<u>Spin Dynamics</u> (2^{nd} edition)

1.2, 1.4

Chapter 2

3.1, 3.2, 3.7, 3.8

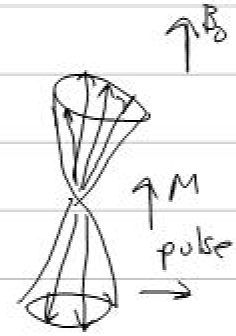
Announcement:

Experiment: http://128.252.35.98/322/~~Exp~~ Experiments/Physics/PulsedNMR/ExpNMR.pdf

<u>Vector Model</u>

Σ magnetic moments → macroscopic magnetization (M)

- no resultant magnetization $\perp$ to B_0



Interaction energy between μ and B_0, M and B_0

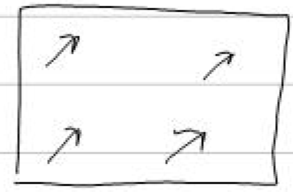
- single spin, $E = -\mu_z B$
- many spins, $E_{tot} = -\sum \mu_z B$

$$\frac{E_{tot}}{V} = -\sum \frac{\mu_z}{V} B = -MB$$

magnetization to be calculated

N = total number of nuclei

Total energy of an ensemble of spins (isolated)



$$= \sum_m E_m N_m = E$$

Boltzmann Distribution, $\frac{N_m}{N_{tot}} = \frac{e^{-E_m/kT}}{\sum_n e^{-E_n/kT}}$

Taylor series expansion: $e^{-E_m/kT} = 1 - \frac{E_m}{kT} + \frac{1}{2}\left(\frac{E_m}{kT}\right)^2 + \ldots$

$$\sum_m e^{-E_m/kT} = \sum_m \left(1 - \frac{E_m}{kT} + \frac{1}{2}\left(\frac{E_m}{kT}\right)^2 + \ldots\right)$$

- compare E_m to thermal energy (protons)
  - 1 mole at 14.6T
    - $E_m = -m\gamma B N_A = \frac{1}{2}(1.05 \cdot 10^{-34}\,\mathrm{J})(2.7 \cdot 10^{8}\,T^{-1}\frac{\mathrm{rad}}{s}) \cdot 14.6\,T \cdot 6.02 \cdot 10^{23}$

$$= 0.12\ \mathrm{J}$$

- Thermal energy $= N_A kT \approx 2500$ J at 300K

~~So~~ We can make a high temperature approximation to knock off the squared terms in the expansions

$$\frac{N_m}{N_{tot}} = \frac{1 + \frac{m\hbar\gamma B}{kT}}{\sum_m 1 + \sum_m \frac{\hbar\gamma B m}{kT}}$$

$$\Downarrow \qquad\qquad \Downarrow$$

$$2I+1 \qquad\qquad \frac{\hbar\gamma B}{kT}\sum_{m_I} m_I = 0$$

So, $$\frac{N_m}{N_{tot}} = \frac{1 + \frac{m_I\hbar\gamma B}{kT}}{2I+1}$$

$$\frac{E_{tot}}{V} = -MB = \sum_{m_I} \frac{E_m N_m}{V} = \sum_m (-m\hbar\gamma B)\left(\frac{1 + m\hbar\gamma B/kT}{2I+1}\right)\frac{N_{tot}}{V}$$

$$= \frac{-\hbar\gamma B}{2I+1}\left(\frac{N_{tot}}{V}\right)\left[\sum_{m_I}\left(\frac{\hbar\gamma B}{kT}\right)m^2\right]$$

$$= \frac{-\hbar^2\gamma^2 B^2}{(2I+1)(kT)}\left(\frac{N_{tot}}{V}\right)\sum m^2$$

Note, $\sum_{\cancel{I}} m^2 = I^2 + (I-1)^2 + \dots + (-I)^2$

math handbook, $\sum_{x=1}^{n} x^2 = \frac{n(n+1)(2n+1)}{3!}$

$$\sum_{m_I=-I}^{I} m^2 = \frac{\cancel{2}I(I+1)(2I+1)}{3\cdot\cancel{2}\cdot 1}$$

$$\frac{E_{tot}}{V} = \frac{-\hbar^2\gamma^2 B^2}{(2I+1)kT}\left(\frac{N_{tot}}{V}\right)\left(\frac{I(I+1)(2I+1)}{3}\right) = \frac{-\hbar^2\gamma^2 B^2 I(I+1)}{3kT}\left(\frac{N_{tot}}{V}\right)$$

