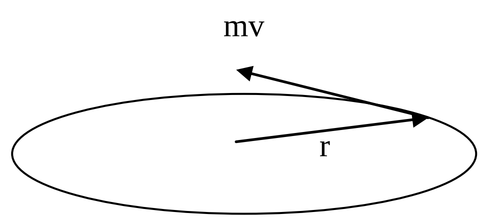
$$\mu = i \cdot A \qquad (1)$$

where i represents the current and A the area enclosed by the circular loop (of radius r). Hence:

$$i = q\upsilon = \frac{q\upsilon \cdot 2\pi}{2\pi} = \frac{q\omega}{2\pi} \quad and \quad A = \pi r^2 \quad \Rightarrow \quad \mu = \frac{1}{2} q\omega r^2 \qquad (2)$$

From the definition of the angular momentum (**L**); **L** = **r** x m**v,** we obtain;

$L = r \cdot mv \cdot \sin\theta = rmv\sin(\pi/2) = rmv = rm \cdot \omega\, r = m\omega r^2$ (see Figure 1) (3)



Combining Eqs 1 and 3;

$$\mu = \frac{q}{2m} L = \gamma L \qquad (4)$$

Exercise 1.2

We start by differentiating the angular momentum **L** with respect to time;

$$\frac{d\vec{L}}{dt} = \frac{d}{dt}\left[\vec{r} \times m\vec{v}\right] = \frac{d\vec{r}}{dt} \times m\vec{v} + \vec{r} \times \frac{d(m\vec{v})}{dt} = \vec{v} \times m\vec{v} + \vec{r} \times \vec{F} = 0 + \vec{r} \times \vec{F} = \vec{\tau} \qquad (1)$$

The symbol F represents the force and τ represents the torque (dreiemoment).

From classical physics we know that a magnetic dipole moment ($\boldsymbol{\mu}$) within a magnetic field $\mathbf{B_0}$ experiences a torque, given by;

$$\boldsymbol{\tau} = \boldsymbol{\mu} \times \mathbf{B_0} \qquad (2)$$

From the previous exercise;

$$\boldsymbol{\mu} = \gamma\mathbf{L} \qquad (3)$$

By combining Eqs 1 – 3, we obtain;

$$\frac{d\vec{\mu}}{dt} = \gamma\vec{\mu} \times \vec{B} \qquad (4)$$

Exercise 1.2 continue

From:

$$\frac{d\vec{\mu}}{dt} = \gamma\vec{\mu} \times \vec{B} \qquad \textbf{(4)}$$

Let us choose $\mathbf{B_0}$ = $B_0\mathbf{k}$**.** Upon inserting this into Eq. 4, we obtain;

$$\frac{d\mu_x}{dt} i + \frac{d\mu_y}{dt} j + \frac{d\mu_z}{dt} k = \gamma \begin{vmatrix} i & j & k \\ \mu_x & \mu_y & \mu_z \\ 0 & 0 & B_0 \end{vmatrix} = \gamma\mu_y B_0 i - \gamma\mu_x B_0 j + 0k \qquad (5)$$

Resulting in the following 3 equations:

$$\frac{d\mu_x}{dt} = \gamma\mu_y B_0 \qquad (5a)$$

$$\frac{d\mu_y}{dt} = -\gamma\mu_x B_0 \qquad (5b)$$

$$\frac{d\mu_z}{dt} = 0 \qquad (5c)$$

If multiplying Eq. 5b by i ($= \sqrt{-1}$) and adding Eq. 5a, the following result appears;

$$\frac{d(\mu_x + i\mu_y)}{dt} = -i\gamma(\mu_x + i\mu_y)B_0 \qquad (6)$$

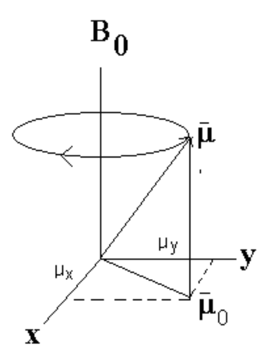
Since we can always write a complex number $\mu_x + i\mu_y$ in the form;

$$\mu_x + i\mu_y = \vec{\mu}_0 = \mu_0 e^{i\omega_0 t} \qquad (= \mu_0 \cos(\omega_0 t) + i\,\mu_0 \sin(\omega_0 t)) \qquad (7)$$

We obtain, by inserting Eq.7 into Eq. 6;

$$\frac{d\vec{\mu}_0}{dt} = -i\gamma B_0\vec{\mu}_0 \Leftrightarrow i\omega_0\mu_0 e^{i\omega_0 t} = -i\gamma B_0\mu_0 e^{i\omega_0 t} \quad \Leftrightarrow \quad \omega_0 = -\gamma B_0 \qquad (8)$$

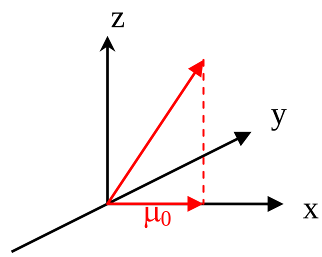
Equation 8 (right) represents the basic NMR equation, or the Larmor equation and shows that the magnetic moment rotates clockwise around the static magnetic field B_0 with a frequency ω_0 ($=-\gamma B_0$) The component of the magnetic moment along the z-axis is constant and independent on time (Eq. 5c).



Exercise 1.2 Alternative:

By combining Eqs 5a and 5b we obtain:

$$\frac{d^2\mu_Y}{dt^2} = -\gamma B_0 \frac{d\mu_X}{dt} = -\gamma^2 B_0^2 \mu_Y \Leftrightarrow \frac{d^2\mu_Y}{dt^2} + \gamma^2 B_0^2 \mu_Y = 0 \qquad (9a)$$



Which the characteristic equation reading;

$$k^2 + \gamma^2 B_0^2 = 0 \quad \Leftrightarrow \quad k = \pm\ i\gamma B_0$$

implying that the general solution can be written:

$$\mu_Y = Ae^{i\gamma B_0 t} + Be^{-i\gamma B_0 t} \qquad (9b)$$

where A and B are constants. By choosing the initial condition to be (see Figure):

$\mu_Y(0) = 0$ and $\mu_X(0) = \mu_0$ we note that B = -A and:

$$\mu_Y = A(e^{i\gamma B_0 t} - e^{-i\gamma B_0 t}) = 2A\frac{e^{i\gamma B_0 t} - e^{-i\gamma B_0 t}}{2i} = 2Ai\sin(\gamma B_0 t) \qquad (9c)$$

According to Eq 5b we find:

$$\mu_X = -\frac{1}{\gamma B_0}\frac{d\mu_y}{dt} = -2Ai\cos(\gamma B_0 t) \qquad (9d)$$

Inserting the initial condition $\mu_X(0) = \mu_0$ we find; $\mu_0 = -2Ai$
After inserting this relation into Eqs 9c and 9d we obtain the general solution:

$$\begin{aligned} \mu_X &= \mu_0\cos(\gamma B_0 t) = \mu_0\cos(-\gamma B_0 t) \\ \mu_Y &= -\mu_0\sin(\gamma B_0 t) = \mu_0\sin(-\gamma B_0 t) \end{aligned} \qquad (10)$$

Hence, the motional frequency ω is identified by $-\gamma B_0$, showing that the vector component μ_0 of the magnetization in the xy-plane rotates anti-clockwise, i.e, along the negative z-axis.

Exercise 1.3

It follows that the macroscopic magnetization M_z^0:

$$M_z^0 = N_+ < u_z^+ > + N_- < \mu_z^- >$$

Energy diagram

N_- (β)

$\Delta E = \hbar\omega = \hbar\gamma B_0$ (where we have used $\omega = \gamma B_0$ in the last term)

N_+(α)

From quantum mechanics:

$$< \mu_z^+ > = \frac{\langle\alpha|\mu_z^+|\alpha\rangle}{\langle\alpha|\alpha\rangle} = \frac{\langle\alpha|\gamma\hbar I_z|\alpha\rangle}{\langle\alpha|\alpha\rangle} = \gamma\hbar\frac{\langle\alpha|I_z|\alpha\rangle}{\langle\alpha|\alpha\rangle} = \frac{\gamma\hbar}{2}\frac{\langle\alpha|\alpha\rangle}{\langle\alpha|\alpha\rangle} = \frac{\gamma\hbar}{2}$$

And

$$< \mu_z^- > = \frac{\langle\beta|\mu_z^+|\beta\rangle}{\langle\beta|\beta\rangle} = \frac{\langle\beta|\gamma\hbar I_z|\beta\rangle}{\langle\beta|\beta\rangle} = \gamma\hbar\frac{\langle\beta|I_z|\beta\rangle}{\langle\beta|\beta\rangle} = -\frac{\gamma\hbar}{2}\frac{\langle\beta|\beta\rangle}{\langle\beta|\beta\rangle} = -\frac{\gamma\hbar}{2}$$

Hence:

$$M_z^0 = (N_+ - N_-)\gamma\hbar/2$$

We will tentatively assume the spin population ratio N_-/N_+ between the two energy levels shown in the Figure to follow a Boltzmann distribution, i.e.;

$$\frac{N_-}{N_+} = \exp\left[-\frac{\Delta E}{kT}\right] = \exp\left[-\frac{\hbar\gamma B_0}{kT}\right] \qquad (1)$$

$\hbar = 1.05 \cdot 10^{-34}$ Js, k = 1.3805x10^{-23} J/K = $\omega = \gamma B_0 \approx 3.9 \cdot 10^7 s^{-1}$

$$\left[\frac{\hbar\gamma B_0}{kT}\right] = \frac{1.05 \cdot 10^{-34} Js \times 3.9 \cdot 10^7 s^{-1}}{1.3810^{-23} J/K \times 300K} \approx 10^{-6} << 1$$

$$\frac{N_-}{N_+} = \exp\left[-\frac{\hbar\gamma B_0}{kT}\right] \approx 1 - \frac{\hbar\gamma B_0}{kT} \text{ (Taylor expansion)}$$

We also have:

$$N_+ + N_- = N_0 \qquad (2)$$

Where N_0 is the total number of spins (or NMR active nuclei) in the sample.

Combining Eqs 1 and 2 we obtain;

$$N_+ = \frac{N_0}{2} \cdot \frac{1}{1 - \hbar\gamma B_0 / 2kT} \approx \frac{N_0}{2}\left[1 + \frac{\hbar\gamma B_0}{2kT}\right] \qquad (3a)$$

The last term in Eq 3a is obtained by noting that:

$$\frac{1}{1-x} = 1 + x \qquad \mathit{for} \qquad x << 1$$

Substituting Eq 3a into Eq 2 we obtain:

$$N_- = \frac{N_0}{2}\left[1 - \frac{\hbar\gamma B_0}{2kT}\right] \qquad (3b)$$

The difference in the number of spins (Δn) between the two energy levels is therefore:

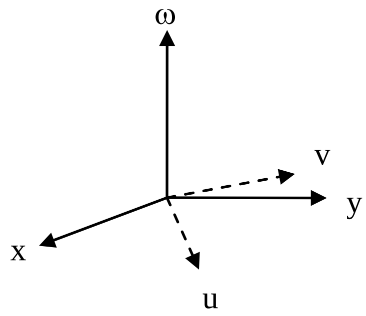
$$\Delta n = N_+ - N_- = \frac{\gamma\hbar B_0 N_0}{2kT} \qquad (3c)$$

The observable, macroscopic magnetization M_z for a spin-1/2 particle is thus;

$$M_z = \mu_z \Delta n = \frac{(\gamma\hbar)^2}{4kT} B N_0$$

Exercise 1.4

We can always describe a motion in a rotating frame (uvz-) of reference rather than in the laboratory frame (xyz-). For instance, in Figure 1 we have introduced a rotating frame of reference, which rotates with a circular frequency ω around the laboratory z-axis (**k**).



