Pulse Nuclear Magnetic Resonance

Spin Echoes, Viscosity, and Paramagnetic Doping

Bhaskar Mookerji Charles Herder

8.13 Experimental Physics I
MIT Department of Physics

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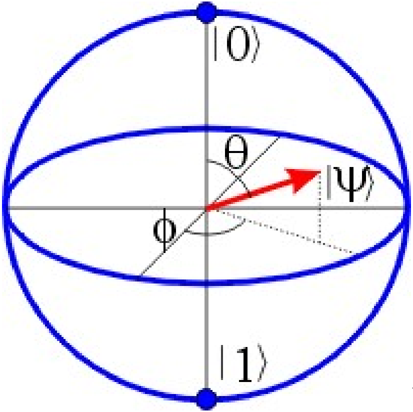
Outline

1 Introduction
- Magnetic Resonance and Relaxation
- Mechanisms of Transverse Decay & Spin Echoes

2 Experimental
- Signal Chain and Sample Preparation
- Calibration, ΔH Field Homogeneity, Timing Parameters

3 Results and Error Analysis
- Random/Systematic Error Accounting
- T_2^* from $\frac{\pi}{2}$ Pulse
- T_2 from $\frac{\pi}{2}$–τ–π
- T_2 from Carr-Purcell Pulse Sequence
- Relaxation from Viscosity in Glycerin
- Relaxation of Paramagnetic Ion Doping with $Fe(NO_3) \cdot 9H_2O$



[1]

$$|\psi(t)\rangle = a_+(t)\,|\uparrow\rangle + a_-(t)\,|\downarrow\rangle \tag{1}$$

[1] http://qt.tn.tudelft.nl/research/qc/bloch.jpg

Energy of magnetic moment in field $\mathbf{B} = B_0 \hat{e}_z$

$$H = -\mu \cdot \mathbf{B}, \tag{2}$$

Ehrenfest's Theorem, Larmor procession about mean moment:

$$\frac{\partial \langle \mu \rangle}{\partial t} = -\frac{i}{\hbar} \langle [\mu, H] \rangle = \gamma \langle \mu(t) \rangle \times \mathbf{B}(t) \,. \tag{3}$$

Oscillating perpendicular field, $B_0 >> B_1$:

$$H = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix} \tag{4}$$

Transformation via $|\phi(t)\rangle = e^{i\omega t S_z/\hbar} |\psi(t)\rangle$:

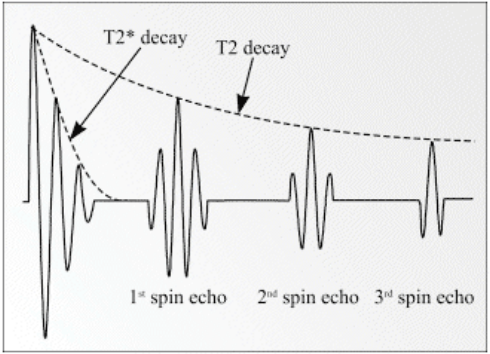
$$\tilde{H} = \frac{\hbar}{2} \begin{pmatrix} -\Delta\omega & \omega_1 \\ \omega_1 & \Delta\omega \end{pmatrix} \tag{5}$$

Driving at resonance $\Delta\omega \approx 0$, Rabi oscillations occur:

$$|\langle\downarrow|\phi(t)\rangle|^2 = \frac{\omega_1^2}{\omega_1^2 + (\Delta\omega)^2} \sin^2\left[\frac{1}{2}\sqrt{(\Delta\omega)^2 + \omega_1^2}\,t\right]. \tag{6}$$

π-pulse: $|\langle\downarrow|\phi(t)\rangle|^2 = 1 \rightarrow t = \pi/\gamma B_1$.

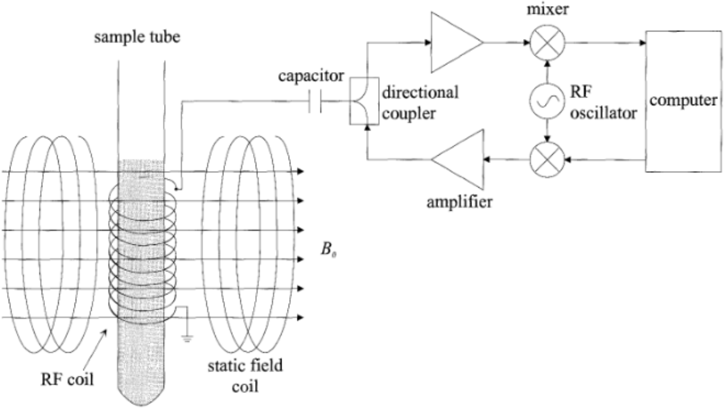
Relations to equilibrium Maxwell-Boltzmann distribution occurs in time T_1