$= $ also $-MB$

So, $$M = \frac{\hbar^2\gamma^2 B I(I+1)}{3kT}\cdot\frac{N_{tot}}{V}$$

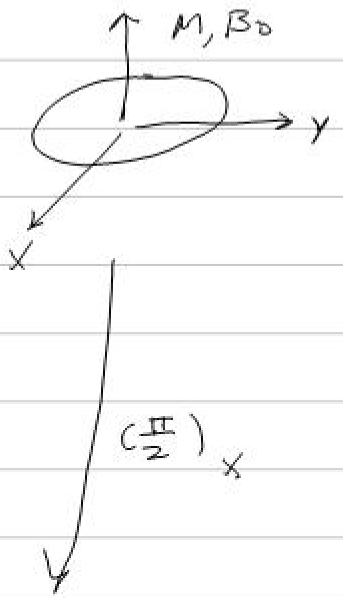
Curie Law

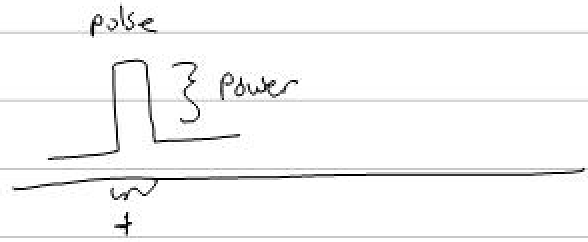
Affects detection limit

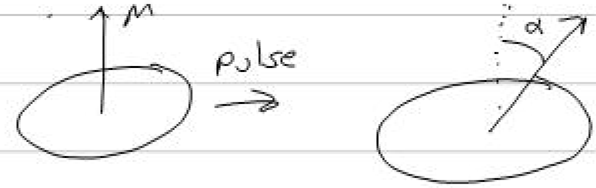
H $\rightarrow 10^{13}$

^{13}C $\rightarrow 10^{17}$

Thermal Equilibrium



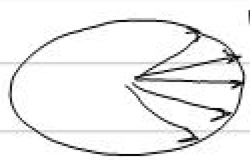




Commonly a 90X pulse puts the magnetization along y. (Let's say)

A pulse on y would put the magnetization on −x.

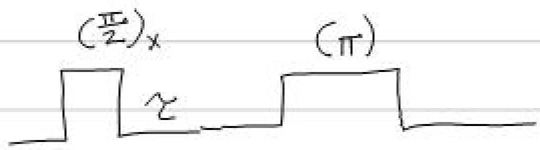
time



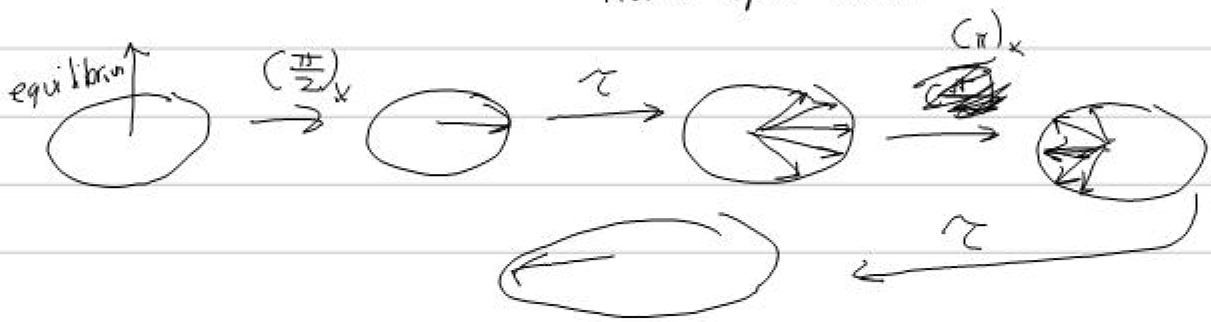
range of frequencies cause spins to dephase

T_2 (transverse relaxation)

To examine T_2,

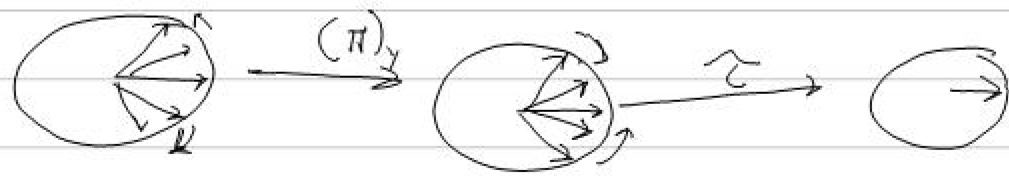


Hahn Spin Echo

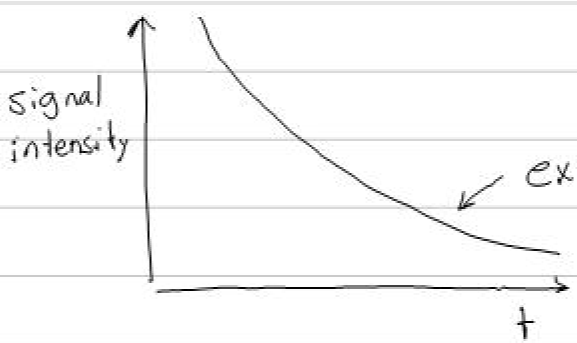


Record negative echo signal. Gaussian.

Or, let it be a $(\pi)_y$ pulse

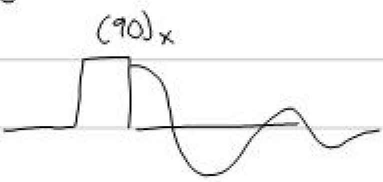


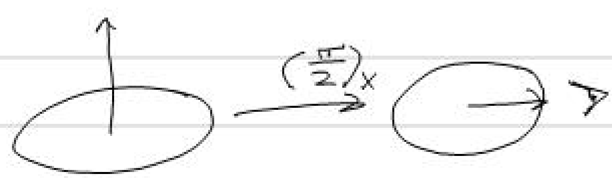
As you lengthen τ, the echo produced will get shorter.



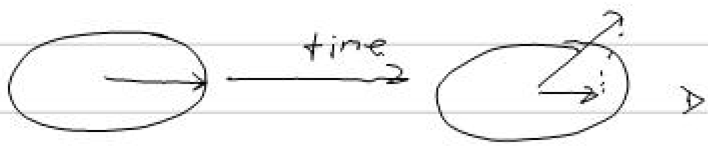
(T_2^*, T_2' also exist)

Again consider Bloch decay.





Return to thermal equilibrium (T_1) (longitudinal, spin-lattice.)



T_1 determines required delay before another acquisition