Appendix 17.11: Bloch Equations **p 626-627** **2 pages**

In my MRI document entitled "MRI notes and sources.doc" I derived the following Bloch Equations and I repeat some of that text here:

In my physics questions doc, I show that the torque on a mag dipole is $\boldsymbol{\mu}$ x **B** = d**J**/dt and we know also that $\boldsymbol{\mu} = \gamma \mathbf{J}$. We can then rewrite the previous as $\gamma\boldsymbol{\mu}$ x **B** = d$\boldsymbol{\mu}$/dt . If we then sum up all our μ_i in a cm^3 say, then we have $M = \Sigma_i \mu_i$ and then we have d**M**/dt = γ**M** x **B** . This is the first required ingredient and appears as (7) on Kittel page 580. This equation of course ignores frictional forces which we refer to as the T1 and T2 relaxation mechanisms.

$$dM_x/dt = \gamma[\mathbf{M} \times \mathbf{B}]_x - M_x/T2$$
$$dM_y/dt = \gamma[\mathbf{M} \times \mathbf{B}]_y - M_y/T2$$
$$dM_z/dt = \gamma[\mathbf{M} \times \mathbf{B}]_z - (M_z - M_{0z})/T1$$

Felix Bloch shared the Nobel with Purcell. So I think these equations are fairly obvious, just combining the rate of change of precession with the rate of change due to relaxation "frictional" forces. If we rescale **M** in units of M_{0z}, then $M_{0z} = 1$. The equations are linear and so keep the same form by any scaling. So it appears that Malcolm has done this in (17.74), so we have a complete understanding of the "frictional terms" in his equations.

But what about the "rotational terms"? The magnetic field with an RF pulse active could be expressed as

$$\mathbf{B} = B^{\circ}\hat{\mathbf{z}} + (B_{RF}/2)\,[\cos(\omega t + \phi)\,\hat{\mathbf{x}} + \sin(\omega t+\phi)\,\hat{\mathbf{y}}\,] \qquad \text{// see page 179}$$

where ω and ϕ are the frequency and phase of the RF pulse (as measured in the lab), and we have assumed B_{RF} was applied in the x direction, and we take 1/2 of it in the correct resonant rotation sense. If we put this B into our Bloch equations, we get this:

$$dM_x/dt = \gamma[\mathbf{M} \times \mathbf{B}]_x = \gamma\,[\,M_yB_z - M_zB_y] = \gamma[\,B_oM_y - (B_{RF}/2)\sin(\omega t+\phi)M_z]$$
$$dM_y/dt = \gamma[\mathbf{M} \times \mathbf{B}]_y = \gamma\,[\,M_zB_x - M_xB_z] = \gamma[\,(B_{RF}/2)\cos(\omega t+\phi)M_z - B_oM_x\,]$$
$$dM_z/dt = \gamma[\mathbf{M} \times \mathbf{B}]_z = \gamma\,[\,M_xB_y - M_yB_x] = \gamma[\,(B_{RF}/2)\sin(\omega t+\phi)M_x - (B_{RF}/2)\cos(\omega t+\phi)M_y\,]$$

Now replace $(B_{RF}/2)\gamma = \omega_{nut}$ and $\gamma B_o = \omega_0$ (Larmor) and we get

$$\begin{aligned}
dM_x/dt &= 0 + \omega_0 M_y - \omega_{nut}\sin(\omega t+\phi)\,M_z \\
dM_y/dt &= -\omega_o M_x + 0 + \omega_{nut}\cos(\omega t+\phi)M_z \\
dM_z/dt &= \omega_{nut}\sin(\omega t+\phi)\,M_x - \omega_{nut}\cos(\omega t+\phi)\,M_y + 0
\end{aligned}$$

So this gives us a 3x3 matrix which is valid **in the laboratory frame**.

How would we get this into the **rotating frame**? I don't remember how to convert mechanics like this to a rotating frame (Coriolis to worry about), but I have another method. We *already know* the Hamiltonian in the rotating frame to be this:

$H = \Omega_o I_z + \omega_{nut}(I_x \cos\phi + I_y \sin\phi)$ page 260 Levitt $\omega_{nut} = \gamma(B_{RF}/2)$

Then quantum mechanics tells us that $\mathbf{M} = \langle \mathbf{I} \rangle$ [ignore scale here, in some unnamed state] so we have

$d\mathbf{M}/dt = d\langle \mathbf{I} \rangle/dt = (1/i\hbar) \langle [\, \mathbf{I}, H \,] \rangle$ // Schiff page 169 bottom. Schrodinger picture

Now let's compute the commutators:

$[\, I_x, H] = [\, I_x, \Omega_o I_z + \omega_{nut}(I_x \cos\phi + I_y \sin\phi)] = -\Omega_o i\hbar\, I_y + \omega_{nut} \sin\phi\, i\hbar I_z$