Form classical mechanics we can describe the motion of a vector **μ** by the equation:

$$\left(\frac{d\boldsymbol{\mu}}{dt}\right)_{lab} = \left(\frac{d\boldsymbol{\mu}}{dt}\right)_{rel} + \boldsymbol{\omega}\times\boldsymbol{\mu} \qquad (1)$$

Since:

$$\left(\frac{d\boldsymbol{\mu}}{dt}\right)_{lab} = \gamma\boldsymbol{\mu}\times\mathbf{B}_0 \qquad (2)$$

We may combine Eqs 1 and 2 to read:

$$\left(\frac{d\boldsymbol{\mu}}{dt}\right)_{rel} = \left(\frac{d\boldsymbol{\mu}}{dt}\right)_{lab} - \boldsymbol{\omega}\times\boldsymbol{\mu} = \gamma\boldsymbol{\mu}\times\mathbf{B}_0 - \boldsymbol{\omega}\times\boldsymbol{\mu}$$
$$= \gamma\boldsymbol{\mu}\times\mathbf{B}_0 + \boldsymbol{\mu}\times\boldsymbol{\omega} = \gamma\boldsymbol{\mu}\times(\mathbf{B}_0 + \boldsymbol{\omega}/\gamma) \qquad (3)$$

We notice that $(\frac{d\vec{\mu}}{dt})_{rel} = 0$ if $\boldsymbol{\omega} = -\mathbf{B}_0/\gamma = \boldsymbol{\omega}_0$ which means that in a relative frame of reference which rotates with a frequency $\boldsymbol{\omega} = \omega_0\mathbf{k} = -B_0\mathbf{k}$ around the z-axis the magnetic dipole moment **μ** will be in rest. Furthermore, if we write $\mathbf{B}_{eff} = \mathbf{B}_0 + \boldsymbol{\omega}/\gamma$ the magnetic dipole moment will presess around $\mathbf{B}_{eff}$ with a frequency $\boldsymbol{\omega}_{eff} = \gamma\mathbf{B}_{eff} = \gamma\mathbf{B}_0 + \boldsymbol{\omega} = -\boldsymbol{\omega}_0 + \boldsymbol{\omega}$. This implies that in the rotating frame of reference, **μ** will presses around the z-axis with a frequency $\omega_{eff} = (\omega - \omega_0)$ in an apparent magnetic field $\mathbf{B}_{eff}$. Hence, we may express the motion of the dipole moment $\mu_\perp$ in the rotating frame as:

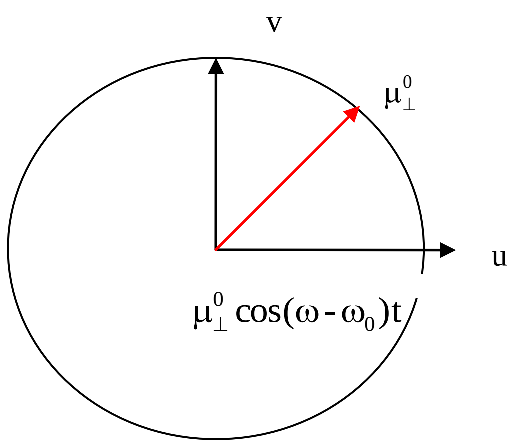
$$\mu_\perp = \mu_\perp^0 e^{i\omega_{eff}t} \qquad = \mu_\perp^0\cos(\omega_{eff}t) + i\mu_\perp^0\sin(\omega_{eff}t)$$

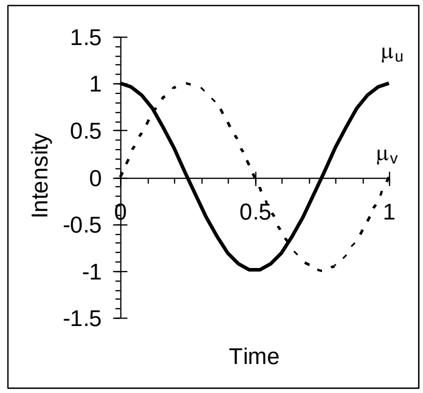
$$= \mu_\perp^0 \cos(\omega - \omega_0)t + i\,\mu_\perp^0 \sin(\omega - \omega_0)t$$

or:

$$\mu_u = \mu_\perp^0 \cos(\omega - \omega_0)t$$

$$\mu_v = \mu_\perp^0 \sin(\omega - \omega_0)t$$





If on resonance, i.e.; $\omega_{eff} = 0$ ($\omega/\gamma = - B_0 = \omega_0/\gamma$), we obtain the solution;

$$\mu_u = \mu_\perp^0$$

$$\mu_u = 0$$

This means that the magnetic dipole is located along the u-axis in the rotating frame of reference. In this frame, the magnetic dipole remains constant and independent of time.

Exercise 1.5

We consider the motion in the rotating frame of reference when on resonance, i.e., $(B_0 - \omega/\gamma)\vec{k} = 0$. This means that:

$$\mathbf{B}_{eff} = B_1\vec{u} + (B_0 - \omega/\gamma)\vec{k} = B_1\vec{u} + 0\vec{k}$$

$$\frac{d\mu_U}{dt}\vec{u} + \frac{d\mu_V}{dt}\vec{v} + \frac{d\mu_Z}{dt}\vec{k} = \gamma\begin{vmatrix} \vec{u} & \vec{v} & \vec{k} \\ \mu_U & \mu_V & \mu_Z \\ B_1 & 0 & 0 \end{vmatrix} = 0\vec{u} + \gamma\mu_Z B_1\vec{v} - \gamma B_1\mu_V\vec{k}$$

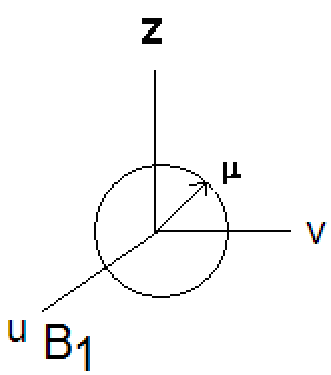
$$\frac{d\mu_U}{dt} = 0 \qquad (5a)$$

$$\frac{d\mu_V}{dt} = \gamma B_1\mu_Z = \quad \omega_1\mu_Z \qquad (5b)$$

$$\frac{d\mu_Z}{dt} = -\gamma B_1\mu_V = \quad -\omega_1\mu_V \qquad (5c)$$

We can easily see that the following solution satisfies the differential equations (by insertion);

$$\mu_V = \mu_0 \sin(\omega_1 t)$$
$$\mu_Z = \mu_0 \cos(\omega_1 t)$$



The magnetic moment is rotating around the negative u-axis with frequency $\boldsymbol{\omega}_1 = -\gamma\mathbf{B}_1$

Exercise 1.6

The local oscillator signal I_{RX}, which is generated internally in the NMR spectrometer, can be represented by a rotating unit vector $\vec{I}_{RX}$ of frequency ω_0. In complex notation we may write:

$$I_{RX} = e^{-\omega_0 t} (= \cos\omega_0 t - i\sin\omega_0 t) \qquad (1)$$

Likewise, the sample signal (only the real part I_S^R is detected) can be written in complex notation:

$$I_S^R = 2I_0 \cos\omega t = I_0 e^{i\omega t} + I_0 e^{-i\omega t} \qquad (2)$$

When mixing (multiplying) the two signals we obtain:

$$I_{obs} = I_{RX} \cdot I_S = 2I_0 \cdot e^{-\omega t} \cdot \left[e^{i\omega_0 t} + e^{-i\omega_0 t}\right] = 2I_0 e^{(\omega_0 - \omega)t} + 2I_0 e^{-(\omega_0 + \omega)t} \qquad (3)$$

Since ω_0 (MHz) ≈ ω, the high-frequency component ($\omega_0 + \omega$) is filtered out by a "low-pass"-filter and we are left with:

$$I_{obs} = e^{(\omega_0 - \omega)t} = \cos((\omega_0 - \omega)t) + i\sin((\omega_0 - \omega)t) \qquad (4)$$

We notice that the signal being detected is identical to the signal in the rotating frame of reference.

Exercise 2.1

In the rotating frame of reference (uvz):

$$d\vec{M}/dt = \gamma\vec{M} \times \vec{B}_{eff} - M_U/T_2\vec{u} - M_V/T_2\vec{v} + (M_0 - M_Z)/T_1\vec{k}$$

$$\vec{B}_{eff} = B_1\vec{u} + (B_0 + \omega/\gamma)\vec{k} = (\omega_1/\gamma)\vec{u} + (-\omega_0 + \omega)/\gamma\vec{k} \qquad (2)$$

$$\frac{d\vec{M}}{dt} = \frac{dM_U}{dt}\vec{u} + \frac{dM_V}{dt}\vec{v} + \frac{dM_z}{dt}k$$
$$= \gamma\begin{vmatrix} \vec{u} & \vec{v} & \vec{k} \\ M_U & M_V & M_Z \\ \omega_1/\gamma & 0 & (-\omega_0+\omega)/\gamma \end{vmatrix} - \frac{M_U}{T_2}\vec{u} - \frac{M_V}{T_2}\vec{v} + \frac{M_0 - M_z}{T_1}\vec{k} \qquad (3)$$

$$\frac{dM_U}{dt} = (\omega - \omega_0)M_V - \frac{M_U}{T_2} \qquad (3a)$$

$$\frac{dM_V}{dt} = -(\omega - \omega_0)M_U + \omega_1 M_z - \frac{M_V}{T_2} \qquad (3b)$$

$$\frac{dM_z}{dt} = -\omega_1 \mathrm{M_V} + \frac{M_0 - M_z}{T_1} \qquad (3c)$$

Case 1
On resonance ($\omega = \omega_0$)

$$\frac{dM_U}{dt} = -\frac{M_U}{T_2} \qquad (3a)$$

$$\frac{dM_V}{dt} = \omega_1 M_z - \frac{\mathrm{M_V}}{T_2} \qquad (3b)$$

$$\frac{dM_z}{dt} = -\omega_1 M_z + \frac{M_0 - M_z}{T_1} \qquad (3c)$$

Exercise 2.2

Using the last set of equations from Exercise 2.1 with $\omega_1 = \gamma B_1 = 0$, we obtain (in the rotating frame);

$$\frac{dM_U}{dt} = -\frac{M_U}{T_2} \qquad (3a)$$

$$\frac{dM_V}{dt} = -\frac{\mathrm{M_V}}{T_2} \qquad (3b)$$

$$\frac{dM_z}{dt} = \frac{M_0 - M_z}{T_1} \qquad (3c)$$

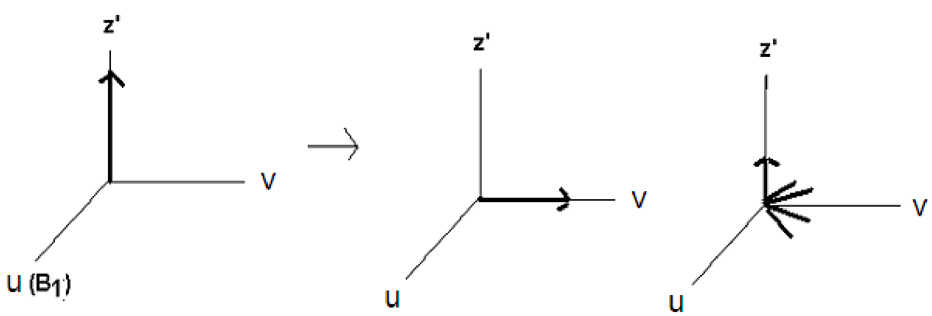
Solution with initial constraints $M_V(0) = M_0$, $M_U(0) = 0$ and $M_z(0) = 0$

$$\frac{\mathrm{dM_V}}{\mathrm{dt}} = -\frac{\mathrm{M_V}}{\mathrm{T_2}} \Leftrightarrow \frac{\mathrm{dM_V}}{\mathrm{M_V}} = -\frac{\mathrm{dt}}{\mathrm{T_2}} \Leftrightarrow \int_{\mathrm{M_0}}^{\mathrm{M_V}} \frac{\mathrm{dM_V}}{\mathrm{M_V}} = -\int_0^{\mathrm{t}} \frac{\mathrm{dt}}{\mathrm{T_2}} \Leftrightarrow \mathrm{M_V} = \mathrm{M_V}(0) \cdot \exp[-\mathrm{t}/\mathrm{T_2}] = \mathrm{M_0} \cdot \exp[-\mathrm{t}/\mathrm{T_2}]$$

$$\frac{dM_z}{dt} = \frac{M_0 - M_z}{T_1} \Leftrightarrow \frac{dM_z}{M_0 - M_z} = \frac{dt}{T_1} \Leftrightarrow \int_{M_z(0)}^{M_z} \frac{dM'_z}{M_0 - M'_z} = \int_0^t \frac{dt}{T_1} \Leftrightarrow -\ln[M_0 - M_z]_0^{M_z} = [t/T_1]$$

$$M_z = M_0 \cdot [1 - \exp(-t/T_1)]$$

Schematics outline of the experiment.



