MAGNETIC RESONANCE IN THE INTERACTION PICTURE

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Reference: Tom Lancaster and Stephen J. Blundell, *Quantum Field Theory for the Gifted Amateur*, (Oxford University Press, 2014), Problem 18.1.

Post date: 28 Jun 2019.

We've looked at magnetic resonance before in the general case where the magnetic field has the form

$$\mathbf{B}=B_{rf}\cos(\omega t)\hat{\mathbf{x}}-B_{rf}\sin(\omega t)\hat{\mathbf{y}}+B_0\hat{\mathbf{z}} \tag{1}$$

That is, there's a constant field of magnitude B_0 along the z axis and an oscillating field with frequency ω that cycles around the z axis. In this case, the hamiltonian is

$$H=-\gamma\mathbf{B}\cdot\mathbf{S} \tag{2}$$

where S is the spin of the particle and γ is the gyromagnetic ration.

In the problem in L&B's book, we look at the special case where the frequency is given by

$$\omega=\gamma B_0 \tag{3}$$

The analysis that follows works only for this special case.

so the hamiltonian is

$$H=\gamma B_0S_z+\gamma B_1\left(S_x\cos\gamma B_0t+S_y\sin\gamma B_0t\right) \tag{4}$$

Our aim is to look at this situation using the interaction picture of quantum theory. To recap, in the interaction picture, we split the hamiltonian into two parts: a part H_0 that doesn't depend on interactions and an auxiliary part H' that does depend on interactions. In our case, we have

$$H_0=\gamma B_0S_z \tag{5}$$

$$H'=\gamma B_1\left(S_x\cos\gamma B_0t+S_y\sin\gamma B_0t\right) \tag{6}$$

We then find the interaction hamiltonian H_I by the formula

$$H_I=e^{iH_0t}H'e^{-iH_0t} \tag{7}$$

This leads to definition of the evolution operator $U(t_2,t_1)$ which, once found, can be used to find the probability amplitude that a system evolves from an initial state (governed solely by H_0) through some interaction (such as scattering) and emerges in some final state (again governed by H_0). This operator is defined by the equation

$$i\frac{d}{dt}U_I(t_2,t_1) = H_I(t_2)\,U_I(t_2,t_1) \tag{8}$$

In the general case, H_I is a function of time, and two instances of H_I evaluated at different times need not commute. This means that what might appear to be a formal solution, namely

$$U_I(t_2,t_1) = e^{-i\int_{t_1}^{t_2} dt\ H_I(t)} \tag{9}$$

does not, in general, work. This is due to the fact that the exponential must be interpreted as a power series, and this power series is valid only if the components $H_I(t)$ commute at different times.

In our case, however, things turn out to be a lot simpler. L&B give us a few identities:

$$S_\pm = S_x \pm iS_y \tag{10}$$
$$S_+e^{i\omega t} = e^{i\omega S_z t}S_+e^{-i\omega S_z t} \tag{11}$$
$$S_-e^{i\omega t} = e^{i\omega S_z t}S_-e^{-i\omega S_z t} \tag{12}$$

The last two identities can be verified using the commutators for spin $[S_x,S_y] = iS_z$ and cyclic permutations (remember we're using units where $\hbar = 1$), but I won't go into that here. We can invert the first identity to get

$$S_x = \frac{1}{2}(S_+ + S_-) \tag{13}$$
$$S_y = \frac{1}{2i}(S_+ - S_-) \tag{14}$$

Applying these identities to 6, we have

$$H' = \gamma B_1\left(\frac{1}{2}S_+(\cos\gamma B_0 t - i\sin\gamma B_0 t) + S_-(\cos\gamma B_0 t + i\sin\gamma B_0 t)\right) \tag{15}$$
$$= \frac{\gamma B_1}{2}\left(S_+e^{-i\gamma B_0 t} + S_-e^{i\gamma B_0 t}\right) \tag{16}$$

We can now use 11 with $\omega = -\gamma B_0$ to get

$$H' = \frac{\gamma B_1}{2} e^{-i\gamma B_0 S_z t} \left(S_+ + S_-\right) e^{i\gamma B_0 S_z t} \tag{17}$$
$$= \gamma B_1 e^{-i\gamma B_0 S_z t} S_x e^{i\gamma B_0 S_z t} \tag{18}$$
$$= \gamma B_1 e^{-iH_0 t} S_x e^{iH_0 t} \tag{19}$$

From 7 we now get the interaction Hamiltonian

$$H_I = \gamma B_1 S_x \tag{20}$$

which is independent of time. Because there is no time dependence, we *can* use 9 to find the evolution operator $U_I(t_2, t_1)$, so we have

$$U_I(t_2, t_1) = e^{-i\int_{t_1}^{t_2} dt\ H_I(t)} \tag{21}$$
$$= e^{-i\gamma B_1 S_x (t_2 - t_1)} \tag{22}$$

