The new solid-state NMR spectrometer (located at SINTEF Oslo) which will be available for researchers at KI/UiO/Sintef from spring 2009.
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.

Relative to the first edition which was prepared in 2007 some few corrections have been made in this second edition. I have no doubt however, that in spite of strenuous efforts, there remain errors of one sort or another. I will be pleased and grateful to hear from any reader who discovers errors (eddýwh@kjem.uio.no)

Eddy W. Hansen
UiO January 2009
Exercise 1.1

A charge $q$ moves in a circular loop with frequency $\nu$. According to classical electromagnetic theory, a magnetic dipole moment $\mu$ is generated, given by:

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

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

$$i = q \nu = \frac{q \nu \pi}{2\pi} = \frac{q \omega}{2\pi} \quad \text{and} \quad A = \pi R^2 \quad \Rightarrow \quad \mu = \frac{1}{2} q \omega R^2 \quad (2)$$

From the definition of the angular momentum ($L$); $L = R \times mv$, we obtain;

$$L = rmv \sin \theta = rmv \sin (\pi/2) = rmv = rm \omega \tau = m \omega \tau^2 \quad (3)$$

Combining Eqs 1 and 3;

$$\mu = \frac{q}{2m} L = \gamma L \quad (4)$$
Exercise 1.2

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

$$\frac{dL}{dt} = \frac{d}{dt}[\vec{r} \times m\vec{v}] = \frac{d\vec{r}}{dt} \times m\vec{v} + \vec{r} \times \frac{d(m\vec{v})}{dt} = \vec{v} \times m\vec{v} + \vec{r} \times \vec{F} = 0 + \vec{r} \times \vec{F} = \vec{r}$$  \hspace{1cm} (1)

The symbol $F$ represents the force and $\tau$ represents the torque (dreiemoment).

From classical physics we know that a magnetic dipole moment ($\mu$) within a magnetic field $B$ experiences a torque, given by;

$$\tau = \mu \times B$$  \hspace{1cm} (2)

From the previous exercise;

$$\mu = \gamma L$$  \hspace{1cm} (3)

By combining Eqs 1 – 3, we obtain;

$$\frac{d\mu}{dt} = \gamma \mu \times B$$  \hspace{1cm} (4)

Solution to Eq 4

Let us choose $B = B_0k$. Upon inserting this into Eq. 4, we obtain;

$$\frac{d\mu_x}{dt}i + \frac{d\mu_y}{dt}j + \frac{d\mu_z}{dt}k = \gamma \left| \begin{array}{ccc} i & j & k \\ \mu_x & \mu_y & \mu_z \\ 0 & 0 & B_0 \end{array} \right| = \gamma \mu_y B_0i - \gamma \mu_x B_0 j + 0k$$  \hspace{1cm} (5)

Resulting in the following 3 equations:

$$\frac{d\mu_x}{dt} = \gamma \mu_y B_0 \hspace{1cm} (5a)$$

$$\frac{d\mu_y}{dt} = -\gamma \mu_x B_0 \hspace{1cm} (5b)$$

$$\frac{d\mu_z}{dt} = 0 \hspace{1cm} (5c)$$

If multiplying Eq. 5b by $i (= \sqrt{-1})$ and adding to Eq. 5a, the following result appears;
\[ \frac{d(\mu_x + i\mu_y)}{dt} = -i\gamma(\mu_x + i\mu_y)B_0 \]  \hspace{1cm} (6)

Since we can always write the complex number \( \mu_x + i\mu_y \) on the form;

\[ \mu_x + i\mu_y = \mu_\perp e^{i\omega t} \quad (= \mu_\perp \cos(\omega t) + i \mu_\perp \sin(\omega t)) \]  \hspace{1cm} (7)

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

\[ i\omega \mu_\perp = -i\gamma \mu_\perp B_0 \quad \Leftrightarrow \quad \omega = -\gamma B_0 \]  \hspace{1cm} (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 with a frequency \( \omega \). The component of the magnetic moment along the z-axis is constant and independent on time (Eq. 5c).
Exercise 1.3

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

\[
N_-/N_+ = \exp\left( -\frac{\Delta E}{kT} \right) = \exp\left( -\frac{\hbar \gamma B}{kT} \right) \approx 1 - \frac{\hbar \gamma B}{kT}
\]  

(1)

The last term is obtained by a Taylor expansion (we have previously shown that \( \frac{\hbar \gamma B}{kT} \ll 1 \))

Energy diagram

\[ \Delta E = \hbar \omega = \hbar \gamma B \] (where we have used \( \omega = \gamma B \) in the last term)

We also have:

\( N_+ + N_- = N_0 \)  

(2)

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

Combining Eqs 1 and 2 we obtain;

\[
N_+ = N_0 \left( 1 - \frac{\hbar \gamma B}{2kT} \right) = N_0 \left( 1 + \frac{\hbar \gamma B}{2kT} \right)
\]  

\[ N_- = \frac{N_0}{2} \left( 1 - \frac{\hbar \gamma B}{2kT} \right) \]  

(3a)

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

\[
\frac{1}{1 - x} = 1 + x \quad \text{for} \quad x \ll 1
\]

Substituting Eq 3a into Eq 2 we obtain:

\[
N_- = \frac{N_0}{2} \left( 1 - \frac{\hbar \gamma B}{2kT} \right)
\]  

(3b)

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

\[
\Delta n = N_+ - N_- = \frac{\hbar \gamma B N_0}{2kT}
\]

(3c)

The observable, macroscopic magnetization \( M \) for a spin-1/2 particle is thus;

\[
M = \mu \Delta n = \frac{(\gamma \hbar)^2}{4kT} BN_0
\]
**Exercise 1.4**

We simply replace $B_0$ in Eq. 8 (see Exercise 1.2) by $B_{\text{eff}} = \omega_{\text{eff}}/\gamma = B_0 + \omega/\gamma$ and obtain the following solution for the magnetic moment ($\mu$) in the xy-plane;