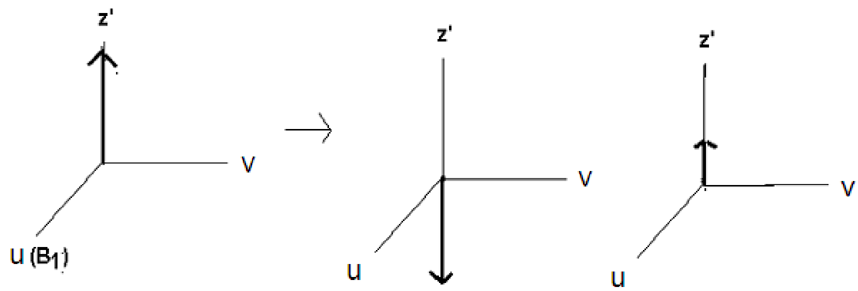
Exercise 2.3

Initial conditions. You first apply an rf-pulse (B_1) such that $M_z(0) = - M_0$.

According to Exercise 2.2, we may write;

$$\frac{dM_z}{dt} = \frac{M_0 - M_z}{T_1} \Leftrightarrow \frac{dM_z}{M_0 - M_z} = \frac{dt}{T_1} \Leftrightarrow \int_{-M_0}^{M_z} \frac{dM_z^{'}}{M_0 - M_z^{'}} = \int_0^t \frac{dt}{T_1} \Leftrightarrow -\ln\left[M_0 - M_z^{'}\right]_{-M_0}^{M_z} = \left[t / T_1\right]$$

$$M_z = M_0 \cdot \left[1 - 2\exp(-t/T)\right]$$



Exercise 2.4

$$\frac{1}{T_1} \propto J(\omega) = \frac{2\tau_c}{1+\omega^2\tau_c^2} \qquad (1)$$

We differentiate Eq. 1 with respect to τ_c and obtain;

$$\frac{d(1/T_1)}{d\tau_c} = \frac{2-2\omega^2\tau_c^2}{\left[1+\omega^2\tau^2\right]^2} \qquad (2)$$

We set Eq 2 equal to 0 and obtain;

$$\tau_c = \frac{1}{\omega}$$

We calculate the second derivative of $1/T_1$ and obtain:

$$f(\omega;\tau_c) = \frac{d^2(1/T_1)}{d\tau_c^2} = -\frac{4\omega^2\tau_c\left[3-\omega^2\tau_c^2\right]}{\left[1+\omega^2\tau^2\right]^3} \qquad (3)$$

$$f(\omega;\tau_c = 1/\omega) = -\omega < 0 \qquad (4)$$

From Eq. 4 we conclude that $1/T_1$ has a maximum for $\tau_c = \frac{1}{\omega}$, i.e.

Note; When increasing the magnetic field strength (increasing ω), the minimum in T_1 shifts to smaller correlation time (Eq 5), i.e., to faster motion (which is equivalent to higher temperature).

Exercise 2.5

Generally the FID can be written:

$$f(t) = e^{-i\omega_0 t} \cdot e^{-t/T_2} \tag{1}$$

Hence, we may write:

$$
\begin{aligned}
F(\omega) &= \int_0^\infty f(t)e^{i\omega t}dt = \int_0^\infty e^{-t/T_2} \cdot e^{-i(\omega-\omega_0)t}dt = \int_0^\infty e^{-t(1/T_2 - i(\omega-\omega_0))}dt \\
&= -\frac{1}{1/T_2 - i(\omega-\omega_0)} e^{-t(1/T_2 - i(\omega-\omega_0))}\Big|_0^\infty = \frac{1}{1/T_2 - i(\omega-\omega_0)} \\
&= \frac{1/T_2 + i(\omega-\omega_0)}{[1/T_2 + i(\omega-\omega_0)][1/T_2 - i(\omega-\omega_0)]} \\
&= \frac{1/T_2}{(1/T_2)^2 + (\omega-\omega_0)^2} + i\frac{\omega-\omega_0}{(1/T_2)^2 + (\omega-\omega_0)^2} \\
&= R(\omega) + iI(\omega)
\end{aligned}
$$

where R(ω) and I(ω) represent the real (u-channel) and imaginary (v-channel) frequency spectra, respectively.

Exercise 2.6

In the rotating frame of reference we may set:

$$d\vec{M}/dt = \gamma\vec{M}\times\vec{B}_{eff} - M_U/T_2\vec{u} - M_V/T_2\vec{v} + (M_0 - M_Z)/T_1\vec{k} \qquad (1)$$

$$\vec{B}_{eff} = B_1\vec{u} + (B_0 + \omega/\gamma + gz)\vec{k} = (\omega_1/\gamma)\vec{u} + (-\omega_0 + \omega + gz)/\gamma\vec{k} \qquad (2)$$

We consider the motion on resonance $(-\omega_0 + \omega) = 0$ and after the magnetization is rotated into the v-axis, i.e., $B_1 = 0$.

Hence:

$$\frac{d\vec{M}}{dt} = \frac{dM_U}{dt}\vec{u} + \frac{dM_V}{dt}\vec{v} + \frac{dM_z}{dt}k$$
$$= \gamma\begin{vmatrix} \vec{u} & \vec{v} & \vec{k} \\ M_U & M_V & M_Z \\ 0 & 0 & gz \end{vmatrix} - \frac{M_U}{T_2}\vec{u} - \frac{M_V}{T_2}\vec{v} + \frac{M_0 - M_z}{T_1}\vec{k}$$

$$\frac{d\vec{M}}{dt} = \frac{dM_U}{dt}\vec{u} + \frac{dM_V}{dt}\vec{v} + \frac{dM_z}{dt}k = \gamma\begin{vmatrix} \vec{u} & \vec{v} & \vec{k} \\ M_U & M_V & M_Z \\ 0 & 0 & gz \end{vmatrix} - \frac{M_U}{T_2}\vec{u} - \frac{M_V}{T_2}\vec{v} + \frac{M_0 - M_z}{T_1}\vec{k} \ (3)$$

$$\frac{dM_U}{dt} = \gamma gzM_V - \frac{M_U}{T_2} \qquad (3a)$$
$$\frac{dM_V}{dt} = -\gamma gzM_U - \frac{M_V}{T_2} \qquad (3b)$$
$$\frac{dM_z}{dt} = \frac{M_0 - M_z}{T_1} \qquad (3c)$$

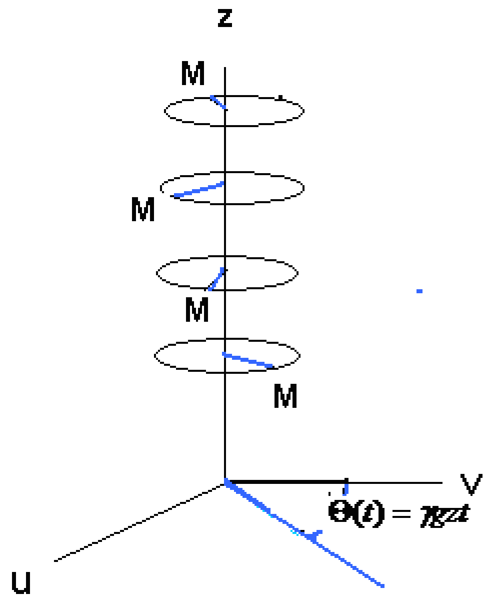
Concerning the transversal magnetization, we multiply Eq. 3b with i $(=\sqrt{-1})$ and add this to Eq. 3a to obtain $M_\perp = M_U + iM_V$:

$$\frac{dM_\perp}{dt} = \gamma gz(M_v - iM_u) - 1/T_2(M_u + iM_v) = -(i\gamma gz - 1/T_2)M_\perp \qquad (4)$$

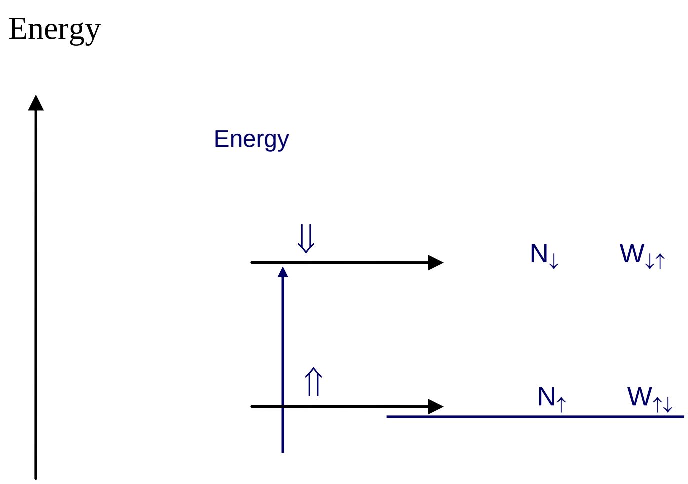
The solution to Eq 4 can be easily found:

$$M_\perp = M_0 e^{-i\gamma gzt}\cdot e^{-t/T_2} = M_0 e^{-\Theta(t)}\cdot e^{-t/T_2}$$

where γgz represents the frequency and $\Theta(t) = \gamma gzt$ represents the phase angle which is proportional to both z and t.



Exercise 2.7



N_i: Number of spins in level i
W_{ij}: Transition probability from level I to j

From general rate-process analysis we may write:

$$\frac{d(N_\downarrow - N_\downarrow^0)}{dt} = -W_{\downarrow\uparrow}(N_\downarrow - N_\downarrow^0) + W_{\uparrow\downarrow}(N_\uparrow - N_\uparrow^0) \tag{1a}$$

$$\frac{d(N_\uparrow - N_\Uparrow^0)}{dt} = -W_{\uparrow\downarrow}(N_\uparrow - N_\uparrow^0) + W_{\downarrow\uparrow}(N_\downarrow - N_\downarrow^0) \tag{1b}$$

Which can be rewritten:

$$\frac{dN_\downarrow}{dt} = -W_{\downarrow\uparrow}(N_\downarrow - N_\downarrow^0) + W_{\uparrow\downarrow}(N_\uparrow - N_\uparrow^0) \tag{1a}$$

$$\frac{dN_\uparrow}{dt} = -W_{\uparrow\downarrow}(N_\uparrow - N_\uparrow^0) + W_{\downarrow\uparrow}(N_\downarrow - N_\downarrow^0) \tag{1b}$$

Subtracting Eq 1a from Eq 1b gives:

$$\frac{d(N_\uparrow - N_\downarrow)}{dt} = -2W_{\uparrow\downarrow}(N_\uparrow - N_\uparrow^0) + 2W_{\downarrow\uparrow}(N_\downarrow - N_\downarrow^0) \tag{2}$$

We introduce the following parameters:

$$\Delta N = N_\uparrow - N_\downarrow \tag{3a}$$

$$N = N_\uparrow + N_\downarrow = N_\uparrow^0 + N_\downarrow^0 \tag{3b}$$

$$\Delta N^0 = N_\uparrow^0 - N_\downarrow^0 \tag{3c}$$

Inserting Eqs 3a – 3c into Eq 2 gives:

$$\frac{d(\Delta N)}{dt} = -W_{\uparrow\downarrow}(\Delta N - \Delta N^0) + W_{\downarrow\uparrow}(\Delta N^0 - \Delta N)$$

$$\frac{d(\Delta N)}{dt} = \Delta N^0 (W_{\uparrow\downarrow} + W_{\downarrow\updownarrow}) - \Delta N (W_{\downarrow\uparrow} + W_{\uparrow\downarrow}) \qquad (4)$$

Since the observed magnetization is proportional to the number of active isotopes (nuclei), we may write $M_Z = k\Delta N$ where k is a constant. Hence, Eq 4 can be reformulated into:

$$\frac{dM_z}{dt} = (W_{\uparrow\downarrow} + W_{\downarrow\uparrow})(M_0 - M_z) \qquad (5)$$

The spin-lattice relaxation rate $1/T_1$ is defined as the sum of the transition probabilities, i.e.;

$$\frac{1}{T_1} = W_{\uparrow\downarrow} + W_{\downarrow\uparrow} \qquad (6)$$

Inserting Eq 6 into Eq 5 gives:

$$\frac{dM_z}{dt} = \frac{M_0 - M_z}{T_1} \qquad (7)$$

Eq 7 is identical to the corresponding Equation presented by the Bloch Equation !!!

