

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

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

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

$$H = -\gamma \mathbf{B} \cdot \mathbf{S} \quad (2)$$

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

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

The hamiltonian matrix is then

$$H = -\frac{\gamma \hbar}{2} \begin{bmatrix} B_0 & B_{rf} (\cos \omega t + i \sin \omega t) \\ B_{rf} (\cos \omega t - i \sin \omega t) & -B_0 \end{bmatrix} \quad (4)$$

$$= -\frac{\hbar}{2} \begin{bmatrix} \omega_0 & \Omega e^{i\omega t} \\ \Omega e^{-i\omega t} & -\omega_0 \end{bmatrix} \quad (5)$$

where

$$\omega_0 \equiv \gamma B_0 \quad (6)$$

$$\Omega \equiv \gamma B_{rf} \quad (7)$$

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

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

Starting with the Schrödinger equation we have

$$i\hbar \dot{\chi}(t) = H\chi \quad (9)$$

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

so the ODEs for the spin states are

$$\dot{a}(t) = \frac{i}{2} (\Omega e^{i\omega t} b + \omega_0 a) \quad (11)$$

$$\dot{b}(t) = \frac{i}{2} (\Omega e^{-i\omega t} a - \omega_0 b) \quad (12)$$

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

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

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

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

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

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

This gives a second order ODE with constant coefficients:

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

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

The characteristic equation is

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

with roots

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

where

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

The general solution is

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

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):

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

The initial conditions are

$$a_0 = A + B \quad (25)$$

$$b_0 = C + D \quad (26)$$

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

$$\dot{a} = A \frac{i}{2} (\omega + \omega') e^{i(\omega+\omega')t/2} + B \frac{i}{2} (\omega - \omega') e^{i(\omega-\omega')t/2} \quad (27)$$

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

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

$$A \frac{i}{2} (\omega + \omega') + B \frac{i}{2} (\omega - \omega') = \frac{i\Omega}{2} (C + D) + \omega_0 a_0 \quad (29)$$

$$\omega a_0 + (A - B) \omega' = \frac{i\Omega}{2} b_0 + \omega_0 a_0 \quad (30)$$

$$A - B = \frac{1}{\omega'} (b_0 \Omega + a_0 (\omega_0 - \omega)) \quad (31)$$

Writing 23 in terms of cosine and sine, we get

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

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

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

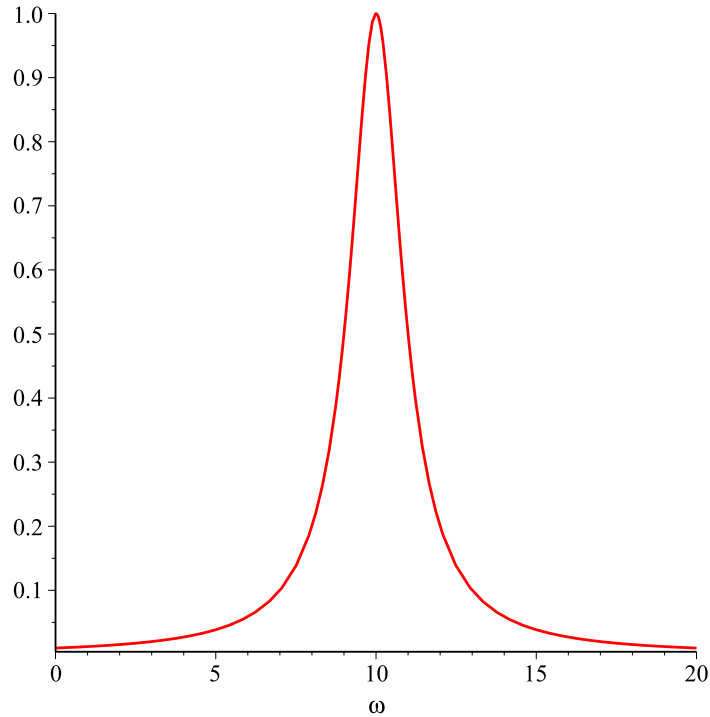
$$b(t) = \left[b_0 \cos \frac{\omega't}{2} + \frac{i}{\omega'} (a_0 \Omega - b_0 (\omega_0 - \omega)) \sin \frac{\omega't}{2} \right] e^{-i\omega t/2} \quad (34)$$

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

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

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

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 $\frac{\Omega^2}{(\omega - \omega_0)^2 + \Omega^2}$ 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

$$\gamma = \frac{g_p e}{2m_p} \quad (37)$$

Its value (as of 2010) is

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

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

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

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

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

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