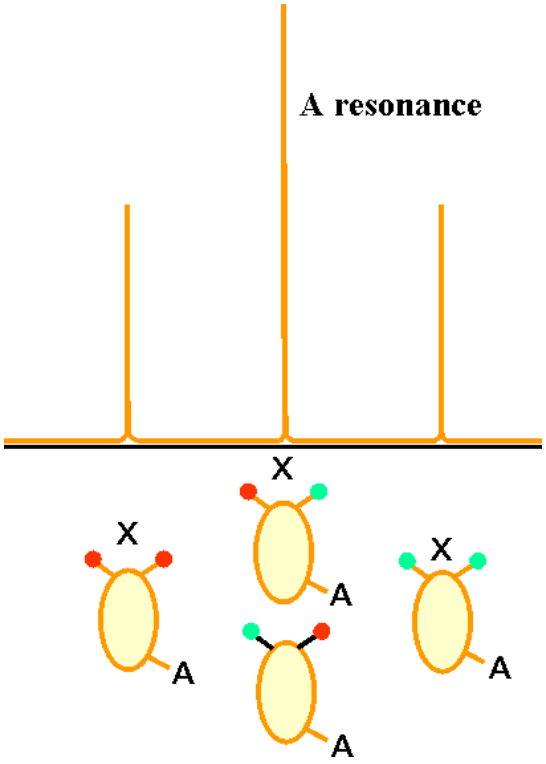
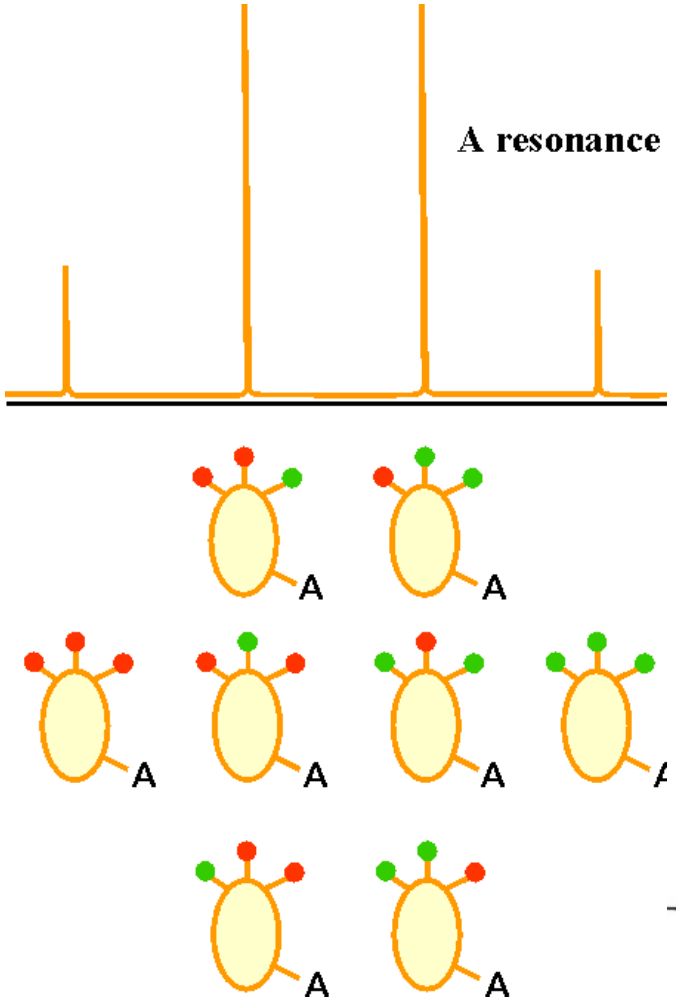
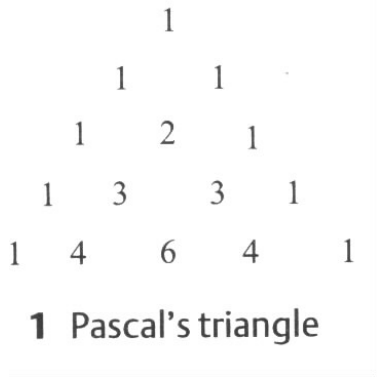
Fine structure: Multiple equivalent nuclei