Exercise 3.1

If introducing a gradient field $\vec{g}$ along any direction $\vec{r}$ in space we obtain:

$$\vec{g} = \frac{\partial B_x}{\partial x}\vec{i} + \frac{\partial B_y}{\partial y}\vec{j} + \frac{\partial B_z}{\partial z}\vec{k} \tag{1}$$

$$\vec{r} = \vec{x}\vec{i} + y\vec{j} + z\vec{k} \tag{2}$$

In the following we will consider only a gradient field in the direction of the external field, i.e., along the z-direction. Hence,

$$\vec{g}\cdot\vec{r} = \vec{g}\cdot\bar{k} = z\frac{\partial B_z}{\partial z} = z\cdot g_0(t) \tag{3}$$

Eq 3 implicitly assumes that the field gradient $\partial B_z / \partial z$ is constant (= g_0), and hence independent on the space-coordinates). This implies that the total magnetic field B_Z along the z-axis is:

$$B_z = B_0 + z\cdot g_0(t) \tag{4a}$$

Hence, if on resonance, the following magnetic field appears within the rotating frame of reference:

$$\vec{B}_{eff} = zg_0\vec{k} \tag{4b}$$

Again, within the rotating frame of reference:

$$\frac{dM_u}{dt}\vec{u} + \frac{dM_v}{dt}\vec{v} + \frac{dM_z}{dt}k = \gamma\begin{vmatrix} u & v & k \\ M_u & M_v & M_z \\ 0 & 0 & zg_0 \end{vmatrix} - \frac{M_u}{T_2}\vec{u} - \frac{M_v}{T_2}\vec{v} + \frac{M_0 - M_z}{T_1}k + \mathrm{D}\nabla^2\mathrm{M}$$

$$\frac{\partial \mathrm{M_u}}{\partial \mathrm{t}} = \gamma \mathrm{g_0 z}\cdot\mathrm{M_v} - \frac{\mathrm{M_u}}{\mathrm{T_2}} + \mathrm{D}\nabla^2\mathrm{M_u} \tag{5a}$$

$$\frac{\partial \mathrm{M_v}}{\partial \mathrm{t}} = \gamma \mathrm{g_0 z}\cdot\mathrm{M_u} - \frac{\mathrm{M_v}}{\mathrm{T_2}} + \mathrm{D}\nabla^2\mathrm{M_v} \tag{5b}$$

$$\frac{\partial \mathrm{M_z}}{\partial \mathrm{t}} = -\frac{\mathrm{M_z} - \mathrm{M_0}}{\mathrm{T_1}} + \mathrm{D}\nabla^2\mathrm{M_z} \tag{5c}$$

Since we are interested only in the transversal magnetization (uv-plane), we will apply a “complex-number-technique”, i.e., introducing the complex magnetization $\hat{M}$ defined by: $\widehat{M} = M_u + iM_v$. After multiplying Eq 5b by the complex number i and adding Eq 5a, we obtain:

$$\frac{\partial \widehat{M}}{\partial t} = -i\gamma g_0 z\widehat{M} - \frac{\widehat{M}}{T_2} + D\nabla^2\widehat{M} \tag{6}$$

Exercise 3.2

From Eq 7:

$$\frac{\partial \widehat{M}}{\partial t} = -i\gamma g_0 z\widehat{M} - \frac{\widehat{M}}{T_2} + D\nabla^2 \widehat{M} \tag{7}$$

Noting that B_z may be a function of both z and t (Eq 4a) we will look for a solution in which also $\hat{M}$ is a function of z and t and independent of x and y, i.e., $\hat{M} = \hat{M}(z,t)$. This implies that $\nabla^2 \widehat{M} = \frac{\partial^2 \widehat{M}}{\partial z^2}$. If we try to find a solution of the form:

$$\widehat{M}(z,t) = M_0 e^{-t/T_2} \widehat{m}(z,t) \tag{8}$$

where the T_2-term is factored out, we notice by inserting Eq 8 into Eq 7 that;

$$-\frac{1}{T_2} M_0 e^{-t/T_2} \widehat{m} + M_0 e^{-t/T_2} \frac{\partial \widehat{m}}{\partial t} = -i\gamma z g_0 M_0 e^{-t/T_2} \widehat{m} - M_0 e^{-t/T_2} \frac{\widehat{m}}{T_2} + M_0 e^{-t/T_2} D \frac{\partial^2 \widehat{m}}{\partial z^2} \tag{9}$$

which simplifies to:

$$\frac{\partial \widehat{m}}{\partial t} = -i\gamma z g_0 \widehat{m} + D\frac{\partial^2 \widehat{m}}{\partial z^2} \tag{10}$$

Exercise 3.3

A general solution to Eq 10 can be written as a complex function with amplitude $\Psi(t')$ and a phase factor $\Omega(z,t')$, i.e.;

$$\hat{m}(z,t') = \Psi(t') \cdot \Omega(z,t') \tag{11}$$

where:

$$\Omega(z,t') = \exp\left[-i\gamma z \int_0^{t'} g_o(t'')dt''\right] \tag{12}$$

As can be easily seen the term $\theta = \left[-i\gamma z \int_0^{t'} g_o(t'')dt''\right]$ represents the phase angle with $\Omega(z,t')$ having modulus 1 (Eq 13)_

$$abs(\Omega(z,t')) = \Omega(z,t') \cdot \Omega^*(z,t') = \exp\left[-i\gamma z 0\int_0^{t'} g_0(t'')dt'''\right] \cdot \exp\left[\gamma z \int_0^{t'} g_0(t'')dt''\right] = 1 \tag{13}$$

Noting that:

$$\frac{\partial \hat{m}}{\partial t'} = \Psi \frac{\partial \Omega}{\partial t'} + \Omega \frac{\partial \Psi}{\partial t'} = \Psi\Omega \cdot \left[-i\gamma z g_0(t')\right] + \Omega \frac{\Psi}{\Psi}\frac{\partial \Psi}{\partial t'} = \hat{m} \cdot \left[-i\gamma z g_0(t') + \frac{1}{\Psi}\frac{\partial \Psi}{\partial t'}\right] \tag{14a}$$

$$\frac{\partial \hat{m}}{\partial z} = \Psi \cdot \frac{\partial \Omega}{\partial z} = \Psi \cdot \Omega \cdot \left[-i\gamma \int_0^{t'} g_0(t'')dt''\right] \tag{14b}$$

$$\frac{\partial^2 \hat{m}}{\partial z^2} = \Psi \frac{\partial^2 \Omega}{\partial z^2} = \Psi\Omega \cdot \left[-i\gamma \int_0^{t'} g_0(t'')dt''\right]^2 = \hat{m}\left[-i\gamma \int_0^{t'} g_0(t'')dt''\right]^2 \tag{14c}$$

We obtain the following simple Eq for Ψ when substituting Eqs 14a) –c) into Eq 10:

$$\begin{aligned}
\frac{1}{\Psi}\frac{d\Psi}{dt'} &= D\left[-i\gamma \int_0^{t'} g_0(t'')dt''\right]^2 = -D\gamma^2\left[\int_0^{t'} g_0(t'')dt''\right]^2 \\
\frac{d\ln\Psi}{dt'} &= -D\gamma^2\left[\int_0^{t'} g_0(t'')dt''\right]^2 \\
\Psi(t) &= \exp\left[-D\gamma^2 \int_0^{t}\left[\int_0^{t'} g_0(t'')dt''\right]^2 dt'\right]
\end{aligned} \tag{15}$$

Additional 1

Let us consider the phase term $\Omega(z,t')$ (see Eq 12 in Exercise 4) of the magnetization;

$$\Omega(z,t') = \exp\left[-i\gamma z\int_0^{t'} g_o(t'')dt''\right] \tag{1}$$

After the gradient pulse has been on for a time τ, the phase angle θ at position z_0 can be written:

$$\theta(\tau) = -\gamma z_0 \int_0^{\tau} g_0(t'')dt'' \tag{2}$$

This means that the magnetization $\hat{m}$ can be written;

$$\hat{m} = \Psi(\tau)\cdot\Omega(z,\tau) = \Psi(\tau)\cdot\exp\left[-i\theta(\tau)\right] \tag{3}$$

What happens to the phase when applying a π-pulse (rf-pulse) along the x-axis?

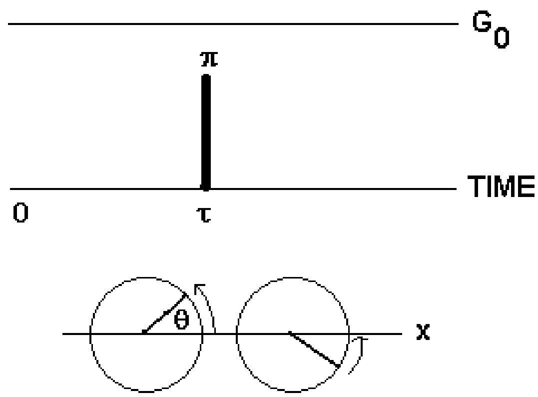


Figure 1A

Since g_0 (= $\delta B_z/\delta z$) is a constant, the phase angle $\theta(\tau)$ equals:

$$\theta(\tau) = \gamma g_0 z\int_0^{\tau} dt = \gamma g_0 z\tau \tag{4}$$

The question is now, what will be the phase angle θ(τ+) just after the π-pulse?
The angle will be $\theta(\tau+) = -\theta(\tau)$. Hence, the effect of a π-pulse (regarding the change in phase angle) is the same as changing the sign of the gradient pulse, i.e., changing g = G_0 to g = – G_0. In short, we may consider the following analogous situation (Figure 1B):

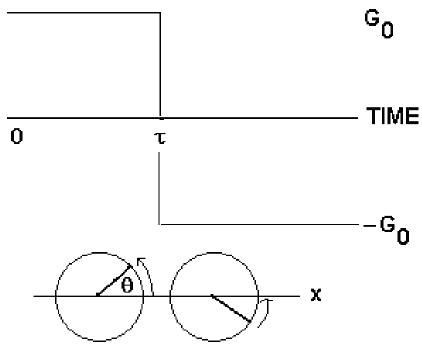


Figure 1B

One question remains, how can we express the phase angle θ as a function of time when considering the pulse-gradient scheme in Figure 1B?

