Basic Theory: Nuclear Overhauser Effect
Albert Overhauser (1953)

Single Quantum Transition
\(~\text{Larmor precession} \ 10^6 \text{ to } 10^9 \text{ Hz}\).

Double quantum transition Probability \(~\text{very fast}\).

\(~\text{Twice Larmor Frequencies}\).

Zero Quantum
\(~\text{difference in Larmor Frequencies}\).
\(~\text{very slow field fluctuation}\).

References:
David Nusbaum and Michael Williamson "The Nuclear Overhauser Effect"
Timothy Claridge "High-Resolution NMR Techniques" Chapter 8.

Steady State Solomon Equation
Two spins system

\[
f_i(S) = \frac{Y_s}{Y_i} \times \left\{ \frac{W_{2IS} - W_{0IS}}{2W_{1IS} + W_{2IS} + W_{0IS}} \right\}
\]

Function of
gyromagnetic ratio, \(I/\hbar\), Molecular motion, Larmor Frequencies

\[
W_{2IS} = \gamma_i^2 \gamma_s^2 r_{2s}^2 \tau_s / [1 + (\omega_i - \omega_s)^2 \tau_s^2]
\]

\[
W_{0IS} = \gamma_i^2 \gamma_s^2 r_{2s}^2 \tau_s / [1 + (\omega_i + \omega_s)^2 \tau_s^2]
\]

\[
W_{1IS} = \gamma_i^2 \gamma_s^2 r_{2s}^2 \tau_s / [1 + \omega_i^2 \tau_s^2]
\]

\[
W_{1II} = \gamma_i^2 \gamma_s^2 r_{2s}^2 \tau_s / [1 + \omega_s^2 \tau_s^2]
\]

Figures sourced from Guilermo Minya, U of the Sciences.
**NOE application**

Cross relaxation

Perturbation from one spin
Inducing changes in the intensity of other spins

- Transient NOE
- Using Shaped pulse
  - e.g. 1D Selective NOE,
  - 2D NOESY

- Steady state NOE
  - e.g. C-13 with all H-1 decoupled

*1D-NOE Review Y.F. Lam, U. of Maryland*
C-13 Application — Steady state NOE

\[ t_1(S) - \frac{Y_{CH}}{Y_{C13}} = \sim 2 \text{ to } 4 \]

CPD : Composite Pulse Decoupling
A repeated series of strong pulses
To obtain the effect of random broad band decoupling

1D proton Transient NOE

- Selective excitation H-1 (essential variable: mixing time)

☐ To estimate the distance between nuclei. ( < 5 – 6 Å )
The sign of NOE can be positive, zero, or negative.

☐ To detect existence of Conformers (Slow conformation change)
The sign of the NOE is negative
(negative NOE, also known as Chemical exchange NOE)
Any other NOE? ROE

- Depends on mixing time and spin-lattice relaxation;
- Large molecules such as protein D8 ~ 100 to 50 ms
- Small molecules D8: range 0.2s to 0.9s.
- Can show either positive NOE, negative NOE, and/or zero!
- ROESY: to distinguish positive and negative NOE.

END of Basic NOE review