[2]

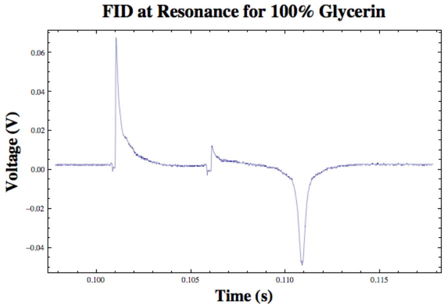
$$\mathbf{B}_i = \mathbf{B}_0 + \mathbf{b}_i \rightarrow \mathbf{b}_i = \frac{\mu_0}{4\pi} \sum_j \left[\frac{\mu}{r_{ij}^3} - \frac{(\mu \cdot \mathbf{r}_{ij})\, \mathbf{r}_{ij}}{r_{ij}^5} \right] \rightarrow M(2\tau) = M(0) \tag{7}$$

[2] http://www.easymeasure.co.uk/webs/3/html/510/fig9.gif



[3]

[3] Quantum Information and Computation, Chuang and Nielsen.



Parameters:

- Pulse width calibration, matching capacitance, minimizing ΔH_0 from FID
- Maximum FID with $\frac{\pi}{2}$-pulse $\rightarrow T_2^*$
- Carr-Purcell and $\frac{\pi}{2} - \tau - \pi$ for T_2

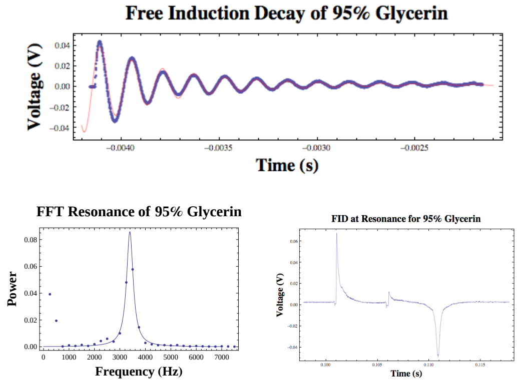
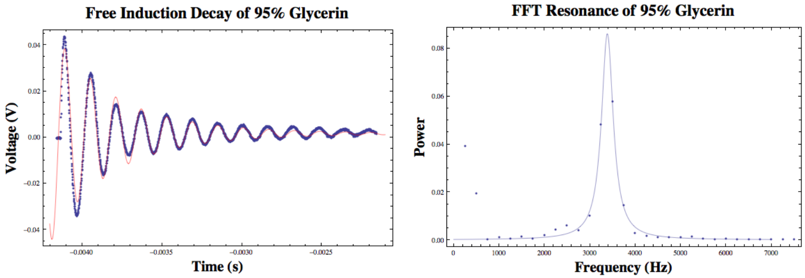


Figure: Caption of subfigures (a), (b) and (c)

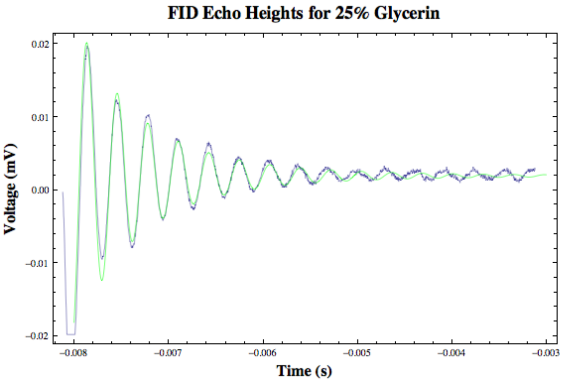
Consider,

- Instrumental scope uncertainty: 1mV
- Statistical uncertainty (sampling error): 0.4mV
- Natural line width
- Inhomogeneity of $H \rightarrow$ Extrapolated from T_2, T_2^*
- Pulse Angle and concentration
- Concentration from samples, contamination

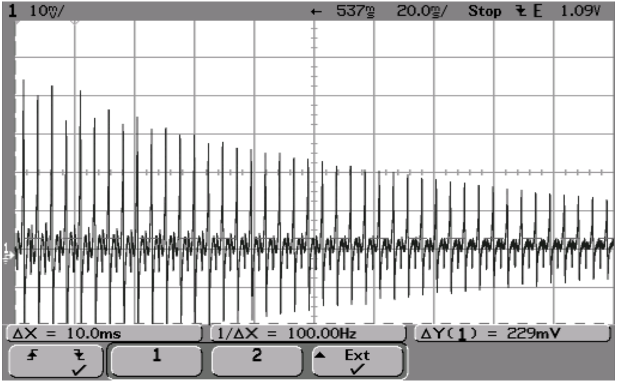


$$V = V_0 \exp\left[-\frac{2\tau}{T_2^*}\right] \cos\left[(\Delta\omega)(t - t_0)\right] \qquad \tilde{V} = \tilde{V}_0 \frac{\sigma}{(f - f_0)^2 + \sigma^2} \qquad T_2^* = \frac{2}{\sigma} \quad (8)$$