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

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

$$\mu = \mu_{\perp} e^{i \omega_{\text{eff}} t} = \mu_{\perp} + i 0$$

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

If not on resonance, the magnetic dipole (in the rotating frame of reference; $\omega_0 = \gamma B_0$) will have the following components;

$$\mu = \mu_{\perp} e^{i \omega_{\text{eff}} t} = \mu_{\perp} \cos(\omega - \omega_0)t + i \mu_{\perp} \sin(\omega - \omega_0)t$$

or;

$$\mu_{x'} = \mu_{\perp} \cos(\omega - \omega_0)t$$

$$\mu_{y'} = \mu_{\perp} \sin(\omega - \omega_0)t$$

Normally, the experiment is set up to observe the signal along $x'$ (rotating frame).
Exercise 1.5

We consider the motion in the rotating frame of reference, on resonance. This means that

\[
\frac{d\mu_x'}{dt} + \frac{d\mu_y'}{dt} \cdot j + \frac{d\mu_z'}{dt} \cdot k = \gamma \mu_x \quad \mu_y \quad \mu_z
\]

\[
B_1 \quad 0 \quad 0
\]

\[
= 0 + \gamma \mu_z' B_1 \quad j + \gamma B_1 \mu_y' k
\]

\[
\frac{d\mu_x'}{dt} = 0 \quad (5a)
\]

\[
\frac{d\mu_y'}{dt} = \gamma \mu_z B_1 = \omega_1 \mu_z' \quad (5b)
\]

\[
\frac{d\mu_z'}{dt} = -\gamma \mu_y' B_1 = \omega_1 \mu_y' \quad (5c)
\]

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

\[
\mu_y' = \mu_0 \sin(\omega_1 t)
\]

\[
\mu_z' = \mu_0 \cos(\omega_1 t)
\]

The magnetic moment is rotating around the x'-axis with frequency \( \omega_1 = \gamma B_1 \)
Exercise 2.1

\[
\begin{align*}
\frac{dM'}{dt} &= \gamma M' \times B_{\text{eff}} - u/T_2 - v/T_2 + (M_0-M_z)/T_1 & (1) \\
B_{\text{eff}} &= B_1i' + (B - \omega_{\text{ref}}/\gamma)k = (\omega_1/\gamma)i' + ((\omega - \omega_{\text{ref}})/\gamma)k & (2)
\end{align*}
\]

\[
\begin{bmatrix}
\frac{du}{dt} & \frac{dv}{dt} & \frac{dM_z}{dt}
\end{bmatrix}
= \gamma
\begin{bmatrix}
i' \\
u \\
v
\end{bmatrix}
\begin{bmatrix}
j' \\
v' \\
M_z
\end{bmatrix}
- \frac{u}{T_2} - \frac{v}{T_2} - \frac{M_0 - M_z}{T_1}k & (3)
\]

\[
\begin{align*}
\frac{du}{dt} &= (\omega - \omega_{\text{ref}})v - \frac{u}{T_2} & (3a) \\
\frac{dM_y}{dt} &= -(\omega - \omega_{\text{ref}})u + \omega_1 M_z - \frac{v}{T_2} & (3b) \\
\frac{dM_z}{dt} &= -\omega_1 v + \frac{M_0 - M_z}{T_1} & (3c)
\end{align*}
\]

Case 1
On resonance (\(\omega = \omega_{\text{ref}}\)

\[
\begin{align*}
\frac{du}{dt} &= -\frac{u}{T_2} & (3a) \\
\frac{dv}{dt} &= \omega_1 M_z - \frac{v}{T_2} & (3b) \\
\frac{dM_z}{dt} &= -\omega_1 M_z + \frac{M_0 - M_z}{T_1} & (3c)
\end{align*}
\]
Exercise 2.2

Using the last set of equations in Exercise 2.1 with $\omega_1 = 0$, we obtain;

\[
\frac{du}{dt} = -\frac{u}{T_2} \quad \text{(3a)}
\]
\[
\frac{dv}{dt} = -\frac{v}{T_2} \quad \text{(3b)}
\]
\[
\frac{dM_z}{dt} = +\frac{M_0 - M_z}{T_1} \quad \text{(3c)}
\]

Solution with initial constraints $v(0) = M_0$, $u(0) = 0$ and $M_z(0) = 0$

\[
\frac{du}{dt} = -\frac{u}{T_2} \Leftrightarrow \frac{du}{u} = -\frac{dt}{T_2} \Leftrightarrow \int^t_0 \frac{du}{u} = -\int^t_0 \frac{dt}{T_2} \Leftrightarrow u = u(0) \cdot \exp[-t/T_2] = 0
\]

\[
\frac{dv}{dt} = -\frac{v}{T_2} \Leftrightarrow \frac{dv}{v} = -\frac{dt}{T_2} \Leftrightarrow \int^v_0 \frac{dv}{v} = -\int^t_0 \frac{dt}{T_2} \Leftrightarrow v = v(0) \cdot \exp[-t/T_2] = M_0 \cdot \exp[-t/T_2]
\]

\[
\frac{dM_z}{dt} = \frac{M_0 - M_z}{T_1} \Leftrightarrow \int^t_0 \frac{dM_z}{M_0 - M_z} = \int^M_z \frac{M_z'}{M_z(0)M_0 - M_z} = \int^t_0 \frac{dt}{T_1} \Leftrightarrow -\ln[M_0 - M_z] = \frac{M_z}{M_z(0)} = \frac{t}{T_1}
\]

