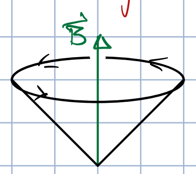
Paramagnetic resonance → Approximation methods

Spin ½ particles : electrons, protons, nuclei

Magnetic moment: $\vec{\mu} = \gamma \vec{S}$ → measured experimentally

in a magnetic field: $H = -\vec{\mu}\cdot\vec{B}$ → precession in a $\vec{B}$ field



$\vec{B} = B_0 \hat{e}_z$

$E_\pm = \mp \frac{\omega_0 \hbar}{2}$ $\qquad \omega_0 = \gamma B_0$

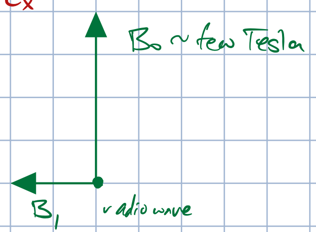
$$\chi(t) = \begin{pmatrix} a e^{i\omega_0 t/2} \\ b e^{-i\omega_0 t/2} \end{pmatrix} \qquad \chi(0) = \begin{pmatrix} a \\ b \end{pmatrix}$$

prob of spin up along z $\qquad$ prob $= (1, 0)\begin{pmatrix} a e^{i\omega_0 t/2} \\ b e^{-i\omega_0 t/2} \end{pmatrix} = |a e^{i\omega_0 t/2}|^2 = |a_0|^2$

precession along z doesn't change w/time

let's induce transitions between spin up & spin down

$H = -\gamma \frac{\hbar}{2}\, \vec{\sigma}\cdot\vec{B}$ $\qquad \vec{B} = B_0 \hat{e}_z + B_1 \cos(\omega t)\, \hat{e}_x$



$$H = -\frac{\gamma\hbar}{2}\begin{pmatrix} B_0 & B_1\cos(\omega t) \\ B_1\cos(\omega t) & B_0 \end{pmatrix}$$

⚬̈ H depends on time! → energy not conserved in this system

can still compute prob. of spin up or down

3 frequencies

ω

$\omega_0 = \gamma B_0$

$\omega_1 = \gamma B_1$

$$\chi(t) = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} \qquad |a|^2 + |b|^2 = 1$$

when $B_1=0$ we have

$$a(t) = a(0)\ e^{i\omega_0 t/2} \quad b(t) = b(0)\ e^{-i\omega_0 t/2}$$

$$\left.\begin{aligned} A(t) &= a(t)\, e^{-i\omega_0 t/2} \\ B(t) &= b(t)\, e^{i\omega_0 t/2} \end{aligned}\right\} \text{ when } B_1=0 \text{ } A, B \text{ are indpt. of time}$$

into SE for $\omega \simeq \omega_0$

① $$i\frac{dA}{dt} = \frac{-\omega}{4}\left(e^{it(\omega-\omega_0)} + \cancel{e^{it(-\omega-\omega_0)}}\right) B(t)$$

② $$i\frac{dB}{dt} = \frac{-\omega}{4}\left(\cancel{e^{it(\omega-\omega_0)}} + e^{it(-\omega-\omega_0)}\right) A(t)$$

allowed to tune ω

make ω close to ω_0 s.t. $\omega-\omega_0 \ll \omega+\omega_0$

$e^{\pm it(\omega+\omega_0)}$ varies rapidly ← drop averages to zero

$e^{\pm it(-\omega+\omega_0)}$ varies slowly

Solve ① for $B(t) = -\frac{4}{\omega_1}\, e^{-it(\omega-\omega_0)}\, \frac{dA}{dt}$, sub into ②

$$\frac{d^2A}{dt^2} - i(\omega-\omega_0)\frac{dA}{dt} + \frac{\omega^2}{16}A(t) = 0$$

2nd order ODE w/constant coefficients $\quad A = A_0 e^{i\lambda t}$

$$\left(-\lambda^2 + (\omega-\omega_0)\lambda + \frac{\omega^2}{16}\right) A e^{i\lambda t} = 0$$

$$\lambda_\pm = \frac{\omega-\omega_0}{2} \pm \frac{1}{2}\sqrt{(\omega-\omega_0)^2 + \frac{\omega^2}{16}}$$

$$\rightarrow A(t) = A_+ e^{i\lambda_+ t} + A_- e^{i\lambda_- t}$$

$\chi(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\quad a(0) = 1 = A_+ + A_-$

$b(0) = 0 = \lambda_+ A_+ + \lambda_- A_-$

$$A_+ = \frac{\lambda_-}{\lambda_- - \lambda_+} \qquad A_- = \frac{-\lambda_+}{\lambda_- - \lambda_+}$$

prob of spin down @ time t

$$\left| (0,1) \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} \right|^2 = |b(t)|^2$$

$$= \left(\frac{\omega_1^2}{4} \frac{1}{(\omega - \omega_0)^2 + \omega_1^2/4} \right) \left(\frac{1 - \cos\left(t \sqrt{(\omega-\omega_0)^2 + \omega_1^2/4}\right)}{2} \right)$$

$\omega \ll \omega_0$