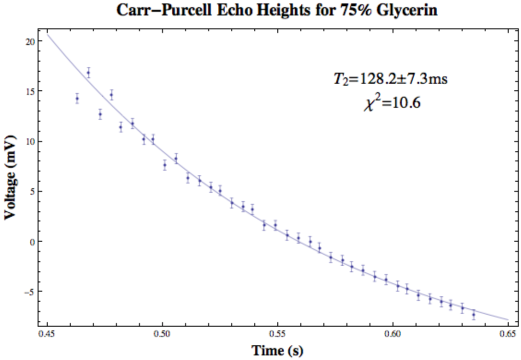
For both $T_2^* \approx 0.51$



$$V = V_0 \exp\left[-\frac{2\tau}{T_2} - \frac{2}{3}\gamma^2 D G^2 \tau^3\right] \cos\left[(\Delta\omega)(t - t_0)\right] \qquad (9)$$



$$\pi/2 - \tau - \pi - 2\tau - \pi - 2\tau - \pi - \cdots$$



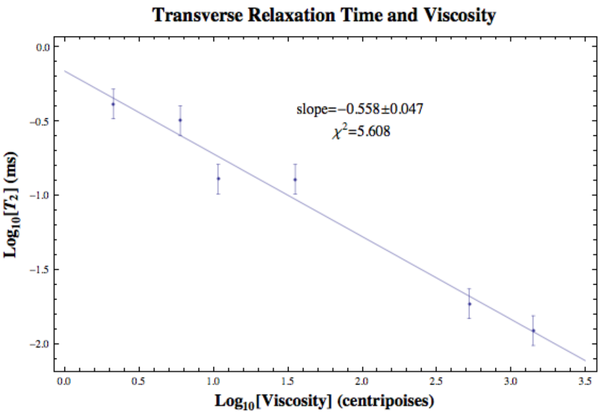
$$V = V_0 \exp\left[-\frac{2n\tau}{T_2}\right] \tag{10}$$

Table: Transverse relaxation time at 23.6±0.5°C.

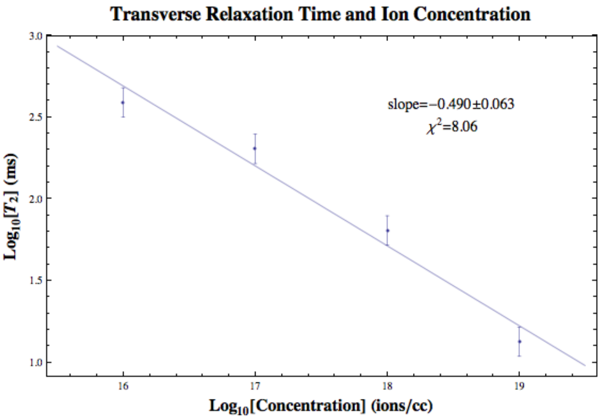
$\eta_{\text{Glyc.}}$ (%)	T_2 (ms)	T_2^* (ms)	ΔH_0 (Gauss)
100	12.13 ± 0.82	0.44 ± 0.07	0.23 ± 0.08
95	18.50 ± 0.73	0.51 ± 0.07	0.24 ± 0.07
75	127.8 ± 1.23	0.99 ± 0.13	0.28 ± 0.03
60	128.0 ± 4.79	0.51 ± 0.08	0.53 ± 0.05
50	318.4 ± 5.52	0.74 ± 0.09	0.80 ± 0.10
25	410.6 ± 11.9	0.83 ± 0.10	0.14 ± 0.11

$$\frac{1}{T_2^*} = \frac{1}{T_2} + \gamma \Delta H \tag{11}$$

Errors determined as 1σ from fits.



See K. Luszczyski, J. A. E. Kail and J.G. Powles. *Molecular Motion in Liquid Glycerol by Proton Magnetic Relaxation*, 1959.


Transverse Relaxation Time and Ion Concentration
slope=−0.490±0.063
χ^2=8.06
$\mathrm{Log}_{10}[T_2]$ (ms)
3.0
2.5
2.0
1.5
1.0
16
17
18
19
Log_{10}[Concentration] (ions/cc)

Summary

- Qualitative agreement on viscosity and ion doping effects on relaxation.
- Magnetic field homogeneity determined from transverse decay constants.
- Problems: Beer's law for measuring concentration: Why doesn't 8.13 have a colorimeter?

Acknowledgements

- Charles Herder
- JLab staff: For being helpful despite knowing more than we do.
- E.M. Purcell: You can't spell NMR without "enema"+"r".