2 X nuclei:

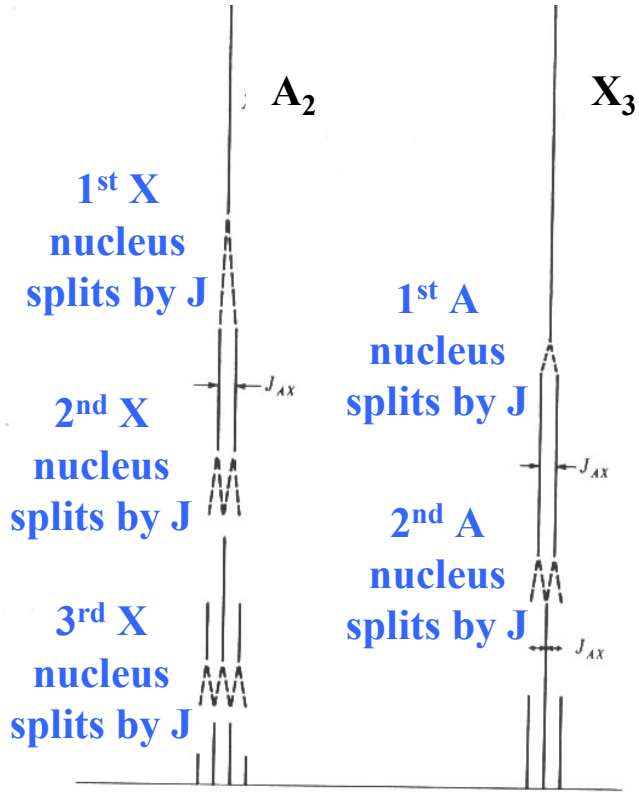


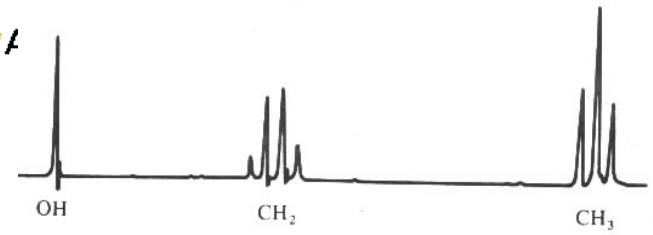
3 X nuclei:





1 Pascal's triangle

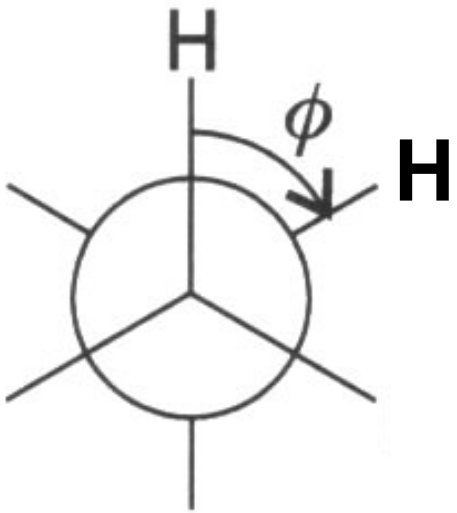




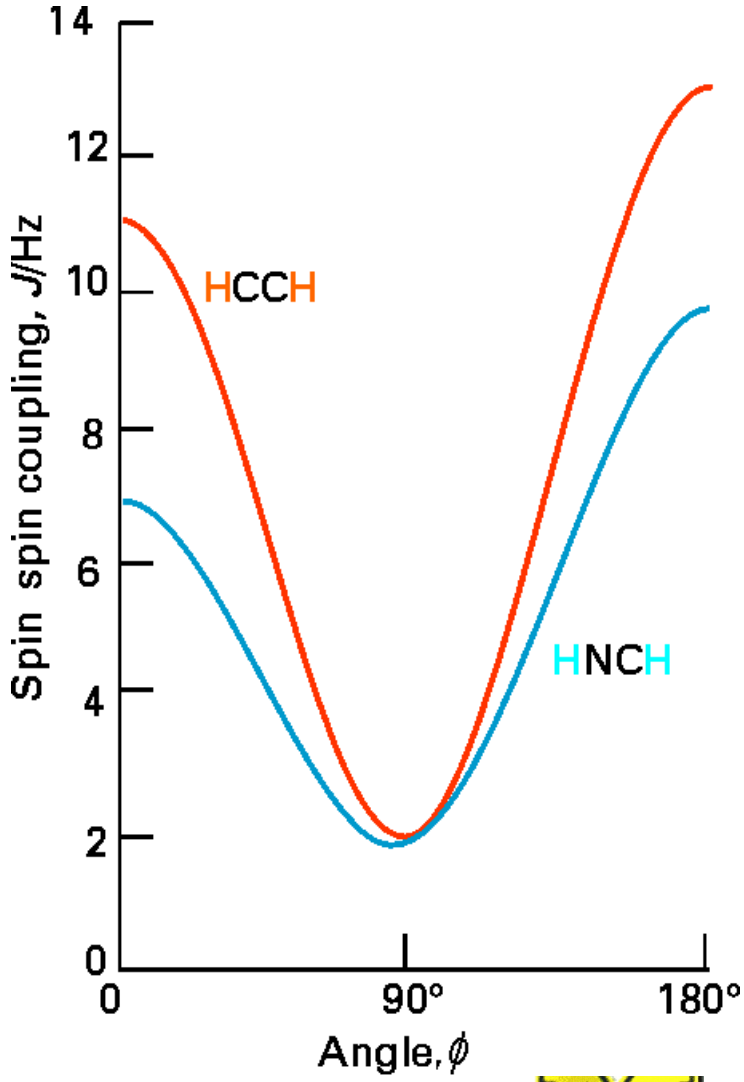
Fine structure: Values of J reveal geometry

