Superoperators for NMR Quantum Information Processing

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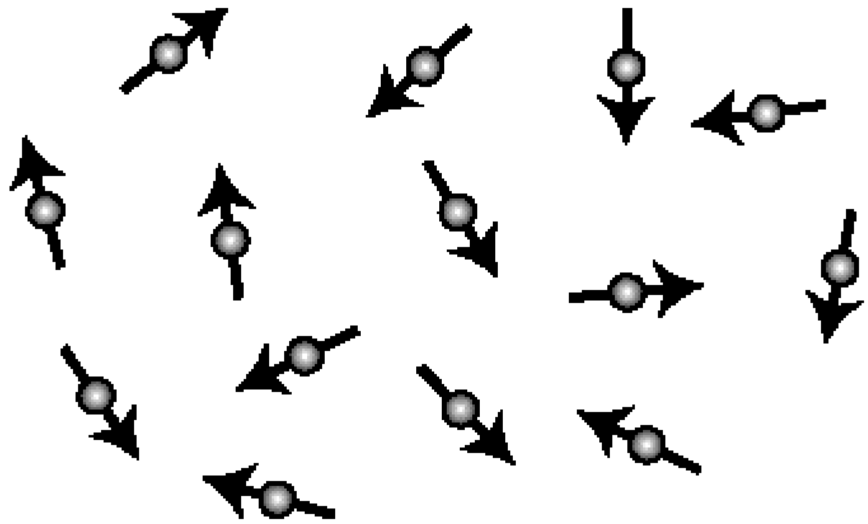
Outline

1. Prerequisites
2. Relaxation and spin Echo
3. Spherical Tensor Operators
4. Superoperators
5. My research work
6. References.

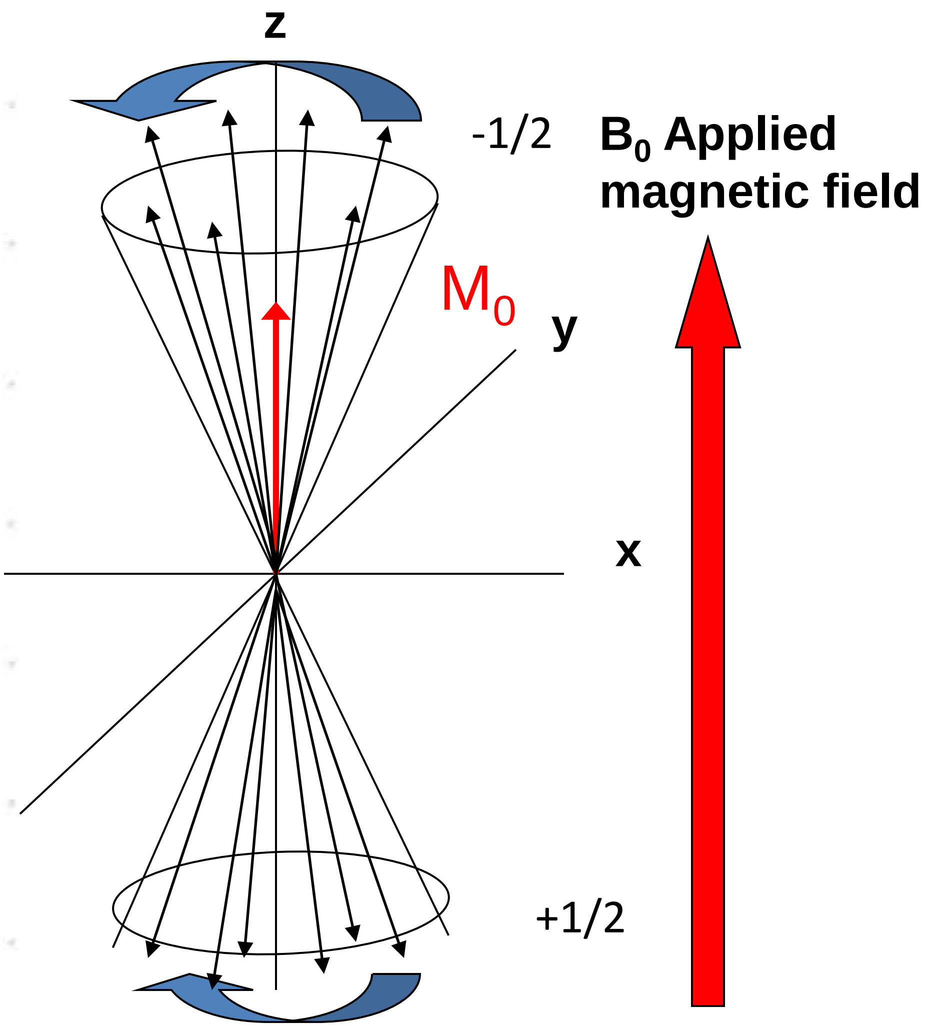
NMR

- NMR is a phenomenon in which the resonance frequencies of nuclear magnetic systems are investigated.
- NMR always employs some form of magnetic field (usually a strong externally applied field B_0 and a RF field)
- Nucleis have a magnetic moment and spin angular momentum

