MAGNETIC RESONANCE

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 9.20.

We've looked at the behaviour of a spin 1/2 particle in a constant magnetic field. Now we can see what happens if we turn on a small time-varying magnetic field in addition to the constant field. The total field is

$$\mathbf{B}=B_{rf}\cos(\omega t)\,\hat{\mathbf{x}}-B_{rf}\sin(\omega t)\,\hat{\mathbf{y}}+B_0\hat{\mathbf{z}} \tag{0.1}$$

where B_{rf} is the (small) magnitude of the time-varying field, which is assumed to be a radio frequency (rf) field (that is, very long wavelength). The spin hamiltonian is

$$H=-\gamma\mathbf{B}\cdot\mathbf{S} \tag{0.2}$$

where γ is the *gyromagnetic ratio,* and $\mathbf{S}=\frac{\hbar}{2}\sigma$ is the vector of 3 spin matrices.

$$\sigma_x=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix};\quad \sigma_y=\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix};\quad \sigma_z=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \tag{0.3}$$

The hamiltonian matrix is then

$$H=-\frac{\gamma\hbar}{2}\begin{bmatrix}B_0 & B_{rf}(\cos\omega t+i\sin\omega t)\\ B_{rf}(\cos\omega t-i\sin\omega t) & -B_0\end{bmatrix} \tag{0.4}$$

$$=-\frac{\hbar}{2}\begin{bmatrix}\omega_0 & \Omega e^{i\omega t}\\ \Omega e^{-i\omega t} & -\omega_0\end{bmatrix} \tag{0.5}$$

where

$$\omega_0\equiv\gamma B_0 \tag{0.6}$$

$$\Omega\equiv\gamma B_{rf} \tag{0.7}$$

We can now see how the spin state of the particle evolves with time. Let the spin state at time t be

$$\chi(t)=\begin{bmatrix} a(t) \\ b(t) \end{bmatrix} \tag{0.8}$$

Starting with the Schrödinger equation we have

$$i\hbar\dot{\chi}(t) = H\chi \tag{0.9}$$

$$i\hbar\begin{bmatrix} \dot{a}(t) \\ \dot{b}(t) \end{bmatrix} = -\frac{\hbar}{2}\begin{bmatrix} \omega_0 & \Omega e^{i\omega t} \\ \Omega e^{-i\omega t} & -\omega_0 \end{bmatrix}\begin{bmatrix} a(t) \\ b(t) \end{bmatrix} \tag{0.10}$$

so the ODEs for the spin states are

$$\dot{a}(t) = \frac{i}{2}\left(\Omega e^{i\omega t}b+\omega_0 a\right) \tag{0.11}$$

$$\dot{b}(t) = \frac{i}{2}\left(\Omega e^{-i\omega t}a-\omega_0 b\right) \tag{0.12}$$

To solve these equations exactly (without perturbation theory) we solve for b in the first equation and then differentiate again:

(0.13)
$$b=\frac{1}{\Omega}e^{-i\omega t}\left(\frac{2}{i}\dot{a}-\omega_0 a\right)$$

(0.14)
$$\ddot{a}=\frac{i}{2}\left(\Omega i\omega e^{i\omega t}b+\Omega e^{i\omega t}\dot{b}+\omega_0\dot{a}\right)$$

(0.15)
$$=\frac{i}{2}\left(\Omega i\omega e^{i\omega t}\frac{1}{\Omega}e^{-i\omega t}\left(\frac{2}{i}\dot{a}-\omega_0 a\right)+\Omega e^{i\omega t}\frac{i}{2}\left(\Omega e^{-i\omega t}a-\omega_0 b\right)+\omega_0\dot{a}\right)$$

(0.16)
$$=-\frac{\omega}{2}\left(\frac{2}{i}\dot{a}-\omega_0 a\right)-\frac{1}{4}\Omega e^{i\omega t}\left(\Omega e^{-i\omega t}a-\omega_0\frac{1}{\Omega}e^{-i\omega t}\left(\frac{2}{i}\dot{a}-\omega_0 a\right)\right)+\frac{i}{2}\omega_0\dot{a}$$