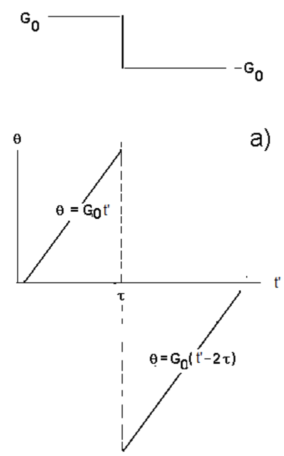


Figure 1C

Figure a) shows how the phase angle $\theta = \gamma \int_0^{t'} g_0(t'')dt''$ changes with time t′ and reveals a discontinuity in θ at t′ = τ because of the π-pulse.

Additional 2

Objective: We consider a one-dimensional diffusion process along the x-axis. Show that the root-means-squares distance (rms) $\langle x^2 \rangle$ traversed during the diffusion time t equals 2Dt where D is the diffusivity C(x,t) represents the concentration of the species at time t and position x, respectively. The function C(x,t) can be solved by the Fick diffusion equation:

$$\frac{\delta C}{\delta t} = D\frac{\delta^2 C}{\delta x^2}$$

The solution to Eq 1 depends on the initial time- and spatial constraints on C. For free diffusion we may write:

$$C(x,t) = \frac{C_0}{\sqrt{4\pi Dt}}\exp(-x^2/4Dt) \qquad (1)$$

Show that:

$$\langle x^2 \rangle = \frac{\int_0^\infty x^2 C(x,t)dx}{\int_0^\infty C(x,t)dx} = 2Dt \qquad (2)$$

Solution:

Note that we may write Eq 2 according to:

$$\langle x^2 \rangle = \frac{\int_0^\infty x^2 \exp(-x^2/4Dt)dx}{\int_0^\infty \exp(-x^2/4Dt)} \qquad (3)$$

If we start with the following integral:

$$I(t) = \int_0^\infty \exp(-x^2/4Dt)dx$$

and use partial integration technique, i.e.:

$$u' = 1 \qquad \Leftrightarrow u = x$$

$$v = \exp(-x^2/4Dt) \Leftrightarrow v' = (-2x/4Dt)\exp(-x^2/4Dt)$$

We may write:

$$\int_0^\infty 1\cdot \exp(-x^2/4Dt)dx = \int_0^\infty = x\exp(-x^2/4Dt)_0^\infty - (-1/2Dt)\int_0^\infty x^2 \exp(-x^2/4Dt)dx$$

Hence : (4)

$$\int_0^\infty \exp(-x^2/4Dt)dx = 0 + (1/2Dt)\int_0^\infty x^2 \exp(-x^2)dx$$

As can be easily seen, Eq 4 can be written:

Hence : 1

$$\frac{\int_0^\infty x^2 \exp(.x^2/4Dt)}{\int_0^\infty \exp(-x^2/4Dt)dx} = 2Dt$$

qed

Chapter 4. Some introductory remarks and comments

From basic quantum mechanics one may show that for a nucleus of spin I, a number of (2I+1) different spin functions exist. These functions are simply denoted:

$|I,m>$ for m = -I, -I + 1, .., 0, … I – 1, I

In particular, for I = ½ (^{1}H, ^{13}C, ^{31}P, ^{19}F,…) we have only two spin functions denoted, respectively:

$|\alpha> = |1/2,1/2>$ and $|\beta> = |1/2, -1/2>$

Again, from basic quantum mechanics the following operator properties may be defined

$\bar{I}_z|\alpha> = 1/2|\alpha>$ $\bar{I}_z|\beta> = -1/2|\beta>$ (3.1a)

It is frequently useful to apply the so called shift operators, or the "raising" $(\hat{I}^{+})$ and "lowering" $(\hat{I}^{-})$ operators, respectively:

$$\hat{I}^{\pm}|I,m\rangle = [I(I+1) - m(m\pm 1)]^{1/2}|I, m\pm 1\rangle$$

Hence:

$$\hat{I}^{+}|\alpha\rangle = \hat{I}^{+}|1/2,1/2\rangle = 0 \qquad \hat{I}^{+}|\beta\rangle = \hat{I}^{+}|1/2,-1/2\rangle = 1\cdot|1/2,1/2\rangle = |\alpha\rangle$$

$$\hat{I}^{-}|\alpha\rangle = \hat{I}^{-}|1/2,1/2\rangle = 1\cdot[1/2,-1/2) = (\beta) \qquad \hat{I}^{-}|\beta\rangle = 0$$

We define:

$$\hat{I}_x = 1/2\left[I^{+} + I^{-}\right] \qquad \hat{I}_y = -i/2\left[I^{+} - I^{-}\right]$$

Hence;

$\bar{I}_x|\alpha> = 1/2|\beta>$ $\bar{I}_x|\beta> = 1/2|\alpha>$ (3.1b)
$\bar{I}_y|\alpha> = i/2|\beta>$ $\bar{I}_x|\beta> = -i/2|\alpha>$ (3.1c)

What is the classical energy (E) of two interacting magnetic dipoles (μ_A and μ_B) in a magnetic field B_0?

$$E = -\vec{\mu}_A \cdot \vec{B}_0 - \vec{\mu}_B \cdot \vec{B}_0 - \vec{\mu}_A \cdot \vec{\mu}_B$$

The corresponding quantum mechanical energy operator H is:

$$\begin{aligned}\hat{\mathrm{H}} &= -\gamma\hbar\hat{I}_{zA}B_0 - \gamma\hbar\hat{I}_{zB}B_0 - \gamma\hbar\hat{I}_{zA}\cdot\gamma\hbar\hat{I}_{zB} \\ &= -\omega_0\hbar\hat{I}_{zA} - \omega_0\hbar\hat{I}_{zB} - \gamma^2\hbar^2\hat{I}_{zA}\cdot\hat{I}_{zB} \qquad (ergs) \\ &= -\nu_A\hat{I}_{zA} - \nu_B\hat{I}_{zB} - J_{AB}\hat{I}_{zA}\cdot\hat{I}_{zB} \qquad (Hz)\end{aligned}$$

The “constant” J_{AB} is denoted the coupling constant.

Uttrykker produktet av spinnoperatorene I_A og I_B ved operatorene I^+ og I^-:

$$\hat{I}_A\cdot\hat{I}_B = \left[\hat{I}_{XA}i + \hat{I}_{YA}j + \hat{I}_{ZA}k\right]\cdot\left[\hat{I}_{XB}i + \hat{I}_{YB}j + \hat{I}_{ZB}k\right]$$

$$\hat{I}_A\cdot\hat{I}_B = \hat{I}_{XA}\hat{I}_{XB} + \hat{I}_{YA}\hat{I}_{YB} + \hat{I}_{ZA}\hat{I}_{ZB}$$

$$\hat{I}_A\cdot\hat{I}_B = 1/4\left[\hat{I}_A^+ + \hat{I}_A^-\right]\cdot\left[\hat{I}_B^+ + \hat{I}_B^-\right] - 1/4\left[\hat{I}_A^+ - \hat{I}_A^-\right]\cdot\left[\hat{I}_B^+ - \hat{I}_B^-\right] + \hat{I}_{ZA}\hat{I}_{ZB}$$

$$\hat{I}_A\cdot\hat{I}_B = 1/4\left[\hat{I}_A^+\cdot\hat{I}_B^+ + \hat{I}_A^+\cdot\hat{I}_B^- + \hat{I}_A^-\cdot\hat{I}_B^+ + \hat{I}_A^-\cdot\hat{I}_B^- - \hat{I}_A^+\cdot\hat{I}_B^+ + \hat{I}_A^+\cdot\hat{I}_B^- + \hat{I}_A^-\cdot\hat{I}_B^+ - \hat{I}_A^-\cdot\hat{I}_B^-\right] + \hat{I}_{ZA}\hat{I}_{ZB}$$

$$\hat{I}_A\cdot\hat{I}_B = 1/2\left[\hat{I}_A^+\cdot\hat{I}_B^- + \hat{I}_A^-\cdot\hat{I}_B^+\right] + \hat{I}_{ZA}\hat{I}_{ZB}$$

In short, we may write the Hamiltonian for a two-spin system as:

$$\hat{\mathrm{H}} = -\upsilon_A\hat{I}_{ZA} - \nu_B\cdot\hat{I}_{ZB} + J_{AB}/2\left[\hat{I}_A^+\cdot\hat{I}_B^- + \hat{I}_A^-\cdot\hat{I}_B^+\right] + J_{AB}\hat{I}_{ZA}\hat{I}_{ZB}$$

Exercise 4.1

The spin-functions |α> and |β> are defined as orthonormal *eigenfunctions* of the z component of the spin operator I_z (see Eq 3.1) and satisfy the following equations:

$$\int\langle\alpha(X)\|\alpha(X)\rangle d\tau = \int\alpha\alpha d\tau = \int\langle\beta(X)\|\beta(X)\rangle d\tau = \int\beta\beta d\tau = 1 \quad (3.1a)$$
$$\int\langle\alpha(X)\|\beta(X)\rangle d\tau = \int\alpha\beta d\tau = \int\langle\beta(X)\|\alpha(X)\rangle d\tau = \int\beta\alpha d\tau = 0 \quad (3.1b)$$

X refers to the actual nucleus in question. For a two-spin system (X = A, B) we may define 4 product functions $\Theta_i\,(i = 1-4)$;

$$|\Theta_1\rangle = |\alpha(A)\alpha(B)\rangle = |\alpha\alpha\rangle \quad (3.2a)$$
$$|\Theta_2\rangle = |\alpha(A)\beta(B)\rangle = |\alpha\beta\rangle \quad (3.2b)$$
$$|\Theta_3\rangle = |\beta(A)\alpha(B)\rangle = |\beta\alpha\rangle \quad (3.2c)$$
$$|\Theta_4\rangle = |\beta(A)\beta(B)\rangle = |\beta\beta\rangle \quad (3.2d)$$

Since these spin-functions (Θ_i) are orthonormal (see Eq 3.1), we may construct a set of orthonormal *eigenfunctions (* Ψ_i *)*, defined as a linear combination of Θ_i , i.e.;

$$|\Psi_1\rangle = C_{11}|\Theta_1\rangle + C_{12}|\Theta_2\rangle + C_{13}|\Theta_3\rangle + C_{14}|\Theta_4\rangle \quad (3.3a)$$
$$|\Psi_2\rangle = C_{21}|\Theta_1\rangle + C_{22}|\Theta_2\rangle + C_{23}|\Theta_3\rangle + C_{24}|\Theta_4\rangle \quad (3.3b)$$
$$|\Psi_3\rangle = C_{31}|\Theta_1\rangle + C_{32}|\Theta_2\rangle + C_{33}|\Theta_3\rangle + C_{34}|\Theta_4\rangle \quad (3.3c)$$
$$|\Psi_4\rangle = C_{41}|\Theta_1\rangle + C_{42}|\Theta_2\rangle + C_{43}|\Theta_3\rangle + C_{44}|\Theta_4\rangle \quad (3.3d)$$

Since these equations are *eigen-functions* to the Hamiltonian, the following equations must be valid for each i (=1 – 4):

$$\begin{aligned}\hat{H}|\Psi_i\rangle &= E|\Psi_i\rangle \\ &= C_{i1}\hat{H}|\Theta_1\rangle + C_{i2}\hat{H}|\Theta_2\rangle + C_{i3}\hat{H}|\Theta_3\rangle + C_{i4}\hat{H}|\Theta_4\rangle \\ &= EC_{i1}|\Theta_1\rangle + EC_{i2}|\Theta_2\rangle + EC_{i3}|\Theta_3\rangle + EC_{i4}|\Theta_4\rangle\end{aligned} \quad (3.4)$$