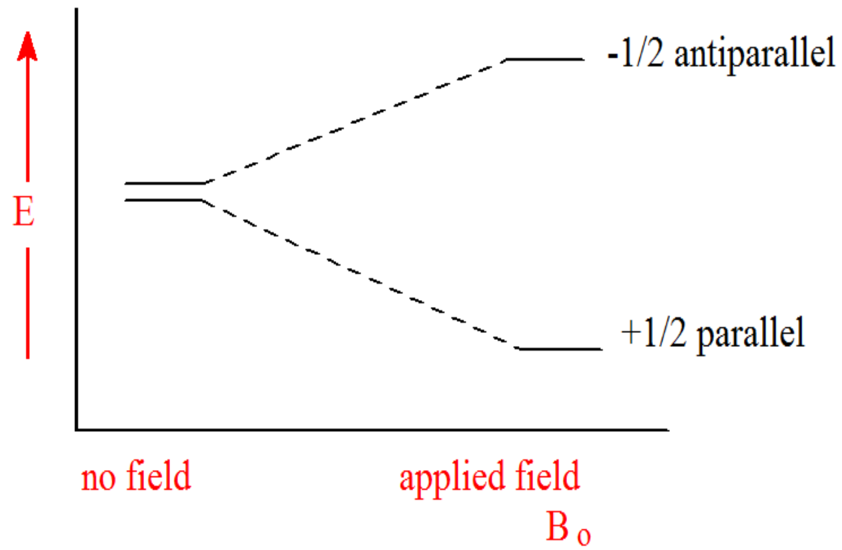
Random direction of spin polarization in the absence of magnetic field.



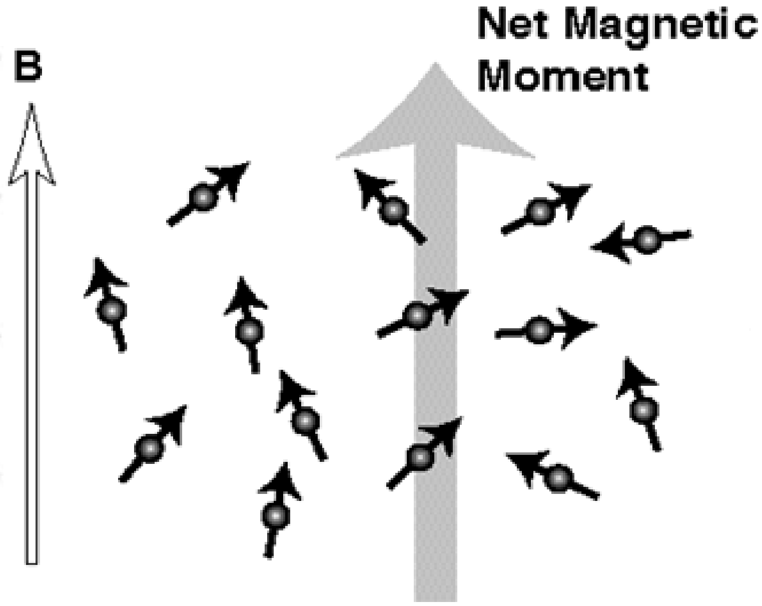
Net magnetic moment from small excess of Nuclei in +1/2 state.

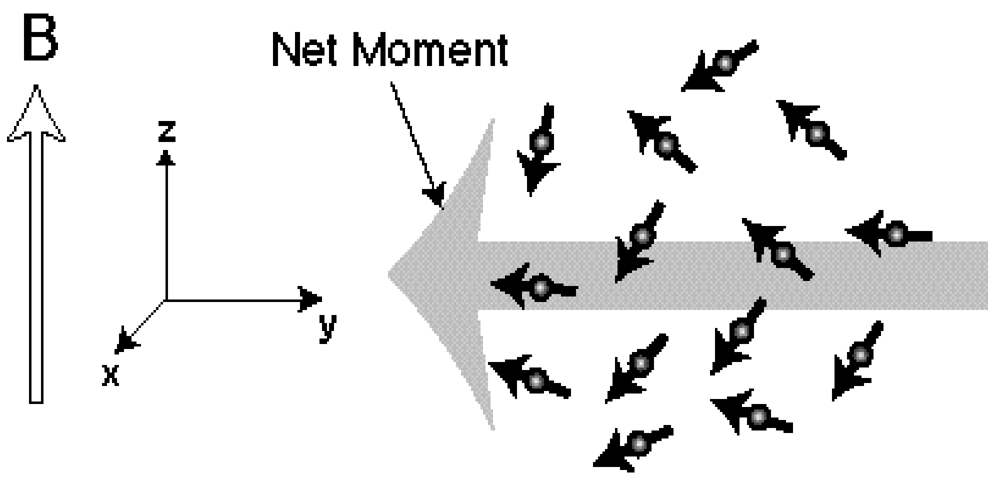


Spin States Split in the presence of B_0



Longitudinal and Transverse Magnetizations





Most commonly studied nuclei

Spin-1/2 nucleus	NMR freq (at 10 T)	abundance
^{1}H	426 MHz	99.9%
^{13}C	107	1.1%
^{15}N	43	0.4%
^{19}F	401	100%
^{28}Si	85	4.7%
^{31}P	175	100%

Applications of NMR

- Physics
  Condensed matter physics
- Chemistry
  Identification of material
- Biophysics
  Analysis of Protein structure
- Medical
  MRI (Magnetic Resonance Image)