Karplus equation

$$^{3}J_{HH} = A + B\cos\phi + C\cos 2\phi$$

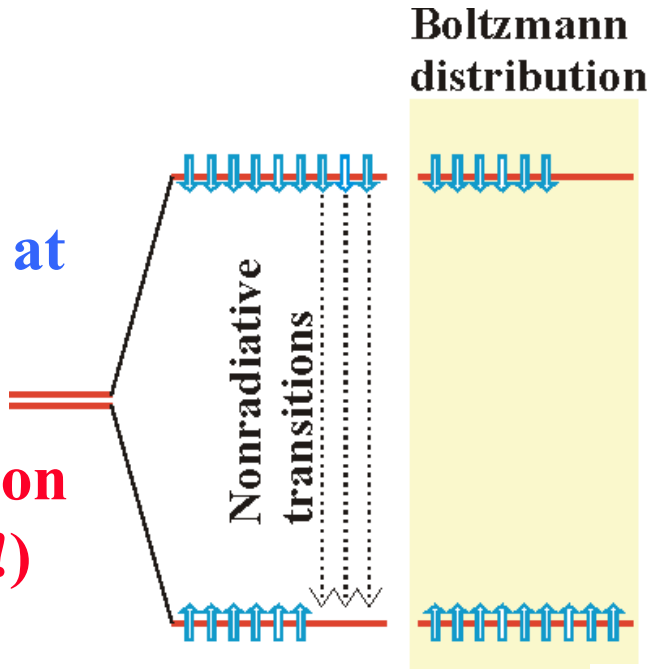


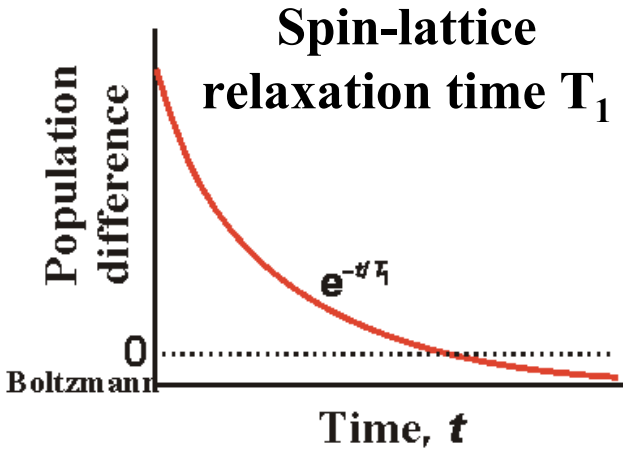
Newman projection



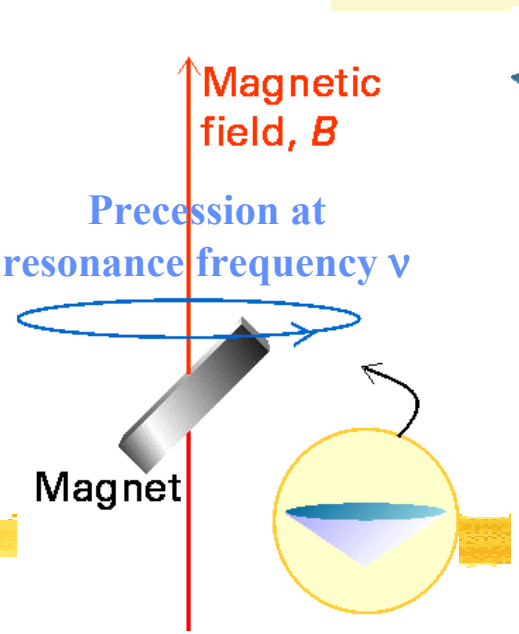
Spin relaxation: Info on molecule dynamics

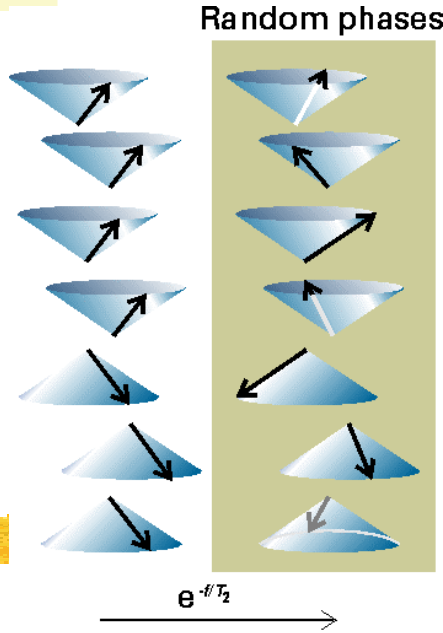
1. Spin-lattice relaxation by molecule tumbling at about resonance frequency (otherwise saturation and loss of signal!)





2. Spin-spin relaxation by transient, yet long-lasting differences in local magnetic fields



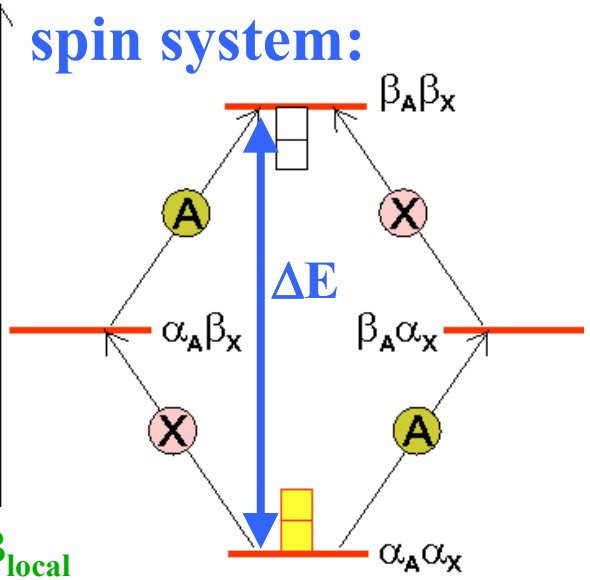


Spin-spin relaxation time T_2

Nuclear Overhauser effect (NOE): Distance constraints to deduce molecule structure

Large molecules have many chemically identical nuclei: How can one identify those that are close together in 3D?