$[\, I_y, H] = [\, I_y, \Omega_o I_z + \omega_{nut}(I_x \cos\phi + I_y \sin\phi)] = +\Omega_o i\hbar\, I_x - \omega_{nut} \cos\phi\, i\hbar I_z$

$[\, I_z, H] = [\, I_z, \Omega_o I_z + \omega_{nut}(I_x \cos\phi + I_y \sin\phi)] = \omega_{nut} \cos\phi\, i\hbar I_y - \omega_{nut} \sin\phi\, i\hbar\, I_x$

so we then get the $i\hbar$'s cancelling and

$dM_x/dt = -\Omega_o M_y + \omega_{nut} \sin\phi\, M_z$ // agrees
$dM_y/dt = +\Omega_o M_x - \omega_{nut} \cos\phi\, M_z$ // agrees
$dM_z/dt = \omega_{nut} \cos\phi M_y - \omega_{nut} \sin\phi\, M_x$ // agrees

and this then gives the exact matrix shown on page 626. I guess we have to assume that the rotation has no effect on the frictional terms and I have already seen evidence elsewhere that this could be an issue.

Now, what happens during a long RF pulse? If on resonance and ϕ=0, we have T_1 restoring to Iz, and the RF continuously knocking down to Iy, so we get a steady state value of M_y as shown.

If you include Ω_0 in this equation you the following steady state solution:

$$\begin{pmatrix} -1/T_2 & -\Omega_0 & 0 \\ \Omega_0 & -1/T_2 & -\omega_n \\ 0 & \omega_n & -1/T_1 \end{pmatrix} \begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -M_{zo}/T_1 \end{pmatrix}$$

I had Maple invert the matrix and the answer I got agrees with what is in the following paper I found:
[it is more on EPR = electron paramagnetic resonance, but same idea]

$$M_x = M_0 \omega_1 \frac{\Omega_0 T_2^2}{1 + \Omega_0^2 T_2^2 + \omega_1^2 T_1 T_2}$$

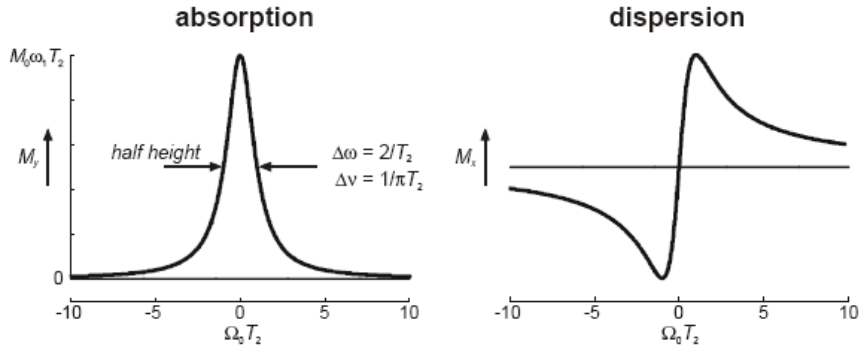
$$M_y = -M_0 \omega_1 \frac{T_2}{1 + \Omega_0^2 T_2^2 + \omega_1^2 T_1 T_2}$$

$$M_z = M_0 \frac{1 + \Omega_0^2 T_2^2}{1 + \Omega_0^2 T_2^2 + \omega_1^2 T_1 T_2}$$

where ω_1 is my ω_{nut} and $M_0 = M_{0z} = 1$ for Levitt. Now if you go close to resonance, $M_x = 0$. To the extent that $\omega_{nut}^2 T_1 T_2 << 1$, the denominator of the M_y term is $1 + \Omega_0^2 T_2^2$ and this shows resonance at $\Omega_0 = 0$.

Before 1962, NMR was done using the continuous-wave steady state method where you either swept the RF frequency or the B_0 field. In the first case, it was just the way my Harvard chem lab IR spectrometer worked with a sweeping fraction grating. You would find the resonances because certain frequencies would absorb and re-emit, and that was how you did NMR. There was no Fourier Transform, there were no RF short pulses. In this context, the Block Equations were the main act, but nowadays they are mostly a curiosity as far as normal NMR theory is concerned, as for example in this book of Levitt.

Note: it turns out that M_x is the D and M_y is the A for the spectrum!



Somehow this must be because the matrix element involves $I^+ = I_x + iI_y$ and the dispersion is the imaginary point, etc etc fudge fudge.

"There are two general types of NMR instrument; continuous wave and Fourier transform. Early experiments were conducted with continuous wave (C.W.) instruments, and in 1970 the first Fourier transform (F.T.) instruments became available. This type now dominates the market."