Interactions in NMR

NRM Interactions

Internal Interactions

External Interactions

1. Chemical shift
2. J-Coupling
3. **DD-Coupling**

1. Applied Magnetic field
2. RF field

Relaxation

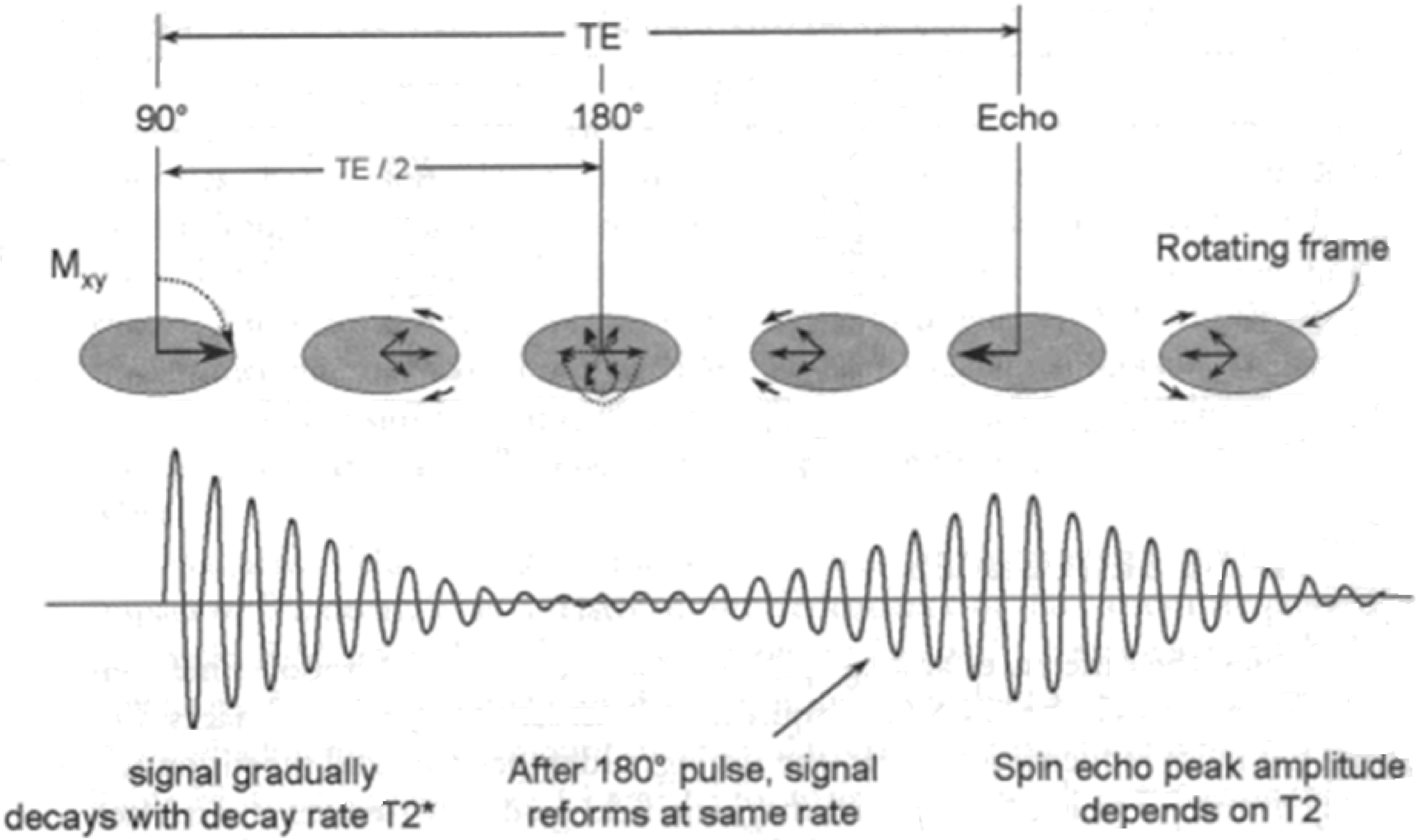
- T1 spin-lattice (relaxing back to precessing about the z axis)

Recovery of Z component of magnetization.