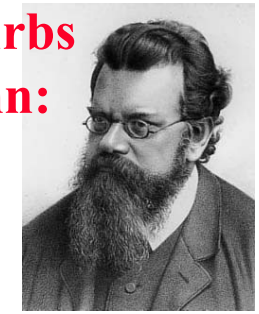
Let's look at a simple AX coupled spin system:



Boltzmann distribution

$$\frac{N_{upper}}{N_{lower}} = e^{-\frac{\Delta E}{kT}}$$

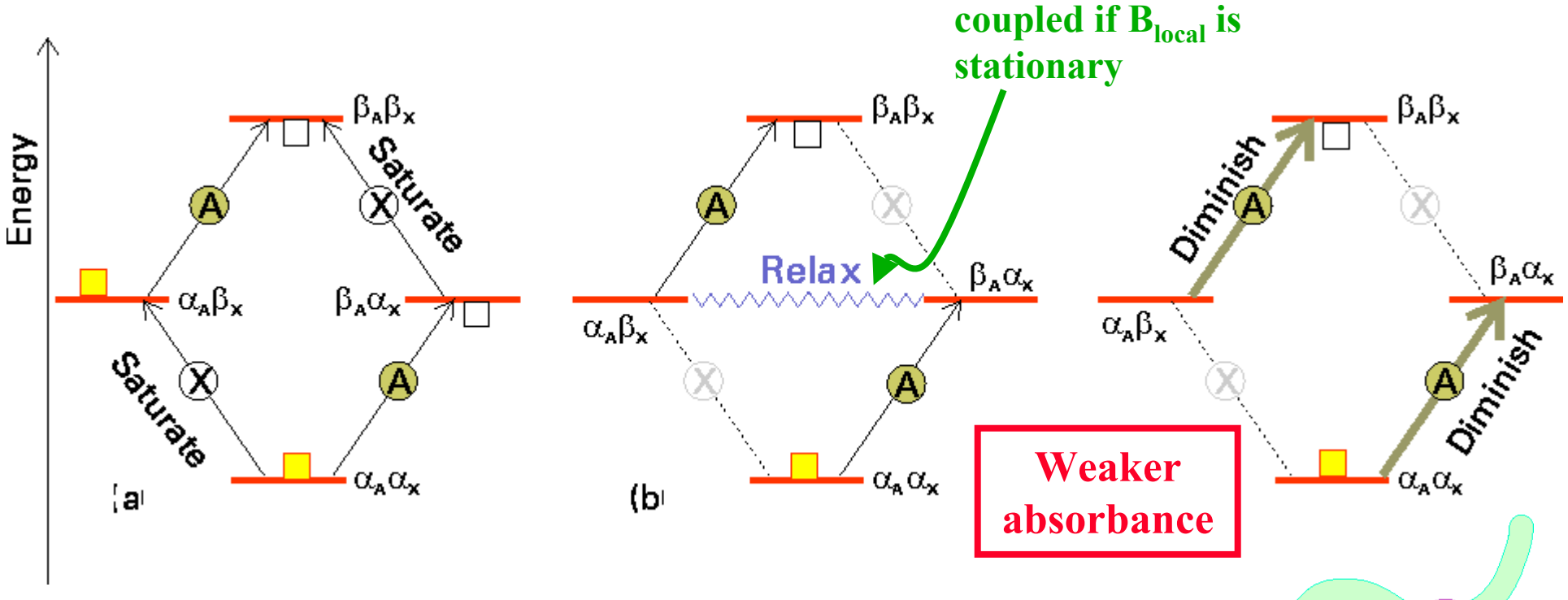
Resonance disturbs Prof. Boltzmann:



coupled if B_{local} modulated at 2ν

Stronger absorbance

NOE: Changes in signal intensity, up or down



The direction and strength of signal intensity changes in an NOE experiment depend on the distance of A and X: Supramolecular structures, e.g., of biomolecules can be studied!