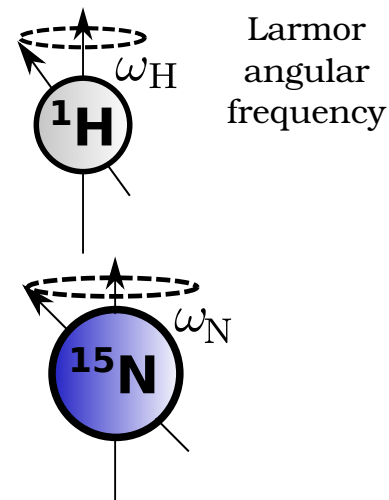


Redfield equations

Dipolar
coupling
constant



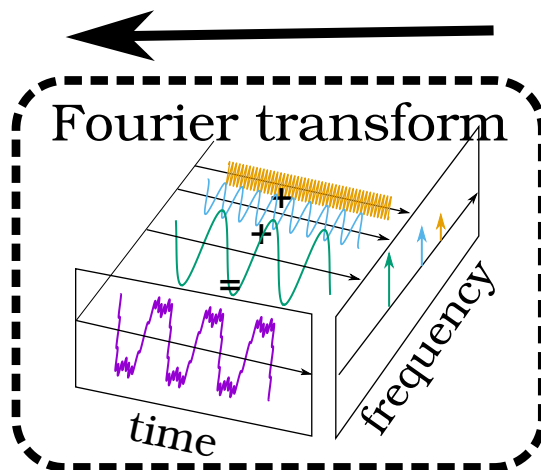
$$\frac{1}{T_1} = \frac{d_{\text{NH}}^2}{20} [J(\omega_{\text{H}} - \omega_{\text{N}}) + 3J(\omega_{\text{N}}) + 6J(\omega_{\text{H}} + \omega_{\text{N}})]$$

$$\frac{1}{T_2} = \frac{1}{2} \frac{d_{\text{NH}}^2}{20} [4J(0) + J(\omega_{\text{H}} - \omega_{\text{N}}) + 3J(\omega_{\text{N}}) + 3J(\omega_{\text{H}}) + 6J(\omega_{\text{H}} + \omega_{\text{N}})]$$

$$\text{NOE} = 1 + \frac{d_{\text{NH}}^2}{20} [J(\omega_{\text{H}}) + 6J(\omega_{\text{H}} + \omega_{\text{N}})] \frac{\gamma_{\text{H}} T_1}{\gamma_{\text{N}}}$$

spectral density

$$J(\omega) = 2 \int_0^\infty C(t) \cos(\omega t) dt$$



second-order rotational
correlation function of N-H
bond vector

$$C(t) = \left\langle \frac{3}{2} \cos^2 \theta_{t'+t} - \frac{1}{2} \right\rangle_{t'}$$