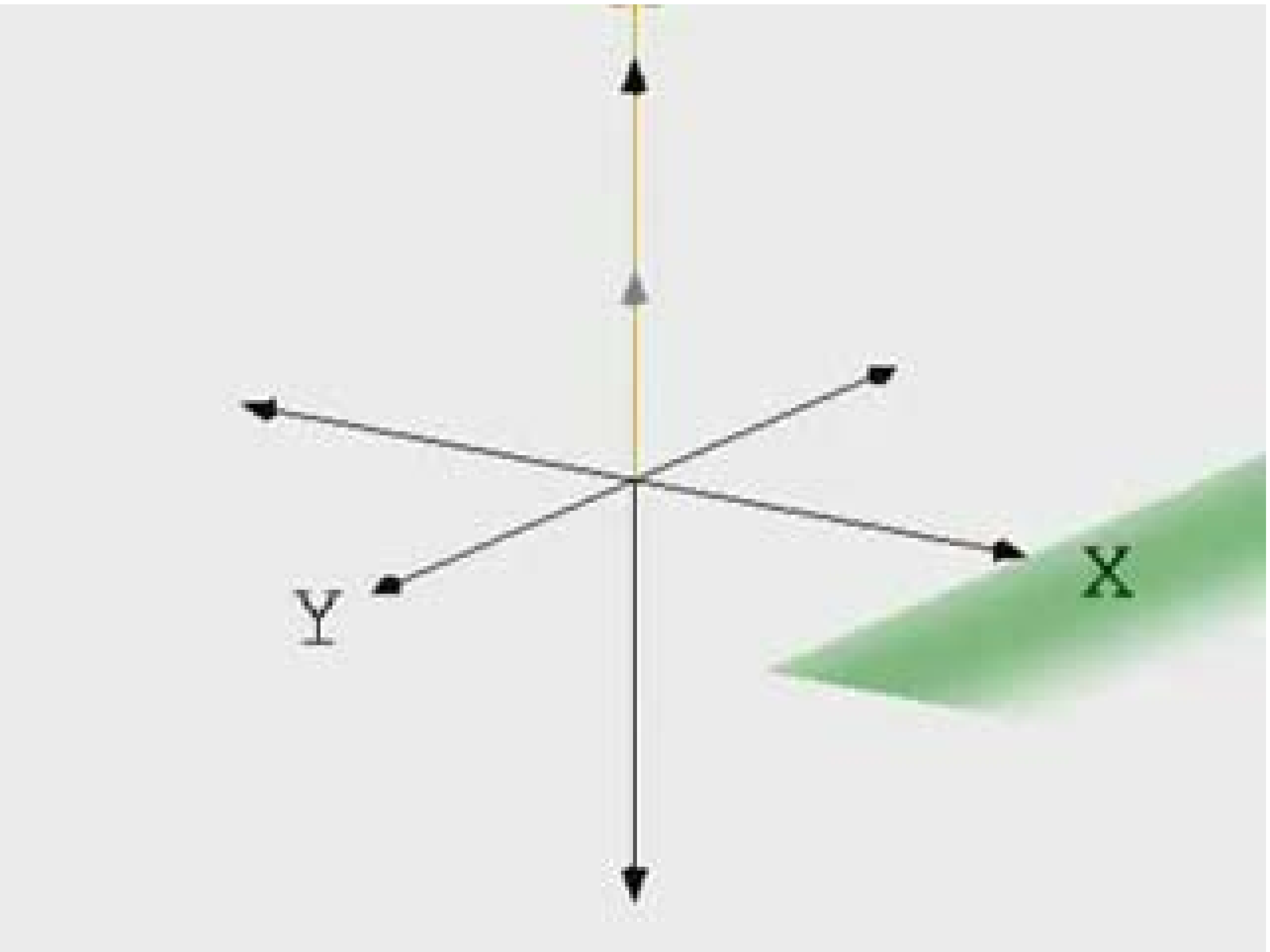
- T2 spin-spin (fanning out)

Decay of x , y component of magnetization.

Spin Echo



TE
90°
180°
Echo
TE / 2
M_{xy}
Rotating frame
signal gradually
decays with decay rate T2*
After 180° pulse, signal
reforms at same rate
Spin echo peak amplitude
depends on T2



X
Y

Density Matrix Formalism

- A tool used to describe the state of a spin ensemble, as well as its evolution in time.

$$\rho \;=\; |\,\psi >< \psi\,|$$

- Average of any observable $\langle A \rangle = \mathrm{Tr}(\rho A)$

- For any state $|\,\psi >= c_\alpha \,|\, \alpha\rangle \,+\, c_\beta \,|\, \beta >$

Diagonal elements = probabilities

$$\rho = \begin{pmatrix} c_\alpha \\ c_\beta \end{pmatrix} \begin{pmatrix} c_\alpha^* & c_\beta^* \end{pmatrix} = \begin{pmatrix} |\, c_\alpha \,|^2 & c_\alpha c_\beta^* \\ c_\beta c_\alpha^* & |\, c^2_{\beta|} \end{pmatrix} \qquad [1]$$

Off-diagonal elements = "coherences" (provide info. about relative phase)

Spherical tensor operators.

- Tensors are very useful simplifying tools that encountered in spherical symmetric problems.
- Any spherical tensor operator can be found by

$$T_{Lm} = \sqrt{\frac{4\pi}{2L+1}} Y_{Lm}$$

- Commutation relations with angular momentum operator.

$$[J^{\pm}, T_{Lm}] = \sqrt{(L \mp m)(L \pm m + 1)} T_{Lm\pm 1}$$

$$[J_z, T_{Lm}] = T_{Lm}$$

[2]

Transformation of Spherical tensor operators

$$T'_{L,m} = \sum_{\acute{m}=-l}^{l} T_{L,\acute{m}} D^{L}_{\acute{m},m}(\alpha,\beta,\gamma)$$

Wigner rotation matrices

$$D^{L}_{\acute{m},m}(\alpha,\beta,\gamma)|L,\acute{m}\rangle = \exp^{-i\acute{m}\alpha}\exp^{-im\gamma} d^{L}_{\acute{m},m}(\beta)$$

Reduced rotation matrix elements

$$d^{L}_{\acute{m},m}(\beta) = \Sigma_k (-1)^{k+\acute{m}-m} \frac{\sqrt{(L+m)!(L-m)!(L+\acute{m})!(L-\acute{m})!}}{(L-\acute{m}-k)!(L+m-k)!(k+\acute{m}-m)!k!} \times (\cos\frac{\beta}{2})^{2L+m-\acute{m}-2k}(\sin\frac{\beta}{2})^{\acute{m}-m+2k}$$

[2]

Total Hamiltonian in terms of Spherical tensor operators.

$$H_{Total} = -\gamma B_\circ T_{10} - 2\pi J\sqrt{3\pi}T_{00}Y_{00} + \frac{3eV_{zzQ}}{4I(2I-1)}\sqrt{\frac{24\pi}{5}}\sum_m (-1)^m T_{2m}Y_{2-m}$$
$$+ \frac{\mu_\circ \gamma^2 \hbar}{4\pi r^3}\sqrt{\frac{24\pi}{5}}(-1)^m T_{2m}Y_{2-m}$$