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

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:

\[
\frac{dM_z}{dt} = \frac{M_0 - M_z}{T_1} \quad \Rightarrow \quad \frac{dM_z}{M_0 - M_z} = \frac{dt}{T_1} \quad \Rightarrow \quad \int_0^{M_z(0)} \frac{dM_z}{M_0 - M_z} = \int_0^{t/T_1} \Rightarrow \quad -\ln[M_0 - M_z] = \frac{M_z}{M_0} = \left[\frac{t}{T_1}\right]
\]

\(M_z = M_0 \left[1 - 2 \exp(-t/T_1)\right]\)
Exercise 2.4

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

(1)

We differentiate Eq. 1 with respect to \(\tau_c\) and obtain;

\[
\frac{d(1/T_1)}{d\tau_c} = \frac{2 - 2\omega^2 \tau_c^2}{[1 + \omega^2 \tau_c^2]^2}
\]

(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:

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

(3)

\[f(\omega, \tau_c = 1/\omega) = -\omega < 0\]

(4)

From Eq. 4 we conclude that \(1/T_1\) has a maximum at \(\tau_c = \frac{1}{\omega}\), i.e., \(T_1\) has a minimum at \(\tau_c = \frac{1}{\omega}\)

(5)

Note; When increasing the magnetic field strength (increasing \(\omega\)), the minimum in \(T_1\) shifts to smaller correlation time (Eq 5), i.e., to higher temperature. From Eq 1 we see that the minimum in \(T_1\) increases with increasing temperature.
Exercise 2.5

\[ F(\omega) = \int_0^\infty e^{-i\omega t} e^{-t/T_2} dt = \int_0^\infty e^{-(i\omega + \frac{1}{T_2})t} dt \]

\[ F(\omega) = -i \frac{1}{i\omega + \frac{1}{T_2}} \left[ e^{-i\omega t} - e^{-\frac{1}{T_2}t} \right]_0^\infty = -i \frac{i\omega - \frac{1}{T_2}}{-\omega^2(\frac{1}{T_2})^2} e^{i\omega t} e^{-\frac{1}{T_2}t} \]

\[ F(\omega) = \frac{i\omega - \frac{1}{T_2}}{\omega^2(\frac{1}{T_2})^2} [0 - 1] = \frac{\frac{1}{T_2}}{\omega^2(\frac{1}{T_2})^2} - i \frac{\omega}{\omega^2(\frac{1}{T_2})^2} \]

The resonance frequency is different from zero \((\omega_0 \neq 0)\) when \(F(\omega)\) is

\[ F(\omega) = \frac{\frac{1}{T_2}}{(\omega - \omega_0)^2 + (\frac{1}{T_2})^2} - i \frac{(\omega - \omega_0)}{(\omega - \omega_0)^2 + (\frac{1}{T_2})^2} \]
Exercise 2.6

\[ \frac{dM'}{dt} = \gamma M' \times B_{\text{eff}} - \frac{u}{T_2} - \frac{v}{T_2} + \frac{(M_0 - M_z)}{T_1} \]  \hspace{1cm} (1)

\[ B_{\text{eff}} = B_{1i'(+ (B + \omega_{\text{ref}}/\gamma + g z)}k = (\omega_{1}/\gamma)i' + ((\omega + \omega_{\text{ref}} + g z)/\gamma)k \]  \hspace{1cm} (2)

Setting \( B_1 = 0 \) and \( \omega = -\omega_{\text{ref}} \) (on resonance)

\[ \frac{du}{dt} + \frac{dv}{dt} + \frac{dM_z}{dt} = \gamma \begin{bmatrix} i' & j' & k \\ u' & v & M_z \\ 0 & 0 & g z \end{bmatrix} - \frac{u}{T_2} - \frac{v}{T_2} + \frac{M_0 - M_z}{T_1} \]  \hspace{1cm} (3a)

\[ \frac{du}{dt} = \gamma g z v - \frac{u}{T_2} \]  \hspace{1cm} (3a)

\[ \frac{dv}{dt} = -\gamma g z u - \frac{v}{T_2} \]  \hspace{1cm} (3b)

\[ \frac{dM_z}{dt} = \gamma \frac{M_0 - M_z}{T_1} \]  \hspace{1cm} (3c)

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

\[ \frac{dM_{\perp}}{dt} = \gamma (g z i - 1/T_2) = \alpha(z)i - 1/T_2 \]  \hspace{1cm} (4)

\( \alpha(z) = \gamma g z t \) represents the phase angle and increases with increasing \( z \). The solution to Eq 4 can be easily found:

\[ M_{\perp} = M_0 e^{\alpha(z) i} e^{-1/T_2} \]
Exercise 2.7

From general rate-process analysis we may write:

\[
\frac{dN_\downarrow}{dt} = -W_{\uparrow\downarrow}N_\downarrow + W_{\downarrow\uparrow}N_\uparrow
\]  

(1a)

\[
\frac{dN_\uparrow}{dt} = -W_{\downarrow\uparrow}N_\uparrow + W_{\uparrow\downarrow}N_\downarrow
\]  

(1b)

Subtracting Eq 1a from Eq 1b gives:

\[
\frac{d(N_\uparrow - N_\downarrow)}{dt} = -2W_{\uparrow\downarrow}N_\uparrow + 2W_{\downarrow\uparrow}N_\downarrow
\]  

(2)

We introduce the following parameters:

\[
\Delta N = N_\uparrow - N_\downarrow
\]  

(3a)

\[
N = N_\uparrow + N_\downarrow
\]  

(3b)

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

\[
\frac{d(\Delta N)}{dt} = -W_{\uparrow\downarrow}(\Delta N + N) + W_{\downarrow\uparrow}(N - \Delta N)
\]  