We'll now consider the case $t_1 = 0$ and $t_2 = t$. We'll also replace the spin matrix S_x by its form using the Pauli matrices, so we have

$$S_x = \frac{1}{2}\sigma_x = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{23}$$

We have

$$U_I(t, 0) = e^{-i\gamma B_1 \sigma_x t/2} \tag{24}$$
$$= \cos\left(\frac{\gamma B_1 t}{2}\sigma_x\right) - i\sin\left(\frac{\gamma B_1 t}{2}\sigma_x\right) \tag{25}$$

We now use the fact that

$$\sigma_x^2 = I \tag{26}$$

where I is the identity matrix. Therefore, all even powers of σ_x are I and all odd powers are just σ_x itself. The series expansion of the cosine contains only even powers, and the expansion of the sine contains only odd powers, so we have

$$\cos\left(\frac{\gamma B_1 t}{2}\sigma_x\right) = I\cos\left(\frac{\gamma B_1 t}{2}\right) \tag{27}$$
$$\sin\left(\frac{\gamma B_1 t}{2}\sigma_x\right) = \sigma_x \sin\left(\frac{\gamma B_1 t}{2}\right) \tag{28}$$

We therefore have

$$U_I(t,0) = I\cos\left(\frac{\gamma B_1 t}{2}\right) - i\sigma_x \sin\left(\frac{\gamma B_1 t}{2}\right) \tag{29}$$

Now consider a particle initially in the spin up (in the z direction) state $|\uparrow\rangle$. In the basis spanned by the z spin states, the spin up state is given by

$$|\uparrow\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{30}$$

If we act on this state with σ_x, we flip the spin:

$$\sigma_x \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{31}$$

The amplitude that a particle starting in the spin up state at $t = 0$ is again in this state at time t is then

$$\langle\uparrow|U_I(t,0)|\uparrow\rangle = \begin{bmatrix} 1 & 0 \end{bmatrix} \left(I\cos\left(\frac{\gamma B_1 t}{2}\right) - i\sigma_x \sin\left(\frac{\gamma B_1 t}{2}\right)\right) \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{32}$$

$$= \begin{bmatrix} 1 & 0 \end{bmatrix} \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \cos\left(\frac{\gamma B_1 t}{2}\right) - i \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \sin\left(\frac{\gamma B_1 t}{2}\right)\right) \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{33}$$

$$= \cos\left(\frac{\gamma B_1 t}{2}\right) \tag{34}$$

Thus the probability of this is

$$P_{\uparrow\uparrow} = |\langle\uparrow|U_I(t,0)|\uparrow\rangle|^2 \tag{35}$$

$$= \cos^2\left(\frac{\gamma B_1 t}{2}\right) \tag{36}$$

The probability amplitude for a spin flip in the same time interval is then

$$\langle\downarrow|U_I(t,0)|\uparrow\rangle = \begin{bmatrix} 0 & 1 \end{bmatrix} \left(I\cos\left(\frac{\gamma B_1 t}{2}\right) - i\sigma_x \sin\left(\frac{\gamma B_1 t}{2}\right)\right) \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{37}$$

$$= \begin{bmatrix} 0 & 1 \end{bmatrix} \left(\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \cos\left(\frac{\gamma B_1 t}{2}\right) - i \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \sin\left(\frac{\gamma B_1 t}{2}\right)\right) \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{38}$$

$$= -i\sin\left(\frac{\gamma B_1 t}{2}\right) \tag{39}$$

with corresponding probability

$$P_{\downarrow\uparrow} = \left|\left\langle \downarrow \left| U_I(t,0) \right| \uparrow \right\rangle\right|^2 \tag{40}$$

$$= \sin^2\left(\frac{\gamma B_1 t}{2}\right) \tag{41}$$

Note that the required condition

$$P_{\uparrow\uparrow} + P_{\downarrow\uparrow} = 1 \tag{42}$$

is satisfied.

The expectation value of S_z at time t is

$$\langle S_z \rangle = \frac{1}{2} P_{\uparrow\uparrow} - \frac{1}{2} P_{\downarrow\uparrow} \tag{43}$$

$$= \frac{1}{2}\left(\cos^2\left(\frac{\gamma B_1 t}{2}\right) - \sin^2\left(\frac{\gamma B_1 t}{2}\right)\right) \tag{44}$$

$$= \frac{1}{2}\cos(\gamma B_1 t) \tag{45}$$

Thus $\langle S_z \rangle$ oscillates between its extreme values of $\pm\frac{1}{2}$.