[3]

$$H_{Total} = H_z + H_{CS} + H_J + H_D$$

Superoperators

- Liouville-von Neumann equation

$$i\hbar \frac{d\rho}{dt} = [H, \rho]$$

- We define a superoperator

$$\hat{\hat{L}} |\rho(t)\rangle = |[H, \rho(t)]\rangle$$

$$i\hbar \frac{d|\rho(t)\rangle}{dt} = \hat{\hat{L}} |\rho(t)\rangle \quad [4]$$

Matrix representation of Superoperators

- Superoperators belong to the superoperator space.
- The difference between the Superoperator space and Hilbert space is dimensionality.
- Different physical conditions.
- Matrix representation

$$\rho = \begin{pmatrix} \rho_{\alpha\alpha} & \rho_{\alpha\beta} \\ \rho_{\beta\alpha} & \rho_{\beta\beta} \end{pmatrix} \qquad |\rho) = \begin{pmatrix} \rho_{\alpha\alpha} \\ \rho_{\beta\alpha} \\ \rho_{\alpha\beta} \\ \rho_{\beta\beta} \end{pmatrix}$$

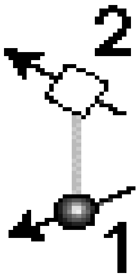
Table

Name	Continuous representation	Continuous scalar product	Discrete representation	Discrete scalar product
Superoperator Space	superoperators	$\sum_{\hat{M}} \langle \hat{M} \| \hat{\hat{P}}^{\dagger} \hat{\hat{Q}} \| \hat{M} \rangle$	*$n^2 \times n^2$ matrices*	$\mathrm{Tr}\left(P^{\dagger} Q\right)$
Liouville space	operators, Density matrices	$\sum_{\varphi} \langle \varphi \| \hat{M}^{\dagger} \hat{K} \| \varphi \rangle$	*$n \times n$ matrices*	$\mathrm{Tr}\left(M^{\dagger} N\right)$
Hilbert space	wavefunctions	$\int \varphi^{*}(x) \psi(x)\, dx$	*n -vectors*	$\sum_{n} \varphi_n^{*} \psi_n$

Long lived Singlet states in solution NMR

Singlet and Triplet states

Two coupled spins

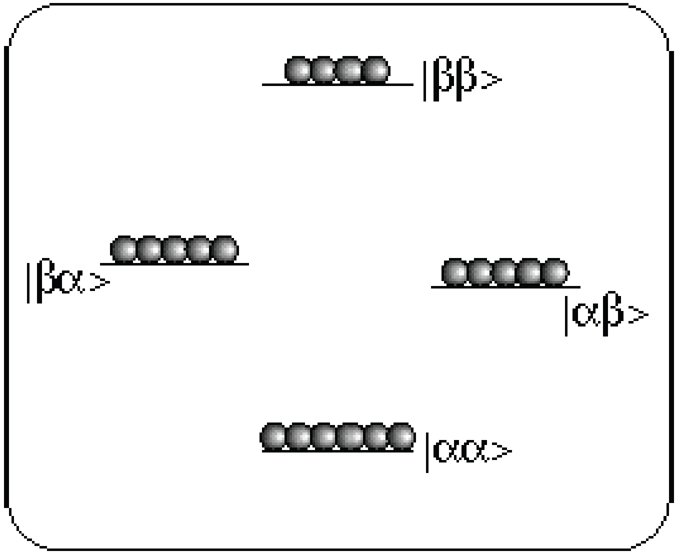


$$|S_\circ\rangle = \frac{1}{\sqrt{2}}(|\alpha\beta\rangle - |\beta\alpha\rangle),$$

$$|T_{+1}\rangle = |\alpha\alpha\rangle,$$

$$|T_0\rangle = \frac{1}{\sqrt{2}}(|\alpha\beta\rangle + |\beta\alpha\rangle),$$

$$|T_{-1}\rangle = |\beta\beta\rangle.$$



Density operator for Spin pair

$$|\psi\rangle = c_{\alpha\alpha}|\alpha\alpha\rangle + c_{\alpha\beta}|\alpha\beta\rangle + c_{\beta\alpha}|\beta\alpha\rangle + c_{\beta\beta}|\beta\beta\rangle$$

$$\hat{\rho} = \begin{pmatrix} c_{\alpha\alpha} \\ c_{\alpha\beta} \\ c_{\beta\alpha} \\ c_{\beta\beta} \end{pmatrix} \left(c_{\alpha\alpha}{}^{*}, \quad c_{\alpha\beta}{}^{*}, \quad c_{\beta\alpha}{}^{*}, \quad c_{\beta\beta}{}^{*} \right)$$

$$\hat{\rho} = \begin{pmatrix} \rho_{\boxed{\alpha\alpha}} & \rho_{\boxed{\alpha+}} & \rho_{\boxed{+\alpha}} & \rho_{\boxed{++}} \\ \rho_{\boxed{\alpha-}} & \rho_{\boxed{\alpha\beta}} & \rho_{\boxed{+-}} & \rho_{\boxed{+\beta}} \\ \rho_{\boxed{-\alpha}} & \rho_{\boxed{-+}} & \rho_{\boxed{\beta\alpha}} & \rho_{\boxed{\beta+}} \\ \rho_{\boxed{--}} & \rho_{\boxed{-\beta}} & \rho_{\boxed{\beta-}} & \rho_{\boxed{\beta\beta}} \end{pmatrix}$$