(4)
At equilibrium, the left hand side of Eq 4 must be equal to 0 \((\frac{d(\Delta N)}{dt} = 0)\), i.e.;

\[
N = \Delta N_0 \frac{W_{\uparrow \downarrow} + W_{\downarrow \uparrow}}{W_{\downarrow \uparrow} - W_{\uparrow \downarrow}}
\]  
(5)

Inserting Eq 5 into Eq 4 results in:

\[
\frac{d(\Delta N)}{dt} = -(W_{\uparrow \downarrow} + W_{\downarrow \uparrow})(\Delta N - \Delta N_0)
\]  
(6)

The spin-lattice relaxation rate \(\frac{1}{T_1}\) is defined as the sum of the transition probabilities, i.e.;

\[
\frac{1}{T_1} = W_{\uparrow \downarrow} + W_{\downarrow \uparrow}
\]  
(7)

Likewise, we recall that the magnetization is proportional to the difference in spin population, i.e.;

\[
M_0 = k\Delta N_0
\]
\[
M = k\Delta N
\]  
(8)

Inserting Eqs 7 and 8 into Eq 6 gives:

\[
\frac{dM_z}{dt} = -\frac{M_z - M_0}{T_1}
\]  
(9)

Eq 9 is identical to the corresponding Equation presented by the Bloch Equation !!!
Exercise 3.0

a) 

b) 

c) 

d) 

e)
Exercise 3.1 – 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:

\[
|I,m> \text{ for } m = -I, -I + 1, \ldots, 0, \ldots I - 1, I
\]

In particular, for \( I = \frac{1}{2} \) \((^1\text{H}, ^13\text{C}, ^31\text{P}, ^19\text{F}, \ldots)\) we have only two spin functions denoted, respectively:

\[
|\alpha> = |1/2,1/2> \quad \text{ and } \quad |\beta> = |1/2,-1/2>
\]

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

\[
\hat{I}_z|\alpha> = 1/2|\alpha>
\]

\[
\hat{I}_z|\beta> = -1/2|\beta>
\]

(3.1a)

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

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

Hence:

\[
\hat{I}^+|\alpha> = \hat{I}^+|1/2,1/2> = 0
\]

\[
\hat{I}^+|\beta> = \hat{I}^+|1/2,-1/2> = 1|1/2,1/2> = |\alpha>
\]

\[
\hat{I}^-|\alpha> = \hat{I}^-|1/2,1/2> = 1|1/2,-1/2> = (\beta)
\]

\[
\hat{I}^-|\beta> = 0
\]

We define:

\[
\hat{I}_x = 1/2\left( \hat{I}^+ + \hat{I}^- \right)
\]

\[
\hat{I}_y = -i/2\left( \hat{I}^+ - \hat{I}^- \right)
\]

Hence:

\[
\hat{I}_x|\alpha> = 1/2|\beta>
\]

\[
\hat{I}_x|\beta> = -i/2|\alpha>
\]

\[
\hat{I}_y|\alpha> = i/2|\beta>
\]

\[
\hat{I}_y|\beta> = -i/2|\alpha>
\]

(3.1b)

(3.1c)

What is the classical energy \((E)\) of two interacting magnetic dipoles \((\mu_A \text{ and } \mu_B)\) 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 $\hat{H}$ is:

$$\hat{H} = -\gamma \hat{h} \hat{z}_A \hat{B}_0 - \gamma \hat{h} \hat{z}_B \hat{B}_0 - \gamma \hat{h} \hat{z}_A \cdot \hat{h} \hat{z}_B$$

$$= -\omega_0 \hat{h} \hat{z}_A - \omega_0 \hat{h} \hat{z}_B - \gamma^2 h^2 \hat{z}_A \cdot \hat{z}_B \quad \text{(ergs)}$$

$$= -\nu_A \hat{z}_A - \nu_B \hat{z}_B - J_{AB} \hat{z}_A \cdot \hat{z}_B \quad \text{(Hz)}$$

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

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

$$\hat{I}_A \cdot \hat{I}_B = \left[ \hat{I}_{xa} i + \hat{I}_{ya} j + \hat{I}_{za} k \right] \cdot \left[ \hat{I}_{xb} i + \hat{I}_{yb} j + \hat{I}_{zb} k \right]$$

$$\hat{I}_A \cdot \hat{I}_B = \hat{I}_{xa} \hat{I}_{xb} + \hat{I}_{ya} \hat{I}_{yb} + \hat{I}_{za} \hat{I}_{zb}$$

$$\hat{I}_A \cdot \hat{I}_B = 1/4 \left[ \hat{I}_{a}^+ + \hat{I}_{a}^- \right] \cdot \left[ \hat{I}_{b}^+ + \hat{I}_{b}^- \right] - 1/4 \left[ \hat{I}_{a}^+ - \hat{I}_{a}^- \right] \cdot \left[ \hat{I}_{b}^+ - \hat{I}_{b}^- \right] + \hat{I}_{za} \hat{I}_{zb}$$

$$\hat{I}_A \cdot \hat{I}_B = 1/2 \left[ \hat{I}_{a}^+ \cdot \hat{I}_{b}^- + \hat{I}_{b}^+ \cdot \hat{I}_{a}^- \right] + \hat{I}_{za} \hat{I}_{zb}$$

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

$$\hat{H} = -\nu_A \hat{z}_A - \nu_B \hat{z}_B + J_{AB} / 2 \left[ \hat{I}_{a}^+ \cdot \hat{I}_{b}^- + \hat{I}_{a}^+ \cdot \hat{I}_{b}^- \right] + J_{AB} \hat{z}_A \hat{z}_B$$
Exercise 3.2