We multiply by $\langle\Theta_j|$ and integrate over the entire spin space:

$$\int \langle \Theta_j | \hat{\mathrm{H}} | \Psi_i \rangle d\tau = E \int \langle \Theta_j || \Psi_i \rangle$$

$$\Updownarrow$$

$$\int C_{i1} \langle \Theta_j | \hat{\mathrm{H}} | \Theta_1 \rangle d\tau + \int C_{i2} \langle \Theta_j | \hat{\mathrm{H}} | \Theta_2 \rangle d\tau + C_{i3} \int \langle \Theta_j | \hat{\mathrm{H}} | \Theta_3 \rangle d\tau + C_{i4} \int \langle \Theta_j | \hat{\mathrm{H}} | \Theta_4 \rangle d\tau$$
$$= EC_{i1} \int \langle \Theta_j || \Theta_1 \rangle d\tau + E \int C_{i2} \langle \Theta_j || \Theta_2 \rangle d\tau + EC_{i3} \int \langle \Theta_j || \Theta_3 \rangle d\tau + EC_{i4} \int \langle \Theta_j || \Theta_4 \rangle d\tau$$

$$\Updownarrow$$

$$C_{i1} H_{j1} + C_{i2} H_{j2} + C_{i3} H_{j3} + C_{i4} H_{j4}$$
$$= EC_{i1} \delta_{j1} + EC_{i2} \delta_{j2} + EC_{i3} \delta_{j3} + EC_{i4} \delta_{j4}$$

For j = 1 to 4, the following set of linear equations arise:

$$\begin{aligned}
C_{i1} H_{11} + C_{i2} H_{12} + C_{i3} H_{13} + C_{i4} H_{14} &= EC_{i1} \\
C_{i1} H_{21} + C_{i2} H_{22} + C_{i3} H_{23} + C_{i4} H_{24} &= EC_{i2} \\
C_{i1} H_{31} + C_{i2} H_{32} + C_{i3} H_{33} + C_{i4} H_{34} &= EC_{i3} \\
C_{i1} H_{41} + C_{i2} H_{42} + C_{i3} H_{43} + C_{i4} H_{44} &= EC_{i4}
\end{aligned} \tag{3.4}$$

Eq 3.4 can be formulated in matrix notation, i.e.;

$$\hat{H} \cdot \vec{C} = 0 \Leftrightarrow \begin{pmatrix} H_{11} - E & H_{12} & H_{13} & H_{14} \\ H_{21} & H_{22} - E & H_{23} & H_{24} \\ H_{31} & H_{32} & H_{33} - E & H_{34} \\ H_{41} & H_{42} & H_{43} & H_{44} - E \end{pmatrix} \cdot \begin{pmatrix} C_{i1} \\ C_{i2} \\ C_{i3} \\ C_{i4} \end{pmatrix} = 0 \tag{3.5}$$

A non-trivial solution $(\vec{C} \neq 0)$ to Eq 3.5 exists only and only if the determinant of $\hat{H}$ is identical to 0, i.e.:

$$\begin{pmatrix} H_{11} - E & H_{12} & H_{13} & H_{14} \\ H_{21} & H_{22} - E & H_{23} & H_{24} \\ H_{31} & H_{32} & H_{33} - E & H_{34} \\ H_{41} & H_{42} & H_{43} & H_{44} - E \end{pmatrix} = 0 \tag{3.6}$$

Which is equivalent to Eq 27.

We will not calculate all the terms H_{pq} (we leave this to the student!) but we illustrate how this can be performed (see Exersice 3.0):

$$\hat{\mathrm{H}} | \Theta_1 \rangle = -\upsilon_A \hat{I}_{ZA} | \Theta_1 \rangle - \nu_B \cdot \hat{I}_{ZB} | \Theta_1 \rangle + J_{AB} / 2 \left[\hat{I}_A^+ \cdot \hat{I}_B^- + \hat{I}_A^- \cdot \hat{I}_B^+ \right] | \Theta_1 \rangle + J_{AB} \hat{I}_{ZA} \hat{I}_{ZB} | \Theta_1 \rangle$$

$$\hat{\mathrm{H}} | \alpha(A) \alpha(B) \rangle = -\upsilon_A \hat{I}_{ZA} | \alpha(A) \alpha(B) \rangle - \nu_B \cdot \hat{I}_{ZB} | \alpha(A) \alpha(B) \rangle +$$

$$J_{AB} / 2 \hat{I}_A^+ \cdot \hat{I}_B^- | \alpha(A) \alpha(B) \rangle + J_{AB} / 2 \hat{I}_A^- \cdot \hat{I}_B^+ | \alpha(A) \alpha(B) \rangle + J_{AB} \hat{I}_{ZA} \hat{I}_{ZB} | \alpha(A) \alpha(B) \rangle$$

$$\hat{\mathrm{H}}|\alpha(A)\alpha(B)\rangle = -\frac{1}{2}\upsilon_A \alpha(B)|\alpha(A)\rangle - \frac{1}{2}\nu_B \cdot \alpha(A)|\alpha(B)\rangle +$$

$$\frac{J_{AB}}{2} \cdot 0 \cdot |\beta(B)\rangle + \frac{J_{AB}}{2}|\beta(A)\rangle \cdot 0 + J_{AB} \cdot \frac{1}{2}|\alpha(A)\rangle \cdot \frac{1}{2}|\alpha(B)\rangle$$

$$\hat{\mathrm{H}}|\Theta_1\rangle = (-\upsilon_A/2 - \nu_B/2 + J_{AB}/4)|\phi_1\rangle = E_1|\Theta_1\rangle_1 \qquad (3.7a)$$

Likewise:

$$\hat{\mathrm{H}}|\Theta_2\rangle = (-\upsilon_A/2 + \nu_B/2 - J_{AB}/4)|\Theta_2\rangle + J_{AB}/2)|\Theta_3\rangle \qquad (3.7b)$$

$$\hat{\mathrm{H}}|\Theta_3\rangle = (\upsilon_A/2 - \nu_B/2 - J_{AB}/4)|\Theta_3\rangle + J_{AB}/2)|\Theta_2\rangle \qquad (3.7c)$$

$$\hat{\mathrm{H}}|\Theta_4\rangle = (\upsilon_A/2 + \nu_B/2 + J_{AB}/4)|\Theta_4\rangle = E_4|\Theta_4\rangle_4 \qquad (3.7d)$$

We easily see that $H_{12} = H_{21} = 0$, $H_{13} = H_{31} = 0$, $H_{14} = H_{41} = 0$, $H_{42} = H_{24} = 0$, $H_{43} = H_{34} = 0$ because $\int\langle\Theta_1\|\Theta_2\rangle d\tau = \int\langle\Theta_1\|\Theta_3\rangle d\tau = \int\langle\Theta_1\|\Theta_4\rangle d\tau = \int\langle\Theta_2\|\Theta_4\rangle d\tau = \int\langle\Theta_3\|\Theta_4\rangle d\tau = 0$

Exercise 4.2

Because two of the spin-functions (Θ_1 and Θ_4) are *eigenfunctions* while Θ_2 og Θ_3 are not.

Exercise 4.3

If we consider the total z-component of our spin-operator (two-spin system AB), as defined by:

$$\hat{F}_Z = \hat{I}_{zA} + \hat{I}_{zB} \tag{3.7}$$

we notice that:

$$\begin{aligned}
\hat{F}_Z|\Theta_1\rangle &= \hat{I}_{zA}|\Theta_1\rangle + \hat{I}_{zB}|\Theta_1\rangle \\
&= \hat{I}_{zA}|\alpha(A)\alpha(B)\rangle + \hat{I}_{zB}|\alpha(A)\alpha(B)\rangle \\
&= 1/2|\alpha(A)\alpha(B)\rangle + 1/2|\alpha(A)\alpha(B)\rangle \\
&= 1\cdot|\alpha(A)\alpha(B)\rangle \\
&= 1\cdot|\Theta_1\rangle
\end{aligned}$$

$$\begin{aligned}
\hat{F}_Z|\Theta_2\rangle &= \hat{I}_{zA}|\Theta_2\rangle + \hat{I}_{zB}|\Theta_2\rangle \\
&= \hat{I}_{zA}|\alpha(A)\beta(B)\rangle + \hat{I}_{zB}|\alpha(A)\beta(B)\rangle \\
&= 1/2|\alpha(A)\beta(B)\rangle - 1/2|\alpha(A)\beta(B)\rangle \\
&= 0\cdot|\alpha(A)\beta(B)\rangle. \\
&= 0\cdot|\Theta_2\rangle
\end{aligned}$$

$$\begin{aligned}
\hat{F}_Z|\Theta_3\rangle &= \hat{I}_{zA}|\Theta_3\rangle + \hat{I}_{zB}|\Theta_3\rangle \\
&= \hat{I}_{zA}|\beta(A)\alpha(B)\rangle + \hat{I}_{zB}|\beta(A)\alpha(B)\rangle \\
&= -1/2|\beta(A)\beta(B)\rangle + 1/2|\beta(A)\alpha(B)\rangle \\
&= 0\cdot|\beta(A)\alpha(B)\rangle \\
&= 0\cdot|\Theta_3\rangle
\end{aligned}$$

$$\begin{aligned}
\hat{F}_Z|\Theta_4\rangle &= \hat{I}_{zA}|\Theta_4\rangle + \hat{I}_{zB}|\Theta_4\rangle \\
&= \hat{I}_{zA}|\beta(A)\beta(B)\rangle + \hat{I}_{zB}|\beta(A)\beta(B)\rangle \\
&= -1/2|\beta(A)\beta(B)\rangle - 1/2|\beta(A)\beta(B)\rangle \\
&= -1\cdot|\beta(A)\beta(B)\rangle \\
&= -1\cdot|\Theta_4\rangle
\end{aligned}$$

This means that the *eigenvalues* F_z of the operator $\hat{F}_Z$ are the same for the two spin-functions Θ_2 and Θ_3, implying that a linear combination of these two functions will define the actual *eigenfunction*

Exercise 4.4

Two find the two remaining energies, we must solve the matrix equation:

$$\begin{pmatrix} H_{22}-E & H_{23} \\ H_{32} & H_{33}-E \end{pmatrix} \cdot \begin{pmatrix} C_{i2} \\ C_{i3} \end{pmatrix} = 0$$

A non-trivial solution exists if and only if the secular determinant is 0, i.e.:

$$\begin{vmatrix} H_{22}-E & H_{23} \\ H_{32} & H_{33}-E \end{vmatrix} = 0 \qquad (3.8)$$

Using Eqs. 7a-d, we can calculate H_{ij}, i.e.:

$$H_{23} = \langle \Theta_2 | \hat{H} | \Theta_3 \rangle = \left\langle \Theta_2 \left| \hat{H} \right| (\frac{1}{2}\nu_A - \frac{1}{2}\nu_B - \frac{1}{4}J_{AB}) | \Theta_3 \rangle + \frac{1}{2}J_{AB} | \Theta_2 \rangle \right\rangle = \frac{1}{2}J_{AB} \qquad (3.9a)$$

Likewise, we derive the following results:

$$H_{22} = -\frac{1}{2}(\nu_A - \nu_B) - \frac{1}{4}J_{AB} \qquad (3.9b)$$

$$H_{33} = \frac{1}{2}(\nu_A - \nu_B) - \frac{1}{4}J_{AB} \qquad (3.9c)$$

Inserting Eqs. 3.9a–c into Eq 3.8 gives:

$$\begin{aligned} E_2 &= -\frac{J_{AB}}{4} - \frac{1}{2}\sqrt{J_{AB}^2 + (\nu_A - \nu_B)^2} \\ E_3 &= -\frac{J_{AB}}{4} + \frac{1}{2}\sqrt{J_{AB}^2 + (\nu_A - \nu_B)^2} \end{aligned} \qquad (3.10)$$

Exercise 4.5

If introducing the following short hand notations:

$$V = \nu_A + \nu_B$$
$$C = \sqrt{J_{AB}^2 + (\upsilon_A - \upsilon_B)^2}$$

we obtain from Exercises 3.1 and 3.4 the following energy level diagrams:

Table 1. Energy levels and corresponding "allowed" transitions

Level	Energy	Fz	Transition	Wave function
1	V/2 + J/4	-1	* *	$\|\Psi_1\rangle = a_{11}\|\Theta_1\rangle$
2	C/2-J/4	0	* * *	$\|\Psi_2\rangle = a_{21}\|\Theta_2\rangle + a_{22}\|\Theta_3\rangle$
3	-C/2-J/4	0	* * *	$\|\Psi_3\rangle = a_{31}\|\Theta_2\rangle + a_{32}\|\Theta_3\rangle$
4	-V/2+J/4	1	* *	$\|\Psi_4\rangle = a_{44}\|\Theta_4\rangle$

Hence, the following transition may be easily derived:

$\Delta E_{1\to2} = E_1 - E_2 = (V - C + J)/2$
$\Delta E_{1\to3} = E_1 - E_3 = (V + C + J)/2$
$\Delta E_{2\to4} = E_2 - E_4 = (V - C + J)/2$
$\Delta E_{3\to4} = E_3 - E_4 = (V - C - J)/2$

Exercise 4.6

In order to determine the *eigenfunctions (Table 1*) we must determine the constants a_{ij} (Table 1). This can be easily performed by noting that these functions are orthonormal, i.e.:

$$\int \langle \Psi_i \| \Psi_j \rangle d\tau = \delta_{ij} \qquad (=1 \quad if \quad i = j\,, \quad = 0 \quad if \quad i \neq j)$$

One may easily show that this results in the following equations (show this!)