Equation of Motion

$$\frac{d}{dt}\rho(t) = \hat{\hat{L}}(t)\rho(t)$$

Liouvillian Space operator

$$\hat{\hat{L}}(t) = \hat{\hat{L}}_{coh}(t) + \hat{\hat{\Gamma}}.$$

Coherent Effects

$$\hat{\hat{L}}_{coh}(t) = -i\hat{\hat{H}}(t).$$

Incoherent Effects

$$\hat{\hat{\Gamma}}$$

- **Dipole-dipole relaxation**
- **External random field relaxation**

Relaxation Superoperator

For DD-relaxation

$$\hat{\hat{\Gamma}}^{jk} = -\frac{2}{5}b_{jk}^2 \int_{-\infty}^{0} d\tau \sum_{m=-2}^{+2} (-1)^m G_{2m}^{jk}(\tau) \times \hat{R}_z(\varphi)\hat{T}_{2m}^{jk}\hat{R}_z(-\varphi)\hat{T}_{2-m}^{jk},$$

For ERF-relaxation

$$\hat{\Gamma}_{j\times k}^{ERF} = C_{jk}\gamma^2 (B_k^{rms})^2 \int_{-\infty}^{0} d\tau \sum_{m=-1}^{+1} (-1)^m G_{1m}(\tau) \times \hat{R}_z(\varphi)\hat{T}_{1m}^{j}\hat{R}_z(-\varphi)\hat{T}_{1-m}^{k}$$

[5]

Autocorrelation function

$$G_{2m}^{jk}(\tau) = \exp\{-|\tau|/\tau_c^{DD}\}$$

Correlation time

$$\tau_c^{DD}$$

Relaxation of singlet-state population

$$[\hat{\Gamma}^{ERF}]^{ST} = \begin{pmatrix} -V_\circ^S - 2V_1^S & V_1^S & V_\circ^S & V_1^S & 0 & 0 \\ V_1^S & -V_1^\Sigma & V_1^T & 0 & -\frac{1}{\sqrt{2}}V_1^\Delta & 0 \\ V_\circ^S & V_1^T & -V_\circ^S - 2V_1^S & V_1^T & 0 & 0 \\ V_1^S & 0 & V_1^T & -V_1^\Sigma & -\frac{1}{\sqrt{2}}V_1^\Delta & 0 \\ 0 & -\frac{1}{\sqrt{2}}V_1^\Delta & 0 & -\frac{1}{\sqrt{2}}V_1^\Delta & -V_1^\Sigma & 0 \\ 0 & 0 & 0 & 0 & 0 & -V^{ST} \end{pmatrix}$$

Final matrix of the coherent Liouvillian Superoperator.

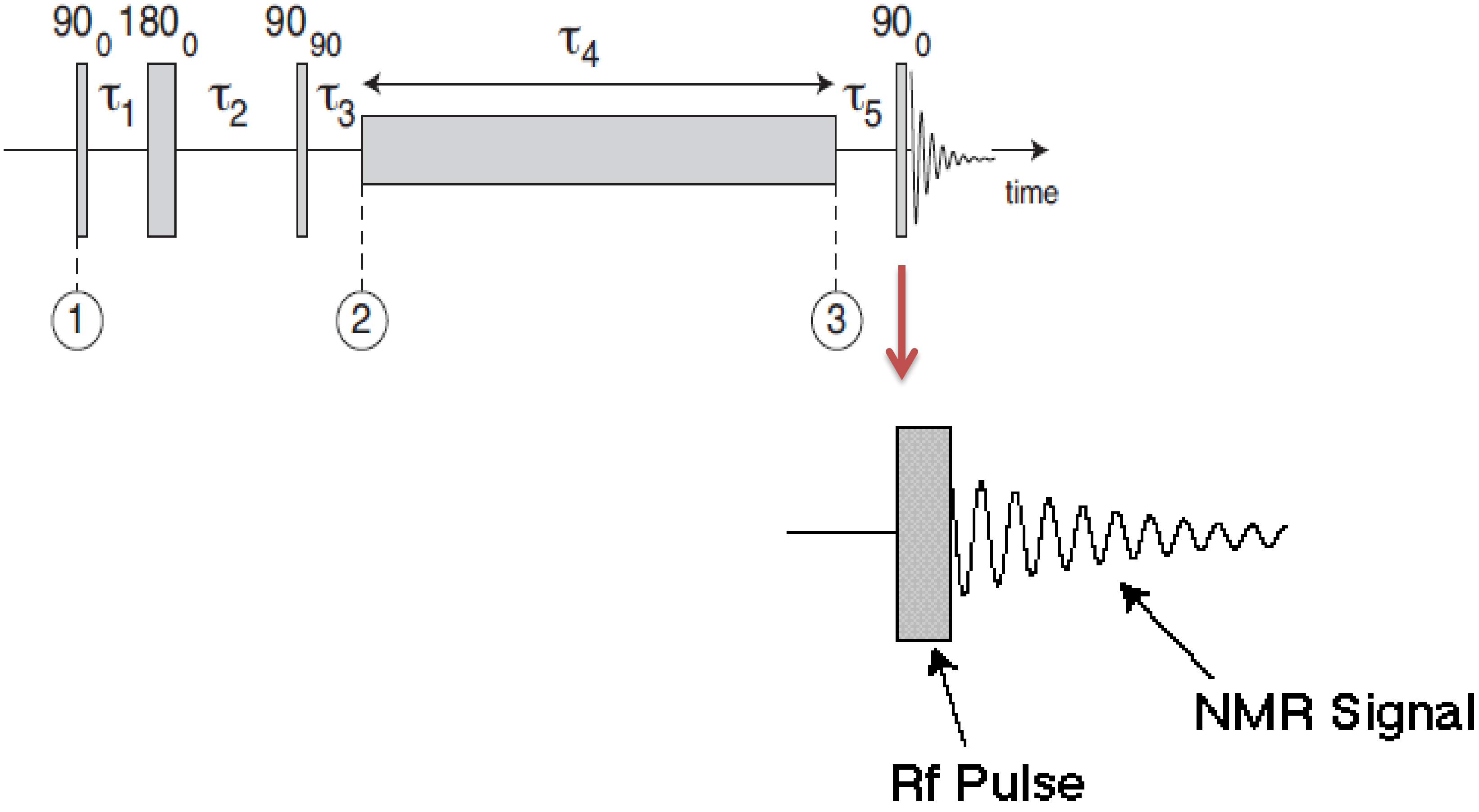
- Shows the conversion of singlet population to singlet-triplet zero-quantum coherence then to triplet population.