(0.17)
$$=i\omega\dot{a}-\frac{1}{4}\left(\Omega^2+\omega_0^2-2\omega\omega_0\right)a$$

This gives a second order ODE with constant coefficients:

$$\ddot{a} - i\omega\dot{a} + \frac{1}{4}\left(\Omega^2 + \omega_0^2 - 2\omega\omega_0\right)a = 0 \tag{0.18}$$

$$\ddot{a} - i\omega\dot{a} + \frac{1}{4}\left(\Omega^2 + (\omega-\omega_0)^2 - \omega^2\right)a = 0 \tag{0.19}$$

The characteristic equation is

$$\lambda^2 - i\omega\lambda + \frac{1}{4}\left(\Omega^2 + (\omega-\omega_0)^2 - \omega^2\right) = 0 \tag{0.20}$$

with roots

$$\lambda = \frac{i}{2}\left(\omega \pm \sqrt{(\omega-\omega_0)^2 + \Omega^2}\right) = \frac{i}{2}\left(\omega \pm \omega'\right) \tag{0.21}$$

where

$$\omega' \equiv \sqrt{(\omega-\omega_0)^2 + \Omega^2} \tag{0.22}$$

The general solution is

$$a(t) = Ae^{i(\omega+\omega')t/2} + Be^{i(\omega-\omega')t/2} \tag{0.23}$$

From the symmetry of equations 0.11 and 0.12, the solution for $b(t)$ is the same, but with signs reversed on ω and ω_0 (thus ω' remains the same):

$$b(t) = Ce^{i(-\omega+\omega')t/2} + De^{i(-\omega-\omega')t/2} \tag{0.24}$$

The initial conditions are

$$a_0 = A + B \tag{0.25}$$

$$b_0 = C + D \tag{0.26}$$

To get additional conditions for determining the constants, we can substitute the solutions back into the original ODEs 0.11 and 0.12.

$$\dot{a} = A\frac{i}{2}\left(\omega+\omega'\right)e^{i(\omega+\omega')t/2} + B\frac{i}{2}\left(\omega-\omega'\right)e^{i(\omega-\omega')t/2} \tag{0.27}$$

$$= \frac{i\Omega}{2}e^{i\omega t}\left[Ce^{i(-\omega+\omega')t/2} + De^{i(-\omega-\omega')t/2}\right] + \omega_0 a \tag{0.28}$$

This equation must be true at all times, so for $t = 0$ we get

$$A\frac{i}{2}\left(\omega+\omega'\right)+B\frac{i}{2}\left(\omega-\omega'\right)=\frac{i\Omega}{2}\left(C+D\right)+\omega_0 a_0 \tag{0.29}$$

$$\omega a_0+\left(A-B\right)\omega'=\frac{i\Omega}{2}b_0+\omega_0 a_0 \tag{0.30}$$

$$A-B=\frac{1}{\omega'}\left(b_0\Omega+a_0\left(\omega_0-\omega\right)\right) \tag{0.31}$$

Writing 0.23 in terms of cosine and sine, we get

$$a\left(t\right)=\left[\left(A+B\right)\cos\frac{\omega' t}{2}+i\left(A-B\right)\sin\frac{\omega' t}{2}\right]e^{i\omega t/2} \tag{0.32}$$

$$=\left[a_0\cos\frac{\omega' t}{2}+\frac{i}{\omega'}\left(b_0\Omega+a_0\left(\omega_0-\omega\right)\right)\sin\frac{\omega' t}{2}\right]e^{i\omega t/2} \tag{0.33}$$

By the symmetry above, we can get $b\left(t\right)$:

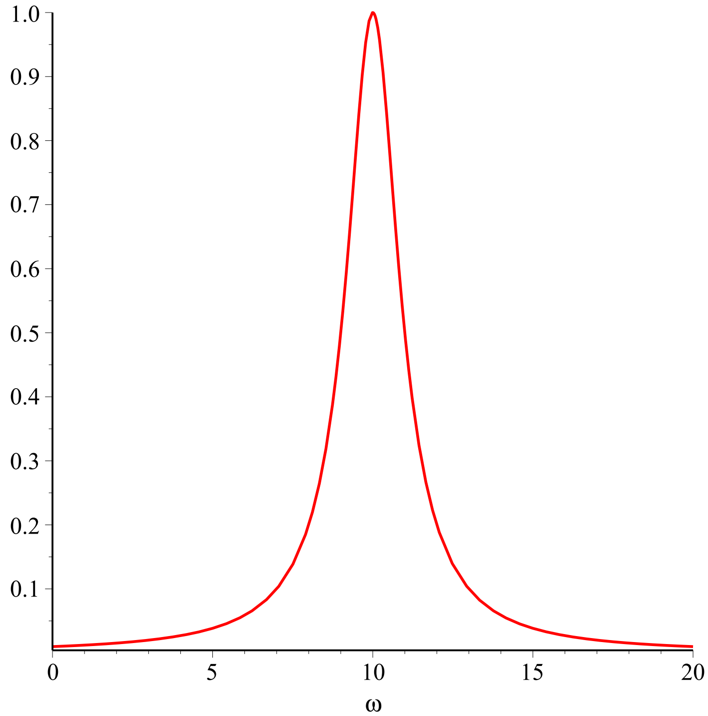
$$b\left(t\right)=\left[b_0\cos\frac{\omega' t}{2}+\frac{i}{\omega'}\left(a_0\Omega-b_0\left(\omega_0-\omega\right)\right)\sin\frac{\omega' t}{2}\right]e^{-i\omega t/2} \tag{0.34}$$

If the particle starts with spin up, then $a_0=1$, $b_0=0$ and the probability of a spin flip is

$$\left|b\left(t\right)\right|^2=\frac{\Omega^2}{\left(\omega'\right)^2}\sin^2\frac{\omega' t}{2} \tag{0.35}$$

$$=\frac{\Omega^2}{\left(\omega-\omega_0\right)^2+\Omega^2}\sin^2\frac{\omega' t}{2} \tag{0.36}$$

The factor multiplying the sine has a resonance at $\omega=\omega_0$, at which frequency the probability of a spin flip can reach its maximum value. Here's a plot of $\frac{\Omega^2}{\left(\omega-\omega_0\right)^2+\Omega^2}$ for $\Omega=1$ and $\omega_0=10$:



At half-maximum, $\frac{\Omega^2}{(\omega-\omega_0)^2+\Omega^2} = 0.5$ so $\omega - \omega_0 = \pm\Omega$ and the full width of the curve at that point is $\Delta\omega = 2\Omega$.

For a proton, the gyromagnetic ratio is given by

$$\gamma = \frac{g_p e}{2m_p} \tag{0.37}$$

Its value (as of 2010) is

$$\gamma = 2.675 \times 10^8 \text{ s}^{-1}\text{Tesla}^{-1} \tag{0.38}$$

In an experiment where the constant field is $B_0 = 10^4$ gauss $= 1$ Tesla and the rf field is $B_{rf} = 0.01$ gauss $= 10^{-6}$ Tesla, we get

$$\omega_0 = \gamma B_0 = 2.675 \times 10^8 \text{ s}^{-1} = 4.26 \times 10^7 \text{ Hz} \tag{0.39}$$

$$\Omega = \gamma B_{rf} = 267.5 \text{ s}^{-1} = 42.6 \text{ Hz} \tag{0.40}$$

$$\Delta\omega = 2\Omega = 535 \text{ s}^{-1} = 85.2 \text{ Hz} \tag{0.41}$$

The magnetic resonance effect results in a narrow peak in which the probability of a spin flip is maximum.