The spin-functions $|\alpha>\text{ and }|\beta>$ are defined as orthonormal eigenfunctions of the z component of the spin operator $I_z$ (see Eq 3.1) and satisfy the following equations:

\[
\int \langle \alpha(X) \rangle \, d\tau = \int a\, d\tau = \int \langle \beta(X) \rangle \, d\tau = \int b\, d\tau = 1
\]

\[
\int \langle \alpha(X) \rangle \, d\tau = \int a\, d\tau = \int \langle \beta(X) \rangle \, d\tau = \int b\, d\tau = 0
\]

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

\[
\begin{align*}
|\Theta_1\rangle &= |\alpha(A)\alpha(B)\rangle = |\alpha\alpha\rangle \\
|\Theta_2\rangle &= |\alpha(A)\beta(B)\rangle = |\alpha\beta\rangle \\
|\Theta_3\rangle &= |\beta(A)\alpha(B)\rangle = |\beta\alpha\rangle \\
|\Theta_4\rangle &= |\beta(A)\beta(B)\rangle = |\beta\beta\rangle
\end{align*}
\]

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

\[
\begin{align*}
|\Psi_1\rangle &= C_{11}|\Theta_1\rangle + C_{12}|\Theta_2\rangle + C_{13}|\Theta_3\rangle + C_{14}|\Theta_4\rangle \\
|\Psi_2\rangle &= C_{21}|\Theta_1\rangle + C_{22}|\Theta_2\rangle + C_{23}|\Theta_3\rangle + C_{24}|\Theta_4\rangle \\
|\Psi_3\rangle &= C_{31}|\Theta_1\rangle + C_{32}|\Theta_2\rangle + C_{33}|\Theta_3\rangle + C_{34}|\Theta_4\rangle \\
|\Psi_4\rangle &= C_{41}|\Theta_1\rangle + C_{42}|\Theta_2\rangle + C_{43}|\Theta_3\rangle + C_{44}|\Theta_4\rangle
\end{align*}
\]

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

\[
\hat{H}|\Psi_i\rangle = E_i|\Psi_i\rangle = C_{i1}\hat{H}|\Theta_1\rangle + C_{i2}\hat{H}|\Theta_2\rangle + C_{i3}\hat{H}|\Theta_3\rangle + C_{i4}\hat{H}|\Theta_4\rangle = E_iC_{i1}|\Theta_1\rangle + E_iC_{i2}|\Theta_2\rangle + E_iC_{i3}|\Theta_3\rangle + E_iC_{i4}|\Theta_4\rangle
\]

We multiply by $\langle \Theta_j |$ and integrate over the entire spin space:
\[
\int \langle \Theta_j | \hat{H} | \Psi_i \rangle d\tau = E \int \langle \Theta_j | \Psi_i \rangle d\tau
\]

\[
\int C_{i1} \langle \Theta_j | \hat{H} | \Theta_1 \rangle d\tau + C_{i2} \langle \Theta_j | \hat{H} | \Theta_2 \rangle d\tau + C_{i3} \langle \Theta_j | \hat{H} | \Theta_3 \rangle d\tau + C_{i4} \langle \Theta_j | \hat{H} | \Theta_4 \rangle d\tau
\]

\[
= EC_{i1} \int \langle \Theta_j | \Theta_1 \rangle d\tau + E \int C_{i2} \langle \Theta_j | \Theta_2 \rangle d\tau + EC_{i3} \int \langle \Theta_j | \Theta_3 \rangle d\tau + EC_{i4} \int \langle \Theta_j | \Theta_4 \rangle d\tau
\]

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

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

\[
C_{i1} H_{11} + C_{i2} H_{12} + C_{i3} H_{13} + C_{i4} H_{14} = EC_{i1}
\]
\[
C_{i1} H_{21} + C_{i2} H_{22} + C_{i3} H_{23} + C_{i4} H_{24} = EC_{i2}
\]
\[
C_{i1} H_{31} + C_{i2} H_{32} + C_{i3} H_{33} + C_{i4} H_{34} = EC_{i3}
\]
\[
C_{i1} H_{41} + C_{i2} H_{42} + C_{i3} H_{43} + C_{i4} H_{44} = EC_{i4}
\]

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

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

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

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

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 Exercise 3.0):

\[
\hat{H} |\Theta_1\rangle = -v_A \hat{I}_{ZA} |\Theta_1\rangle - v_B \hat{I}_{ZB} |\Theta_1\rangle + J_{AB} / 2 \left[ \hat{i}_A^+ \hat{i}_B^- + \hat{i}_B^+ \hat{i}_A^- \right] |\Theta_1\rangle + J_{AB} \hat{I}_{ZA} \hat{I}_{ZB} |\Theta_1\rangle
\]

\[
\hat{H} |\alpha(A)\alpha(B)\rangle = -v_A \hat{I}_{ZA} |\alpha(A)\alpha(B)\rangle - v_B \hat{I}_{ZB} |\alpha(A)\alpha(B)\rangle + J_{AB} / 2 \hat{i}_A^+ \hat{i}_B^- |\alpha(A)\alpha(B)\rangle + J_{AB} \hat{I}_{ZA} \hat{I}_{ZB} |\alpha(A)\alpha(B)\rangle
\]
Likewise:

\[
\hat{H} |\Theta_1\rangle = (-\nu_A / 2 - \nu_B / 2 + J_{AB} / 4) |\phi_1\rangle = E_1 |\Theta_1\rangle_1
\]

(3.7a)

\[
\hat{H} |\Theta_2\rangle = (-\nu_A / 2 + \nu_B / 2 - J_{AB} / 4) |\Theta_2\rangle + J_{AB} / 2 |\Theta_3\rangle
\]

