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

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

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

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

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

$$\sigma_x=\begin{bmatrix}0&1\\1&0\end{bmatrix};\quad\sigma_y=\begin{bmatrix}0&-i\\i&0\end{bmatrix};\quad\sigma_z=\begin{bmatrix}1&0\\0&-1\end{bmatrix} \tag{3}$$

The hamiltonian matrix is then

$$\begin{aligned}H&=-\frac{\gamma\hbar}{2}\begin{bmatrix}B_0&B_{rf}(\cos\omega t+i\sin\omega t)\\B_{rf}(\cos\omega t-i\sin\omega t)&-B_0\end{bmatrix} &(4)\\&=-\frac{\hbar}{2}\begin{bmatrix}\omega_0&\Omega e^{i\omega t}\\\Omega e^{-i\omega t}&-\omega_0\end{bmatrix} &(5)\end{aligned}$$

where

$$\begin{aligned}\omega_0&\equiv\gamma B_0 &(6)\\\Omega&\equiv\gamma B_{rf} &(7)\end{aligned}$$

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

$$\chi(t) = \begin{bmatrix} a(t) \\ b(t) \end{bmatrix} \tag{8}$$

Starting with the Schrödinger equation we have

$$\begin{aligned} i\hbar\dot{\chi}(t) &= H\chi & (9) \\ i\hbar\begin{bmatrix} \dot{a}(t) \\ \dot{b}(t) \end{bmatrix} &= -\frac{\hbar}{2}\begin{bmatrix} \omega_0 & \Omega e^{i\omega t} \\ \Omega e^{-i\omega t} & -\omega_0 \end{bmatrix}\begin{bmatrix} a(t) \\ b(t) \end{bmatrix} & (10) \end{aligned}$$

so the ODEs for the spin states are

$$\begin{aligned} \dot{a}(t) &= \frac{i}{2}\left(\Omega e^{i\omega t} b + \omega_0 a\right) & (11) \\ \dot{b}(t) &= \frac{i}{2}\left(\Omega e^{-i\omega t} a - \omega_0 b\right) & (12) \end{aligned}$$

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

$$b = \frac{1}{\Omega}e^{-i\omega t}\left(\frac{2}{i}\dot{a} - \omega_0 a\right) \tag{13}$$

$$\ddot{a} = \frac{i}{2}\left(\Omega i\omega e^{i\omega t} b + \Omega e^{i\omega t}\dot{b} + \omega_0\dot{a}\right) \tag{14}$$

$$= \frac{i}{2}\left(\Omega i\omega e^{i\omega t}\frac{1}{\Omega}e^{-i\omega t}\left(\frac{2}{i}\dot{a} - \omega_0 a\right) + \Omega e^{i\omega t}\frac{i}{2}\left(\Omega e^{-i\omega t} a - \omega_0 b\right) + \omega_0\dot{a}\right) \tag{15}$$

$$= -\frac{\omega}{2}\left(\frac{2}{i}\dot{a} - \omega_0 a\right) - \frac{1}{4}\Omega e^{i\omega t}\left(\Omega e^{-i\omega t} a - \omega_0\frac{1}{\Omega}e^{-i\omega t}\left(\frac{2}{i}\dot{a} - \omega_0 a\right)\right) + \frac{i}{2}\omega_0\dot{a} \tag{16}$$

$$= i\omega\dot{a} - \frac{1}{4}\left(\Omega^2 + \omega_0^2 - 2\omega\omega_0\right)a \tag{17}$$

This gives a second order ODE with constant coefficients:

$$\ddot{a} - i\omega\dot{a} + \frac{1}{4}\left(\Omega^2 + \omega_0^2 - 2\omega\omega_0\right)a = 0 \tag{18}$$

$$\ddot{a} - i\omega\dot{a} + \frac{1}{4}\left(\Omega^2 + (\omega - \omega_0)^2 - \omega^2\right)a = 0 \tag{19}$$

The characteristic equation is

$$\lambda^2 - i\omega\lambda + \frac{1}{4}\left(\Omega^2 + (\omega-\omega_0)^2 - \omega^2\right) = 0 \tag{20}$$

with roots

$$\lambda = \frac{i}{2}\left(\omega \pm \sqrt{(\omega-\omega_0)^2 + \Omega^2}\right) = \frac{i}{2}\left(\omega \pm \omega'\right) \tag{21}$$

where

$$\omega' \equiv \sqrt{(\omega-\omega_0)^2 + \Omega^2} \tag{22}$$

The general solution is

$$a(t) = Ae^{i(\omega+\omega')t/2} + Be^{i(\omega-\omega')t/2} \tag{23}$$

From the symmetry of equations 11 and 12, the solution for $b(t)$ is the same, but with signs reversed on ω and ω_0 (thus ω' remains the same):

$$b(t) = Ce^{i(-\omega+\omega')t/2} + De^{i(-\omega-\omega')t/2} \tag{24}$$

The initial conditions are

$$a_0 = A + B \tag{25}$$
$$b_0 = C + D \tag{26}$$

To get additional conditions for determining the constants, we can substitute the solutions back into the original ODEs 11 and 12.