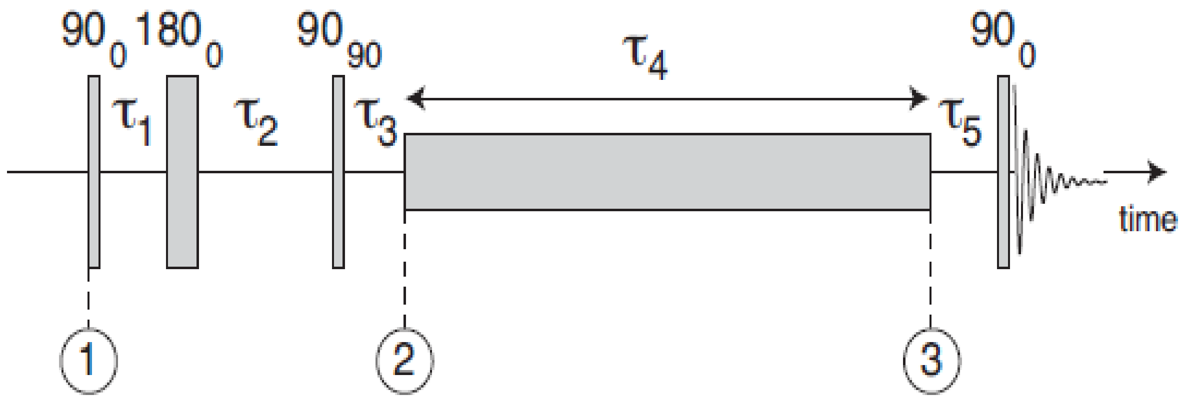
$$[\hat{\hat{L}}_{coh}]^{ST} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & -\frac{\Delta\omega^\circ}{\sqrt{2}} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\Delta\omega^\circ}{\sqrt{2}} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\pi J \\ -\frac{\Delta\omega^\circ}{\sqrt{2}} & 0 & -\frac{\Delta\omega^\circ}{\sqrt{2}} & 0 & -2\pi J & 0 \end{pmatrix}$$

Final matrix of the evolution of spin density operator.

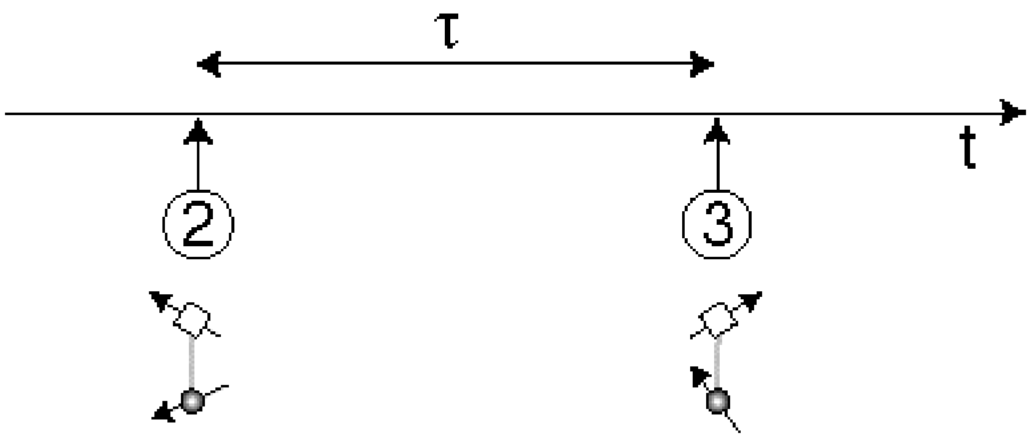
$$\begin{pmatrix} -V_\circ^S - 2V_1^S & V_1^S & V_\circ^S & V_1^S & 0 & -\frac{\Delta\omega^\circ}{\sqrt{2}} \\ V_1^S & WV & W1V1 & W_2^T & -\frac{1}{\sqrt{2}}V_1^\Delta & 0 \\ V_\circ^S & W11 & 2WV & W1V1 & 0 & -\frac{1}{\sqrt{2}}V_1^\Delta \\ V_1^S & W_2^T & W1V1 & WV & \frac{1}{\sqrt{2}}V_1^\Delta & 0 \\ 0 & -\frac{1}{\sqrt{2}}V_1^\Delta & 0 & \frac{1}{\sqrt{2}}V_1^\Delta & -R^{ST} - V_1^\Sigma & 2\pi J \\ \frac{1}{\sqrt{2}}V_1^\Delta & 0 & -\frac{1}{\sqrt{2}}V_1^\Delta & 0 & -2\pi J & -R^{ST} - V^{ST} \end{pmatrix}$$