(3.7b)

\[
\hat{H} |\Theta_3\rangle = (\nu_A / 2 - \nu_B / 2 - J_{AB} / 4) |\Theta_3\rangle + J_{AB} / 2 |\Theta_2\rangle
\]

(3.7c)

\[
\hat{H} |\Theta_4\rangle = (\nu_A / 2 + \nu_B / 2 + J_{AB} / 4) |\Theta_4\rangle = E_4 |\Theta_4\rangle_4
\]

(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 \( \langle \Theta_1 | \Theta_2 \rangle d\tau = \langle \Theta_1 | \Theta_3 \rangle d\tau = \langle \Theta_1 | \Theta_4 \rangle d\tau = \langle \Theta_2 | \Theta_4 \rangle d\tau = \langle \Theta_3 | \Theta_4 \rangle d\tau = 0 \)
Exercise 3.3
Because two of the spin-functions ($\Theta_1$ and $\Theta_4$) are eigenfunctions while $\Theta_2$ and $\Theta_3$ are not.
Exercise 3.4

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

\[ \hat{F}_z = \hat{I}_z A + \hat{I}_z B \]  

we notice that:

\[ \hat{F}_z |\Theta_1\rangle = \hat{I}_z A |\Theta_1\rangle + \hat{I}_z B |\Theta_1\rangle \]
\[ = \hat{I}_z A |\alpha(A)\alpha(B)\rangle + \hat{I}_z B |\alpha(A)\alpha(B)\rangle \]
\[ = \frac{1}{2} |\alpha(A)\alpha(B)\rangle + \frac{1}{2} |\alpha(A)\alpha(B)\rangle \]
\[ = \frac{1}{2} \Theta_1 \]

\[ \hat{F}_z |\Theta_2\rangle = \hat{I}_z A |\Theta_2\rangle + \hat{I}_z B |\Theta_2\rangle \]
\[ = \hat{I}_z A |\alpha(A)\beta(B)\rangle + \hat{I}_z B |\alpha(A)\beta(B)\rangle \]
\[ = \frac{1}{2} |\alpha(A)\beta(B)\rangle - \frac{1}{2} |\alpha(A)\beta(B)\rangle \]
\[ = 0 \]

\[ \hat{F}_z |\Theta_3\rangle = \hat{I}_z A |\Theta_3\rangle + \hat{I}_z B |\Theta_3\rangle \]
\[ = \hat{I}_z A |\beta(A)\alpha(B)\rangle + \hat{I}_z B |\beta(A)\alpha(B)\rangle \]
\[ = \frac{1}{2} |\beta(A)\alpha(B)\rangle + \frac{1}{2} |\beta(A)\alpha(B)\rangle \]
\[ = 0 \]

\[ \hat{F}_z |\Theta_4\rangle = \hat{I}_z A |\Theta_4\rangle + \hat{I}_z B |\Theta_4\rangle \]
\[ = \hat{I}_z A |\beta(A)\beta(B)\rangle + \hat{I}_z B |\beta(A)\beta(B)\rangle \]
\[ = \frac{1}{2} |\beta(A)\beta(B)\rangle - \frac{1}{2} |\beta(A)\beta(B)\rangle \]
\[ = 0 \]

This means that the eigenvalues $F_z$ of the operator $\hat{F}_z$ are the same for the two spin-functions $\Theta_2$ and $\Theta_3$, implying that a linear combination of these two functions will define the actual eigenfunction.
Exercise 3.5

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

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

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

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

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

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

Likewise, we derive the following results:

\[
H_{22} = -\frac{1}{2} (\nu_A - \nu_B) - \frac{1}{4} J_{AB} \] (3.9b)
\[
H_{33} = \frac{1}{2} (\nu_A - \nu_B) - \frac{1}{4} J_{AB} \] (3.9c)

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

\[
E_2 = -\frac{J_{AB}}{4} - \frac{1}{2} \sqrt{J_{AB}^2 + (\nu_A - \nu_B)^2}
\]
\[
E_3 = -\frac{J_{AB}}{4} + \frac{1}{2} \sqrt{J_{AB}^2 + (\nu_A - \nu_B)^2}
\] (3.10)
Exercise 3.6

If introducing the following short hand notations:

\[ V = \nu_A + \nu_B \]
\[ C = \sqrt{J_{AB}^2 + (\nu_A - \nu_B)^2} \]

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

<table>
<thead>
<tr>
<th>Level</th>
<th>Energy</th>
<th>Fz</th>
<th>Transition</th>
<th>Wave function</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>V/2 + J/4</td>
<td>-1</td>
<td>*</td>
<td>[ \Psi_1 &gt; = a_{11}</td>
</tr>
<tr>
<td>2</td>
<td>C/2 - J/4</td>
<td>0</td>
<td>*</td>
<td>[ \Psi_2 &gt; = a_{21}</td>
</tr>
<tr>
<td>3</td>
<td>-C/2 - J/4</td>
<td>0</td>
<td>*</td>
<td>[ \Psi_3 &gt; = a_{31}</td>
</tr>
<tr>
<td>4</td>
<td>-V/2 + J/4</td>
<td>1</td>
<td>*</td>
<td>[ \Psi_4 &gt; = a_{44}</td>
</tr>
</tbody>
</table>

Hence, the following transition may be easily derived:

\[ \Delta E_{1 \rightarrow 2} = E_1 - E_2 = (V - C + J)/2 \]
\[ \Delta E_{1 \rightarrow 3} = E_1 - E_3 = (V + C + J)/2 \]
\[ \Delta E_{2 \rightarrow 4} = E_2 - E_4 = (V - C + J)/2 \]
\[ \Delta E_{3 \rightarrow 4} = E_3 - E_4 = (V - C - J)/2 \]
Exercise 3.7

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.:

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

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;

$$I_{m=-1\Rightarrow m=0} = (\int \psi_{m=-1} \hat{I}^4 + \hat{I}^6 \psi_{m=0} d\tau)^2$$

Vi beregner først;

$$\hat{I}^4 \psi_{m=0} = \hat{I}^4 (\cos \theta \cdot \alpha(A) \beta(B) + \hat{I}^4 \sin \theta \cdot \beta(A) \alpha(B))$$
$$= \cos \theta \cdot \beta(B) \hat{I}^4 \alpha(A) + \sin \theta \cdot \alpha(B) \hat{I}^4 \beta(A)$$
$$= \cos \theta \cdot \beta(B) \beta(A) - \sin \theta \cdot \alpha(B) \cdot 0$$
$$= \cos \theta \cdot \beta(B) \beta(A)$$

Tilsvarende finner vi for;

$$\hat{I}^6 \psi_{m=0} = \hat{I}^6 (\cos \theta \cdot \alpha(A) \beta(B) + \hat{I}^6 \sin \theta \cdot \beta(A) \alpha(B))$$
$$= \cos \theta \cdot \alpha(A) \hat{I}^6 \beta(A) + \sin \theta \cdot \beta(A) \hat{I}^6 \alpha(B)$$
$$= \cos \theta \cdot \alpha(A) \cdot 0 - \sin \theta \cdot \beta(A) \cdot \beta(B)$$
$$= -\sin \beta(A) \beta(B)$$

Innsatt i første likning;
\[ I_{m=-1\to m=0} = \left( \int \psi_{m=1} \hat{\mathbf{i}} \cdot \hat{\mathbf{r}} \, d\tau \right)^2 \]
\[ = \left( \int \beta(A) \beta(B) \left[ \cos \theta \cdot \beta(B) \beta(A) - \sin \theta \beta(A) \beta(B) \right] \, d\tau \right)^2 \]
\[ = (\cos \theta \int \beta(A) \beta(A) d\tau_A \cdot \int \beta(B) \beta(B) d\tau_B - \sin \theta \int \beta(A) \beta(A) d\tau_A \cdot \int \beta(B) \beta(B) d\tau_B)^2 \]
\[ = (\cos \theta - \sin \theta)^2 = \cos^2 \theta - 2 \sin \theta \cos \theta + \sin^2 \theta \]
\[ = 1 - \sin(2\theta) \]
Exercise 4.1

If introducing a gradient field \( \mathbf{g} \) along any direction \( \mathbf{r} \) in space we obtain:

\[
\mathbf{g} = \frac{\partial B_x}{\partial x} \mathbf{i} + \frac{\partial B_y}{\partial y} \mathbf{j} + \frac{\partial B_z}{\partial z} \mathbf{k}
\]

\( \mathbf{r} = x \mathbf{i} + y \mathbf{j} + z \mathbf{k} \quad (1) \)

Without loss of generality we consider the component of the gradient field only in the direction of the external field, i.e., along the z-direction. Hence,

\[
\mathbf{g} \cdot \mathbf{r} = g_z z = \frac{\partial B_z}{\partial z} = g_0(t) \quad (2)
\]

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

\[
B_z = B_0 + z \cdot g_0(t) \quad (4a)
\]

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

\[
\mathbf{B}_{\text{eff}} = z g_0 \mathbf{k} \quad (4b)
\]

Again, within the rotating frame of reference:

\[
\frac{du}{dt} + \frac{dv}{dt} + \frac{dM_z}{dt} = \begin{pmatrix}
M_x' & M_y' & M_z' \\
 M_x'' & M_y'' & M_z'' \\
0 & 0 & -1 \\
\end{pmatrix} - \frac{u}{T_2} - \frac{v}{T_2} + \frac{M_0 - M_z}{T_1} + D \nabla^2 M \quad (5a)
\]

\[
\frac{\partial u}{\partial t} = \gamma g_0 z \cdot v - \frac{u}{T_2} + D \nabla \cdot \nabla u \quad (5b)
\]

\[
\frac{\partial v}{\partial t} = \gamma g_0 z \cdot u - \frac{v}{T_2} + D \nabla \cdot \nabla v \quad (5c)
\]

\[
\frac{\partial M_z}{\partial t} = - \frac{M_z - M_0}{T_1} + D \nabla \cdot \nabla M_z \quad (5d)
\]

Since we are interested only in the transversal magnetization (uv-plane), we will apply a “complex-number-approach”, by introducing the complex magnetization \( \mathbf{M} \) defined by:

\[
\mathbf{M} = M_x + i M_y \quad (6)
\]

Multiplying Eq 5b by the complex number i and adding Eq 5a, we obtain:

\[
\frac{\partial \mathbf{M}}{\partial t} = -i \gamma g_0 z \mathbf{M} - \frac{\mathbf{M}}{T_2} + D \nabla^2 \mathbf{M} \quad (7)
\]
Exercise 4.2

From Eq 7:

\[ \frac{\partial \hat{M}}{\partial t} = -i\gamma_0 z \hat{M} - \frac{\hat{M}}{T_2} + D \nabla^2 \hat{M} \]  \hspace{1cm} (7)

Noting that \( B_z \) may be a function of both \( z \) and \( t \) (Eq 4) we will look for a solution in which also \( \dot{M} \) is a function of \( z \) and \( t \) and independent of \( x \) and \( y \). This implies that:

\[ \nabla \cdot \nabla \hat{M} = \frac{\partial^2 \hat{M}}{\partial z^2} \]  \hspace{1cm} (8)