$|\Psi_1\rangle = |\Theta_1\rangle$
$|\Psi_2\rangle = \cos\theta|\Theta_2\rangle + \sin\theta|\Theta_3\rangle$
$|\Psi_3\rangle = -\sin\theta|\Theta_2\rangle + \cos\theta|\Theta_3\rangle$
$|\Psi_4\rangle = |\Theta_4\rangle$

Vi skal bestemme intensitetet (overgangssannsynligheten) $I_{m=-1 \Rightarrow m=0}$ mellom nivå 3 og 4 og benytter resultatet fra kvantemekanikken;

$$I_{m=-1\to m=0} = (\int \psi_{m=-1}\left[\hat{I}_-^A + \hat{I}_-^B\right]\psi_{m=0} d\tau)^2$$

Vi beregner først;

$$\hat{I}_-^A \psi_{m=0} = \hat{I}_-^A(\cos\theta\cdot\alpha(A)\beta(B) + \hat{I}_-^A \sin\theta\cdot\beta(A)\alpha(B))$$
$$= \cos\theta\cdot\beta(B)\hat{I}_-^A\alpha(A) + \sin\theta\cdot\alpha(B)\hat{I}_-^A\beta(A)$$
$$= \cos\theta\cdot\beta(B)\beta(A) - \sin\theta\cdot\alpha(B)\cdot 0$$
$$= \cos\theta\cdot\beta(B)\beta(A)$$

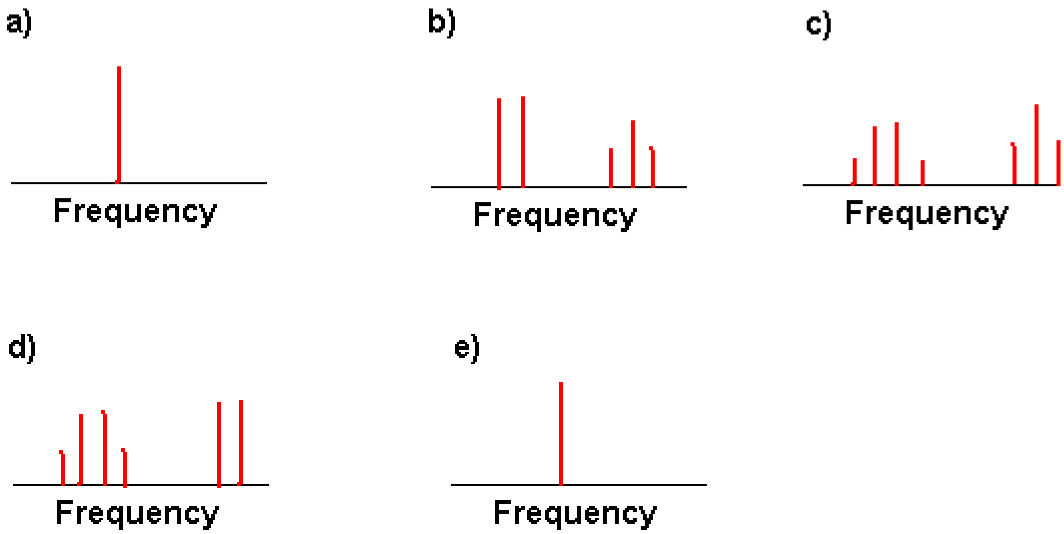
Tilsvarende finner vi for;

$$\hat{I}_-^B \psi_{m=0} = \hat{I}_-^B(\cos\theta\cdot\alpha(A)\beta(B) + \hat{I}_-^B \sin\theta\cdot\beta(A)\alpha(B))$$
$$= \cos\theta\cdot\alpha(A)\hat{I}_-^B\beta(A) + \sin\theta\cdot\beta(A)\hat{I}_-^B\alpha(B)$$
$$= \cos\theta\cdot\alpha(A)\cdot 0 - \sin\theta\cdot\beta(A)\cdot\beta(B)$$
$$= -\sin\beta(A)\beta(B)$$

Innsatt i første likning;

$$I_{m=-1\to m=0} = (\int \psi_{m=-1}\left[\hat{I}_-^A + \hat{I}_-^B\right]\psi_{m=0} d\tau)^2$$
$$= (\int \beta(A)\beta(B)\cdot\left[\cos\theta\cdot\beta(B)\beta(A) - \sin\theta(A)\beta(B)\right]d\tau)^2$$
$$= (\cos\theta\int\beta(A)\beta(A)d\tau_A\cdot\int\beta(B)\beta(B)d\tau_B - \sin\theta\int\beta(A)\beta(A)d\tau_A\cdot\int\beta(B)\beta(B)d\tau_B)^2$$
$$= (\cos\theta - \sin\theta)^2 = \cos^2\theta - 2\sin\theta\cos\theta + \sin^2\theta$$
$$= 1 - \sin(2\theta)$$

Exercise 4.7 and 4.8



Miscellaneous 1

In the rotating frame of reference (uvz):

$$d\vec{M}/dt = \gamma\vec{M} \times \vec{B}_{eff} - M_U/T_2\vec{u} - M_V/T_2\vec{v} + (M_0 - M_Z)/T_1\vec{k}$$

$$\vec{B}_{eff} = B_1\vec{u} + (B_0 + \omega/\gamma)\vec{k} = (\omega_1/\gamma)\vec{u} + (-\omega_0 + \omega)/\gamma\vec{k} \qquad (2)$$

$$\begin{aligned} \frac{d\vec{M}}{dt} &= \frac{dM_U}{dt}\vec{u} + \frac{dM_V}{dt}\vec{v} + \frac{dM_z}{dt}k \\ &= \gamma\begin{vmatrix} \vec{u} & \vec{v} & \vec{k} \\ M_U & M_V & M_Z \\ \omega_1/\gamma & 0 & (-\omega_0+\omega)/\gamma \end{vmatrix} - \frac{M_U}{T_2}\vec{u} - \frac{M_V}{T_2}\vec{v} + \frac{M_0 - M_z}{T_1}\vec{k} \end{aligned} \qquad (3)$$

$$\frac{dM_U}{dt} = (\omega - \omega_0)M_V - \frac{M_U}{T_2} \qquad (3a)$$

$$\frac{dM_V}{dt} = -(\omega - \omega_0)M_U + \omega_1 M_z - \frac{M_V}{T_2} \qquad (3b)$$

$$\frac{dM_z}{dt} = -\omega_1 \mathrm{M_V} + \frac{M_0 - M_z}{T_1} \qquad (3c)$$

Case 1
On resonance ($\omega = \omega_0$)

$$\frac{dM_U}{dt} = -\frac{M_U}{T_2} \qquad (3a)$$

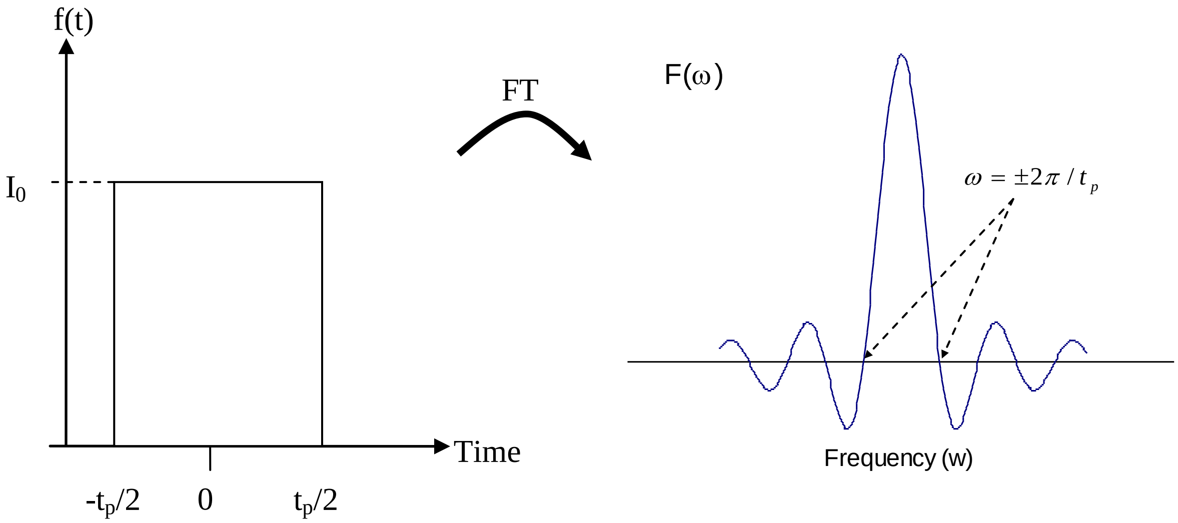
$$\frac{dM_V}{dt} = \omega_1 M_z - \frac{\mathrm{M_V}}{T_2} \qquad (3b)$$

$$\frac{dM_z}{dt} = -\omega_1 M_z + \frac{M_0 - M_z}{T_1} \qquad (3c)$$

Miscellaneous 2

Rf-pulses – bandwidth and all that

Fourier transform F(ω) of a rectangular pulse f(t) in the time domain.