Signal Obtained

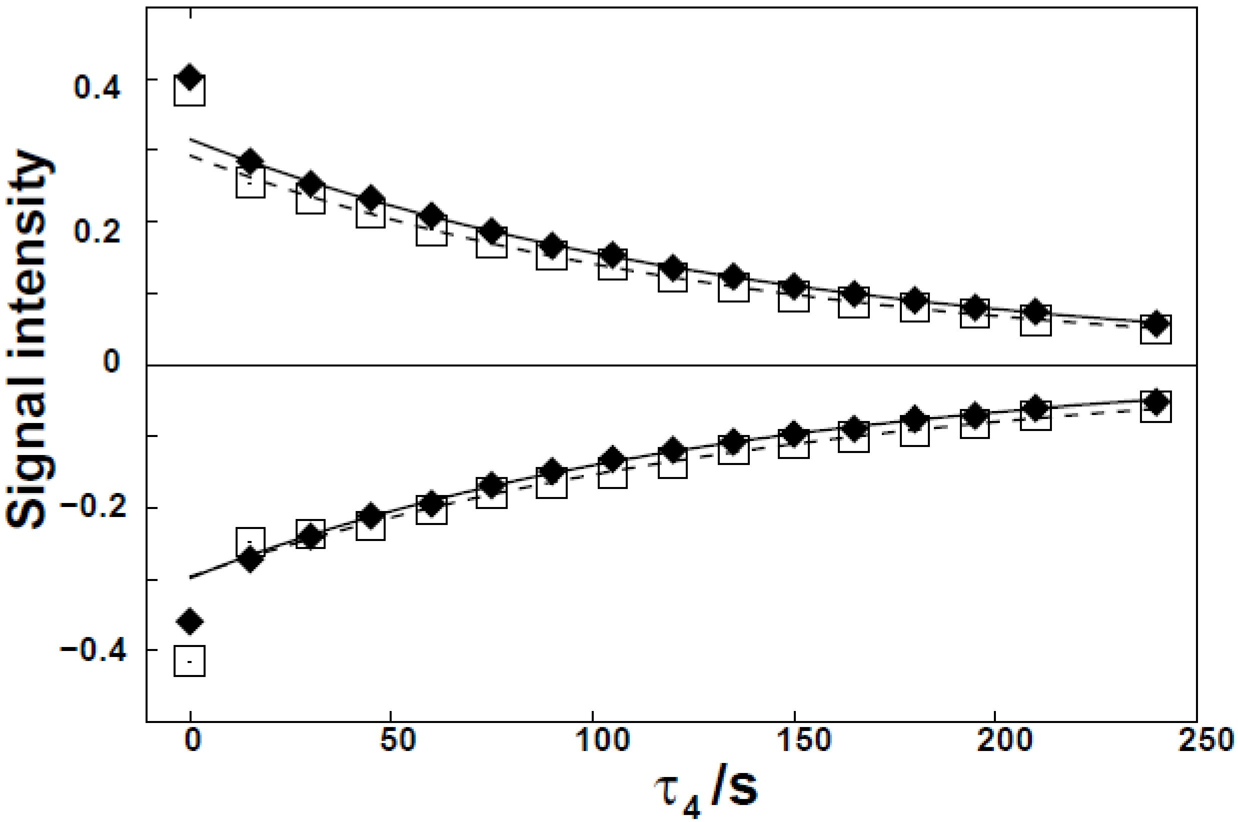




90_0
180_0
90_{90}
90_0
τ_1
τ_2
τ_3
τ_4
τ_5
time
1
2
3



τ
t
2
3



0.4
0.2
0
−0.2
−0.4
Signal intensity
0
50
100
150
200
250
τ4 /s

Advantages and applications of long-lived states

- Store information up to 40 times longer than T1.
- Can be created in both high or low magnetic fields, the latter case very interesting for applications on humans.
- For the study of molecular transportation and storage of polarized nuclear spin coherence.
- Can be used for the investigation of slow-cross relaxation between different molecules in solutions.

NMR for Quantum Information

Advantages	**Disadvantages**
1. Physics of NMR is well described.	1. Noisy signal
2. Long decoherence times	2. No entanglement.
3. Small quantum computer is easy to construct.	3. Limited measurement.

Why NMR?

A major requirement of a quantum information/computer is that the coherence should last long.

- Nuclear spins in liquids retain coherence ~ 100's millisec and their longitudinal state for several seconds.
- A system of N coupled spins (each spin 1/2) form an N qubit Quantum Computer.
- Unitary Transform can be applied using R.F. Pulses and various logical operations and quantum algorithms can be implemented. [7]

References

1. *Levitt M.H*, **Spin Dynamics Basics of Nuclear Magnetic Resonance**, John Wiley & Sons Ltd, 2001.
2. C.P. Slichter. Principles of Magnetic Resonance. Harper , Row, 1963.
3. Melinda J. D, Introduction to Solid-State NMR Spectroscopy, John Wiley & Sons Ltd, 2004.
4. Mayne C.L, Liouville Equation of Motion, Encycl. Nucl. Mag. Res, 2717-2730.
5. M. Carravetta and M. H. Levitt. Theory of long-lived nuclear spin states in solution nuclear magnetic resonance. i. singlet states in low magnetic field. J. Chem. Phys., 122:214505, 2005.
6. *Jeener J,* **Superoperators in Magnetic Resonance**, Adv. Mag. Res, 10 (1982), 1-51.
7. *Jones J.A*, **Quantum Computing with NMR**, Prog. NMR Spectrosc. 38,325-360(2001).

THANKS FOR YOUR PATIENCE