By inserting Eq 9 into Eq 8, we easily derive Eq 10:

\[ \hat{M}(z,t) = e^{-t/T_2} \tilde{m}(z,t) \]  \hspace{1cm} (9)

\[ -\frac{1}{T_2} e^{-t/T_2} \tilde{m} + e^{-t/T_2} \frac{\partial \tilde{m}}{\partial t} = -i\gamma z_0 e^{-t/T_2} \tilde{m} - e^{-t/T_2} \frac{\tilde{m}}{T_2} + e^{-t/T_2} D \frac{\partial^2 \tilde{m}}{\partial z^2} \]  \hspace{1cm} (10)

Which simplifies to:

\[ \frac{\partial \tilde{m}}{\partial t} = -i\gamma z_0 \tilde{m} + D \frac{\partial^2 \tilde{m}}{\partial z^2} \]  \hspace{1cm} (11)
Exercise 4.3

We will try to find a solution to Eq 11 of the form:

\[ \hat{m} = \Psi(t) \cdot \Omega(z,t) \quad (12) \]

where:

\[ \Omega(z,t) = \exp\left(-i \gamma g_0(t) dt'\right) \quad (13) \]

Since \( \Omega(z,t) \) is a complex function of modulus 1, it simply represents a phase shift of the observable (and complex) magnetization \( \hat{m} \). Hence, the modulus (absolute value) of the complex magnetization \( \hat{m} \) will be identical to \( \Psi(t) \) (see Eq 14) and thus represents the observable signal intensity.

\[ \text{abs}(\hat{m}) = \text{abs}(\Psi(t) \cdot \Omega(z,t)) = \Psi(t) \text{abs}(\Omega(z,t)) = \Psi(t) \cdot \Omega(z,t) \cdot \Omega^* (z,t) = \Psi(t) \cdot 1 = \psi(t) \quad (14) \]

*; complex conjugate

Noting that:

\[ \frac{\partial \Omega}{\partial t} + \frac{\partial \Psi}{\partial t} = \Psi \cdot \left[-i \gamma g_0(t) + \Omega \frac{\partial \Psi}{\partial t} \right] = \hat{m} \cdot \left[-i \gamma g_0(t) + \frac{1}{\Psi} \frac{\partial \Psi}{\partial t} \right] \quad (15a) \]

\[ \frac{\partial \hat{m}}{\partial z} = \psi \cdot \frac{\partial \Omega}{\partial z} = \Psi \cdot \Omega \cdot \left[-i \gamma \int_0^t g_0(t') dt'\right] \quad (15b) \]

\[ \frac{\partial^2 \hat{m}}{\partial z^2} = \psi \cdot \frac{\partial^2 \Omega}{\partial z^2} = \Psi \cdot \Omega \cdot \left[-i \gamma \int_0^t g_0(t') dt'\right]^2 = \hat{m} \cdot \left[-i \gamma \int_0^t g_0(t') dt'\right]^2 \quad (15c) \]

We obtain the following simple Eq for \( \psi \) when substituting Eqs 15a)–c) into Eq 11:
\[
\frac{1}{\Psi} \frac{d\Psi}{dt} = D \left[ -i \gamma \int_0^t g_0(t') dt' \right]^2 = -D \gamma^2 \left[ \int_0^t g_0(t') dt' \right]^2
\]

\[
\Rightarrow \quad \frac{d\Psi}{\Psi} = -D \gamma^2 \left[ \int_0^t g_0(t') dt' \right]^2 dt
\]

\[
\Rightarrow \quad \Psi(t) = \exp \left[ -D \gamma^2 \int_0^t \left[ \int_0^{t'} g_0(t'') dt'' \right]^2 dt' \right]
\]
Let us consider the phase term of the magnetization (Eq. 1);

\[
\Omega(z,t) = \exp \left[ -i \gamma \int_0^t g_0(t')dt' \right]
\]

(1)

After the gradient pulse has been on for a time \( \tau \), the phase angle \( \varphi \) at position \( z \) can be written:

\[
\theta = - \gamma \int_0^\tau g_0(t')dt'
\]

(2)

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

\[
\hat{m} = \Psi(t) \cdot \exp[-i\theta]
\]

(3)

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

![Diagram](image.png)

A constant gradient field \( G_0 (=\delta B_x/\delta z) \) is applied along the z-axis (along \( B_0 \)). At time \( \tau \), the phase angle \( \theta_1 \) will be:

\[
\theta_1 = \gamma G_0 z \int_0^\tau dt = \gamma G_0 z \tau
\]

(1)

The magnetization \( M(\tau) \) will then be:

\[
M(\tau) = M_0 \cdot \exp[-t/T_2] \cdot \exp[i\theta_1] \Rightarrow M_0 \cdot \exp[-\tau/T_2] \cdot [i\gamma G_0 \tau]
\]

(2)

What will be the phase angle \( \theta_2 \) after the \( \pi \)-pulse?
The angle will be \( \theta_2 = - \theta_1 \) so the magnetization just after the pulse will be:
\[ M_{t, \text{after}} = M_0 \cdot \exp[-\tau / T_2] \cdot [-i \gamma G_0 \tau] \]

Hence, the effect of a \( \pi \)-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:

\[ \int_{0}^{t} \dot{g}(t') \, dt' \]

How can we express the phase angle \( \theta \) as a function of time when considering the pulse-gradient scheme in Figure 1B?

\[ \theta = \int_{0}^{t} g(t') \, dt' \]

Figure 1B

Figure 1C

Figure a) shows how the phase angle \( \theta = \int_{0}^{t} g(t') \, dt' \) changes with time \( t \) and reveals a discontinuity in \( \theta \) at \( t = \tau \) because of the \( \pi \)-pulse. However, since we are only interested in the time variation of the square of
the phase angle, as given by the integral \[ \left[ \int_0^t g_0(t')dt' \right]^2 \] (see Eq 16) we may alternatively consider the integral illustrated on Figure b).
Additional 2