$$\dot{a} = A\frac{i}{2}\left(\omega+\omega'\right)e^{i(\omega+\omega')t/2} + B\frac{i}{2}\left(\omega-\omega'\right)e^{i(\omega-\omega')t/2} \tag{27}$$
$$= \frac{i\Omega}{2}e^{i\omega t}\left[Ce^{i(-\omega+\omega')t/2} + De^{i(-\omega-\omega')t/2}\right] + \omega_0 a \tag{28}$$

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

$$A\frac{i}{2}\left(\omega+\omega'\right) + B\frac{i}{2}\left(\omega-\omega'\right) = \frac{i\Omega}{2}(C+D) + \omega_0 a_0 \tag{29}$$
$$\omega a_0 + (A-B)\omega' = \frac{i\Omega}{2}b_0 + \omega_0 a_0 \tag{30}$$
$$A - B = \frac{1}{\omega'}\left(b_0\Omega + a_0(\omega_0-\omega)\right) \tag{31}$$

Writing 23 in terms of cosine and sine, we get

$$a(t) = \left[(A+B)\cos\frac{\omega' t}{2} + i(A-B)\sin\frac{\omega' t}{2}\right] e^{i\omega t/2} \tag{32}$$

$$= \left[a_0\cos\frac{\omega' t}{2} + \frac{i}{\omega'}\left(b_0\Omega + a_0\left(\omega_0-\omega\right)\right)\sin\frac{\omega' t}{2}\right] e^{i\omega t/2} \tag{33}$$

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

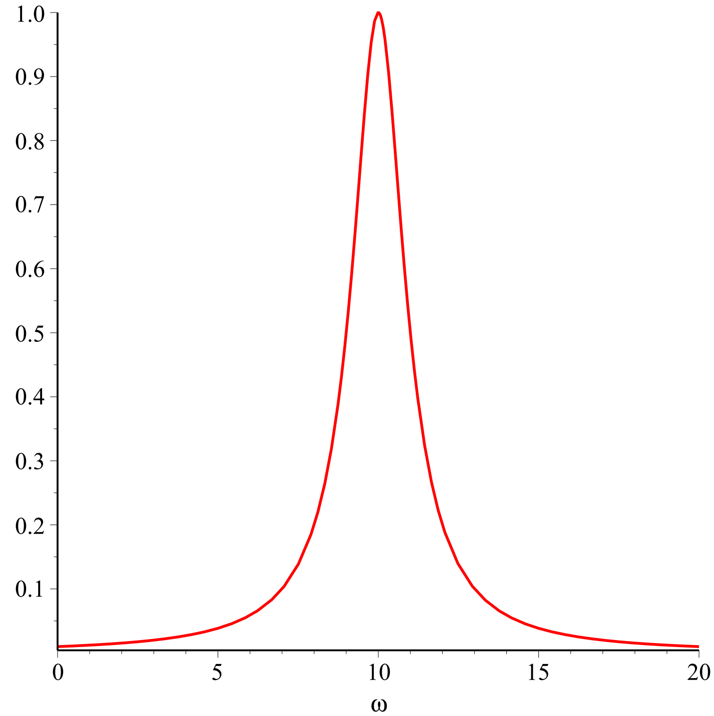
$$b(t) = \left[b_0\cos\frac{\omega' t}{2} + \frac{i}{\omega'}\left(a_0\Omega - b_0\left(\omega_0-\omega\right)\right)\sin\frac{\omega' t}{2}\right] e^{-i\omega t/2} \tag{34}$$

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

$$|b(t)|^2 = \frac{\Omega^2}{(\omega')^2}\sin^2\frac{\omega' t}{2} \tag{35}$$

$$= \frac{\Omega^2}{\left(\omega-\omega_0\right)^2+\Omega^2}\sin^2\frac{\omega' t}{2} \tag{36}$$

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

$$\gamma = \frac{g_p e}{2m_p} \tag{37}$$

Its value (as of 2010) is

$$\gamma = 2.675 \times 10^8 \text{ s}^{-1}\text{Tesla}^{-1} \tag{38}$$

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

$$\omega_0 = \gamma B_0 = 2.675 \times 10^8 \text{ s}^{-1} = 4.26 \times 10^7 \text{ Hz} \tag{39}$$

$$\Omega = \gamma B_{rf} = 267.5 \text{ s}^{-1} = 42.6 \text{ Hz} \tag{40}$$

$$\Delta\omega = 2\Omega = 535 \text{ s}^{-1} = 85.2 \text{ Hz} \tag{41}$$

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