Field Gradients – Uses in NMR

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Pulsed Field Gradients – NMR Applications

Pulsed Field Gradients – How they Work

Magnetization vectors precess at different rates depending on $G(z)$ and $\gamma$ for each volume element. They dephase - net $M_x, M_y = 0$
Effects of Gradients can be Refocussed

Application: Water Suppression

Resonance not affected by 90 refocuses

Resonance affected by 90 dephases (H₂O)
1D $^1H$ Water-Suppressed Spectrum

*Pf*-Rubredoxin in $^1H_2O$
Coherence Selection Using Pulse Field Gradients

• \( H(r) = -\sum_k \gamma_k [B_0 + B_z(r)] I_{kz} \)

  (in radians s\(^{-1}\) and neglecting chemical shifts)

• Effects on product operators for a z gradient:

  • \( I_{kz} \rightarrow -\gamma_k B_z(z) I_{kz} \tau \quad I_{kz} \)

  • \( I_k^+ \rightarrow -\gamma_k B_z(z) I_{kz} \tau \quad \exp[i \gamma_k B_z(z) \tau ] \quad I_k^+ \)

  • \( I_k^- \rightarrow -\gamma_k B_z(z) I_{kz} \tau \quad \exp[-i \gamma_k B_z(z) \tau ] \quad I_k^- \)

• For linear gradients \( B_z(z) = G_z z \)

• Observables are integrals over \( z \) – zero for \( I_k^+ , I_k^- \)
Gradient Selected HSQC

\[ \sigma_{mn}(t2) = \text{Integral}_z \left\{ \sigma_{mn}(t1) \exp[i\gamma_N 2G_1 z] \exp[-i\gamma_H G_2 z] \right\} \]

\[ = \text{Integral}_z \left\{ \sigma_{mn}(t1) \exp[i(\gamma_N 2G_1 z - \gamma_H G_2 z)] \right\} \]

\[ \sigma_{mn}(t2) \text{ finite only if } \gamma_N 2G_1 = \gamma_H G_2 \]

All 1Q proton transverse magnetization eliminated
Translational Diffusion Constants for Macromolecules

- Determine aggregate size
- Determine protein-protein interactions
- Screen for bound ligands

$$<(X_1-X_0)^2> = nDt \text{ where } D = kT/(6\pi\eta r)$$

- Key: if molecule moves, field is different, magnetization doesn’t refocus
Stejskal and Tanner Pulse Sequence for Diffusion Measurement

\[ \ln \left( \frac{S}{S_0} \right) = -\gamma^2 g^2 D \delta^2 (\Delta - \delta/3) \]
Diffusion Measurement Continued

- Measurements are limited by natural $T_2$
- Improved sequence uses $z$ storage
  (Altieri, Hinton and Byrd, 1995)

\[
\ln\left(\frac{S}{S_0}\right)
\]

\[
g^2
\]

- Large molecule
- Small molecule
The Nobel Prize in Physiology or Medicine 2003

"for their discoveries concerning magnetic resonance imaging"

Paul C. Lauterbur

Sir Peter Mansfield
Simple Imaging Strategy

- During gradient spins in each volume element have their own precession frequency
- Can get a 1D image of sample – used in gradient shimming
Simple 2D Image

- For 2D imaging use gradients in different directions (x, z) in different evolution periods (t1, t2)
Echo Planar Imaging – Speeding up Acquisitions

- $t_2$ will have spatial image (needs to be reversed in even $dw$)
- $t_1$ can sample a number of different properties
- $t_1$ could have a gradient in another dimension – 2D map
- $t_1$ could sample chemical shift dispersion - MRSI
Magnetic Resonance Spectroscopy Imaging

Prostate Cancer
B- Spectral Grid
C- MRSI Array