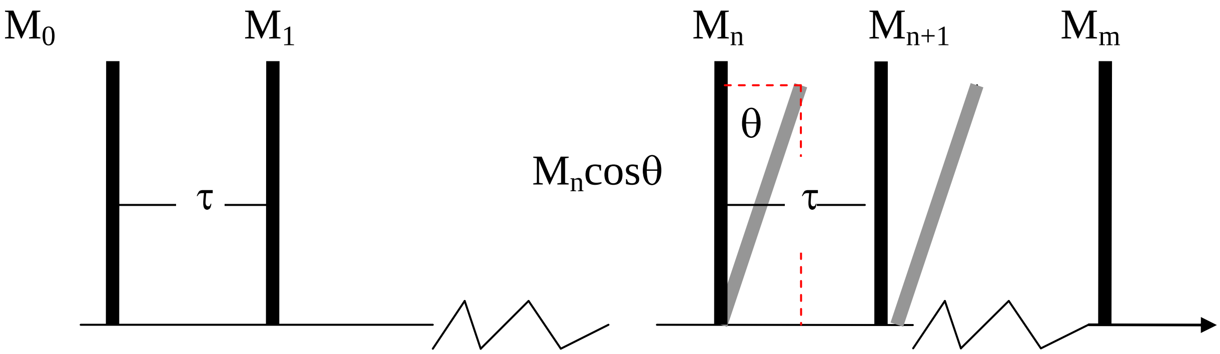
$$F(\omega) = \int_{-t_p/2}^{t_p/2} f(t)\cdot e^{i\omega t}dt = \int_{-t_p/2}^{0} I_0 \cdot e^{i\omega t}dt + \int_{0}^{t_p/2} I_0 \cdot e^{i\omega t}dt \qquad \text{(E1)}$$

By substituting u = -t (du = –dt) in the first integral on the right side of Eq E1 we obtain:

$$\begin{aligned}
F(\omega) &= -\int_{t_p/2}^{0} I_0 \cdot e^{-i\omega u}du + \int_{0}^{t_p/2} I_0 \cdot e^{i\omega t}dt \\
&= \int_{0}^{t_p/2} I_0 \cdot e^{-i\omega u}du + \int_{0}^{t_p/2} I_0 \cdot e^{i\omega t}dt \\
&= \int_{0}^{t_p/2} I_0 \cdot e^{-i\omega t}dt + \int_{0}^{t_p/2} I_0 \cdot e^{i\omega t}dt \\
&= I_0\left[\int_{0}^{t_p/2} \cdot e^{-i\omega t} + \int_{0}^{t_p/2} \cdot e^{i\omega t}\right]dt = 2I_0 \int_{0}^{t_p/2} \frac{\left[e^{i\omega t} + e^{-i\omega t}\right]}{2} = 2I_0 \int_{0}^{t_p/2} \cos[\omega t]dt \\
&= \frac{2I_0}{\omega}\sin[\omega t]\Big|_{0}^{t_p/2} \\
&= I_0 \frac{\sin[\omega t_p/2]}{\omega/2}
\end{aligned} \qquad \text{(E2)}$$

The function on the right of the last equation is denoted a sinc-function and is plotted on the Figure. We note that the first null-point of the F(ω) appears at $\omega = 2\pi/t_p$. If we apply a 90^0-pulse ($t_p = t_{90}$) we must have: $Rotation \quad angle = \omega_1 \cdot t_{90} = \gamma B_1 t_{90} = \pi/2 \Leftrightarrow B_1 = \pi/(2\cdot\gamma t_{90})$

Miscellaneous 3



M_n represents the magnetization along the z-axis after (n+1) rf-pulses. We will assume that $T_2 << T_1$. Hence, according to the Bloch equation we may write:

$$\frac{dM_z}{dt} = \frac{M_0 - M_z}{T_1}$$

$$\int_{M_n\cos\theta}^{M_{n+1}} \frac{dM_z}{M_0 - M_z} = \int_0^{\tau} \frac{dt}{T_1}$$

$$\ln \frac{M_0 - M_{n+1}}{M_0 - M_n \cos\theta} = -\frac{t}{T_1} \qquad (1)$$

$$M_{n+1} = M_0 - (M_0 - M_n \cos\theta)\exp(.-\tau/T_1)$$

$$M_{n+1} = M_0(1 - \exp(-\tau/T_1)) + M_n \cos\theta \cdot \exp(-\tau/T_1)$$

By setting $a = (1 - \exp(-\tau/T_1))\,and \quad b = \cos\theta \cdot \exp(-\tau/T_1)$ we can write:

$$M_{n+1} = aM_0 + bM_n \qquad (2)$$

Eq 2 is a recursion formula leading to:

$$M_1 = aM_0 + bM_0 = (a+b)M_0$$

$$M_2 = aM_0 + bM_1 = M_0(a + ab + b^2)$$

$$M_3 = aM + bM_2 = M_0(a + ab + ab^2 + b^3)$$

We realize the following general expression:

$$M_{n+1} = M_0(a + ab + ab^2 + ... + ab^n + b^{n+1})$$

$$M_{n+1} = aM_0((1 + b + b^2 + ... + b^n) + M_0 b^{n+1}) \qquad (3)$$

From simple algebra we find (by noting that b < 1):

$$1+b+b^2+...+b^n = \frac{(b^{n+1}-1)}{b-1} = \frac{1-b^{n+1}}{1-b} \tag{4}$$

Hence:

$$\begin{aligned} M_{n+1} &= aM_0((1+b+b^2+....+b^n)+M_0b^{n+1}) \\ M_{n+1} &= aM_0\frac{1-b^{n+1}}{1-b}+M_0b^{n+1} \\ M_{n+1} &= M_0(\frac{a(1-b^{n+2})}{1-b}+b^{n+1}) \end{aligned} \tag{5}$$

Since b < 0, we may always find an n such that both b^n and b^{n+1} are close to 0, i.e.,

$$M_{n+1} = M_0\frac{a}{1-b} = M_0\frac{1-\exp(-\tau/T_1)}{1-\cos\theta\cdot\exp(-\tau/T_1)} \tag{6}$$

Note, Eq 6is identical to Eq 2 when setting $M_{n+1} = M_n = M_{ss}$, i.e.,

$$M_{ss} = aM_0 + bMss$$

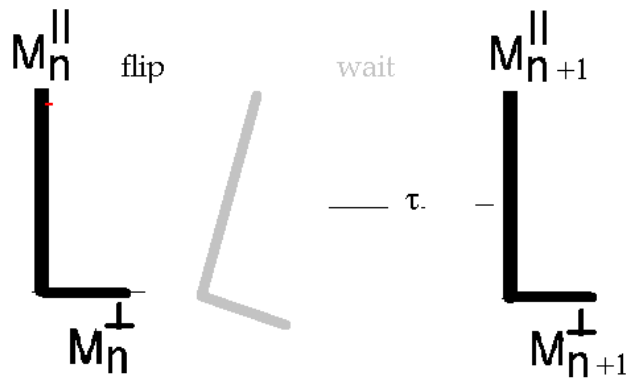
$$M_{ss} = \frac{a}{1-b}M_0$$

Concerning Eq 4, we note that by setting

$$\begin{aligned} &S_n = 1+b+b^2+...+b^n \\ &and \\ &bS_n = b+b^2+....+b^{n+1} \\ &we \quad obtain: \\ &S_n - bS_n = 1-b^{n+1} \\ &S_n = \frac{1-b^{n+1}}{1-b} \end{aligned} \tag{7}$$

Miscellaneous 4

Problem (litt vanskelig)



After performing the same experiment n times with a time delay τ between each experiment the longitudinal magnetization and the transverse magnetization have become M_n^{II} and $M_n^{\perp}$, respectively (see Figure). After applying an rf-pulse, the magnetization components are rotated (flipped) around the negative x-axis (pointed into the paper plane) by an angle θ. Calculate the transverse and longitudinal magnetization component after a time τ has elapsed?

What are the steady-state magnetization components?

Solution

An initial equilibrium magnetization M_0^{II} along the z-axis (same direction as $\mathbf{B}_0$) is rotated an angle θ (along the x-axis) and then left for a time τ before again being flipped an angle θ along the x-axis. After n such sequences of rotation/waiting we denote the longitudinal magnetization component by M_n^{II} and the transversal magnetization component by $M_n^{\perp}$, respectively. After the next (n + 1) rotations or flips, we write:

$$M_n^{II,flip} = M_n^{II}\cos\theta - M_n^{\perp}\sin\theta \quad (1a)$$

$$M_n^{\perp,flip} = M_n^{II}\sin\theta + M_n^{\perp}\cos\theta \quad (1b)$$

After leaving these magnetizations for a time τ they will relax toward M_{n+1}^{II} and $M_{n+1}^{\perp}$ according to:

$$\frac{dM_Z}{dt} = \frac{M_0 - M_Z}{T_1} \Leftrightarrow \int_{M_n^{II,flip}}^{M_{n+1}^{II}} \frac{dM'}{M_0 - M_z'} = \int_0^{\tau} \frac{dt}{T_1}$$

$$-\ln\frac{M_0-M_{n+1}^{II}}{M_0-M_n^{II,flip}}=\frac{\tau}{T_1}$$

$$M_0-M_{n+1}^{II}=\left[M_0-M_n^{II,flip}\right]\exp(-\tau/T_1)=\left[M_0-M_n^{II}\cos\theta+M_n^{\perp}\sin\theta\right]\exp(-\tau/T_1)$$

$$M_{n+1}^{II}=M_0-M_0\exp(-\tau/T_1)+M_n^{II}\cos\theta\exp(-\tau/T_1)-M_n^{\perp}\sin\theta\exp(-\tau/T_1) \qquad (2a)$$

Likewise, for the transversal magnetization we may write:

$$\frac{dM_{\perp}}{dt}=-\frac{M_{\perp}}{T_2}\Leftrightarrow\int_{M_{n+1}^{\perp I,flip}}^{M_{n+1}^{\perp}}\frac{dM_{\perp}'}{M_{\perp}}=-\int_0^{\tau}\frac{dt}{T_2}$$

$$\ln\frac{M_{n+1}^{\perp}}{M_{n+1}^{\perp,flip}}=-\frac{\tau}{T_2}$$

$$M_{n+1}^{\perp}=M_{n+1}^{\perp,flip}\exp(-\tau/T_2)=M_n^{II}\sin\theta\exp(-\tau/T_2)+M_n^{\perp}\cos\theta\exp(-\tau/T_2) \qquad (2b)$$

After a few rotations/waiting periods we obtain a steady state situation in which:

$$M_{n+1}^{II}=M_n^{II}=M_{ss}^{II}$$
$$and \qquad (3)$$
$$M_{n+1}^{\perp}=M_n^{\perp}=M_{ss}^{\perp}$$

Eq 3 inserted into Eqs 2a and 2b gives:

$$M_{ss}^{II}=M_0-M_0\exp(-\tau/T_1)+M_{ss}^{II}\cos\theta\exp(-\tau/T_1)-M_{ss}^{\perp}\sin\theta\exp(-\tau/T_1)$$
$$\Updownarrow \qquad (4a)$$
$$M_{ss}^{II}=\frac{M_0-M_0\exp(-\tau/T_1)-M_{ss}^{\perp}\sin\theta\exp(-\tau/T_1)}{1-\cos\theta\exp(-\tau/T_1)}$$

$$M_{ss}^{\perp}=M_{ss}^{II}\sin\theta\exp(-\tau/T_2)+M_{ss}^{\perp}\cos\theta\exp(-\tau/T_2)$$
$$\Updownarrow \qquad (4b)$$
$$M_{ss}^{\perp}=M_{ss}^{II}\frac{\sin\theta\exp(-\tau/T_2)}{1-\cos\theta\exp(-\tau/T_2)}$$

There are some interesting situations to be discussed from Eqs 4a and 4b.

A) If $\theta=\pi/2$

$$M_{ss}^{\perp}=M_{ss}^{II}\exp(-\tau/T_2) \qquad (5a)$$

Hence:

$$M_{ss}^{II} = M_0 - M_0 \exp(-\tau/T_1) - M_{ss}^{II} \exp(-\tau(1/T_1 + 1/T_2))$$
$$M_{SS}^{II} = M_0 \frac{1-\exp(-\tau/T_1)}{1+\exp(-\tau(1/T_1+1/T_2))} \qquad (5b)$$

B) If $\theta = \pi$

$$M_{ss}^{\perp} = 0 \qquad (6a)$$

$$M_{ss}^{II} = M_0 \frac{1-\exp(-\tau/T_1)}{1+\exp(-\tau/T_1)} \qquad (6b)$$

C) $t/T_2 >> 1$ (this is the same as T_2 is very short (applying a spoiler pulse)) and leads to:

$$M_{ss}^{\perp} = M_{ss}^{II} \frac{\sin\theta \exp(-\tau/T_2)}{1-\cos\theta \exp(-\tau/T_2)} \approx 0$$

Hence:

$$M_{ss}^{II} = M_0 \frac{1-\exp(-\tau/T_1)}{1-\cos\theta \exp(-\tau/T_1)} \quad \Leftrightarrow M_0 = \frac{1-\cos\theta \exp(-\tau/T_1)}{1-\exp(-\tau/T_1)} M_{ss}^{II} \qquad (7a)$$

If $\theta = \pi/2 \Leftrightarrow M_{ss}^{II} = M_0(1-\exp(-\tau/T_1))$ (7b)

If $\theta = \pi \Leftrightarrow M_{ss}^{II} = M_0 \frac{1-\exp(-\tau/T_1)}{1+\exp(-\tau/T_1)}$ (7c)