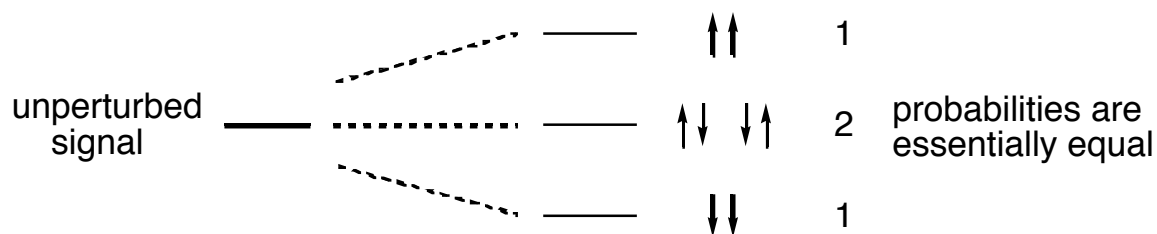


Simple Spin-Spin Coupling

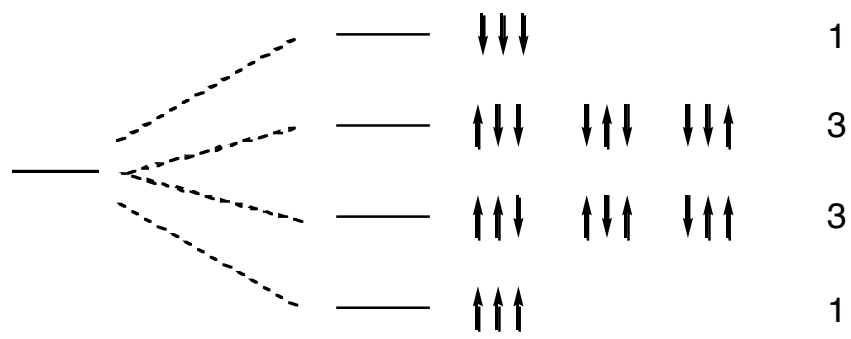
The field experienced by one set of equivalent protons is influenced by the spin of the adjacent protons

Consider a CH₃ resonance perturbed by adjacent CH₂ spins



Magnetic effects of these different arrangements are transmitted through intervening bonds to the methyl group so that it will "feel" one of the three effective fields

for CH₂ perturbed by CH₃

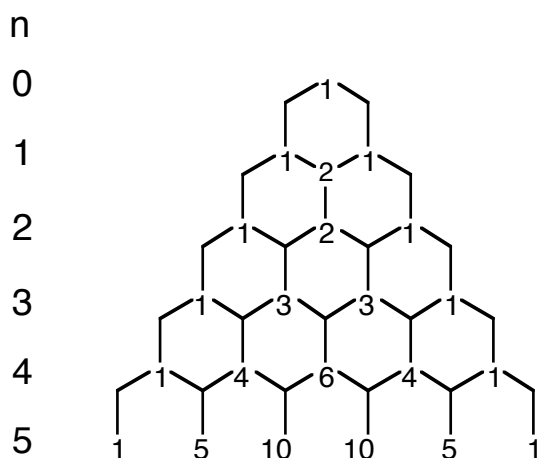


Spacing of lines is a direct measurement of spin-spin coupling constant J (range 0-20 Hz) (constant is not affected by field strength)
multiplicity = singlet, doublet, triplet, quartet, etc.

for a proton coupled to n other protons with *equal coupling constant*
multiplicity = n + 1

general formula for all nuclei $2n(I) + 1$

Intensities follow Pascal's Triangle



This is called first-order splitting

$$\frac{\Delta\nu}{J} \approx 10$$

at higher field, $\Delta\nu$ increases,

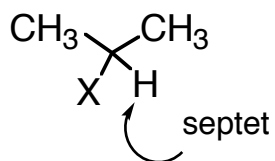
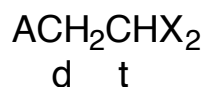
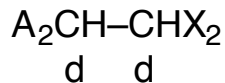
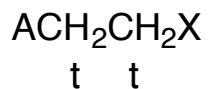
J constant = more like 1st order

$^1\text{H} - ^1\text{H}$ Coupling constants range from 0 to 20 Hz

$J \approx 7$ Hz for normal ethyl groups

Coupling over more than 3 bonds is generally small,
(long range coupling) < 1 Hz

Other simple coupling patterns



^1H , ^{13}C Chemical Shift Summary

TYPE OF ATOMS		^1H CHEMICAL SHIFT (δ , ppm)	^{13}C CHEMICAL SHIFT (δ , ppm)
1°-Alkyl	RCH_3	0.8–1.0	5–20
2°-Alkyl	RCH_2R	1.2–1.4	20–30
3°-Alkyl	R_3CH	1.4–1.7	30–45
allylic	$\begin{array}{c} \text{CH}_3 \\ \diagup \\ \text{R}_2\text{C}=\text{C} \\ \diagdown \\ \text{R} \end{array}$	1.6–1.9	20–40
α -ketone	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RC}^{\text{b}}\text{C}^{\text{a}}\text{H}_3 \end{array}$	2.5–3.0	a, 25–40 b, 190–210
alkyne	$\text{R}-\text{C}\equiv\text{C}-\text{H}$	2.1–2.6	65–95
alkyl bromide	RCH_2Br	3.4–3.6	~20
alkyl chloride	RCH_2Cl	3.6–4.0	~35
alcohol or ether	RCH_2OH RCH_2OR	3.5–4.0	60–70
vinylic	$\text{R}_2\text{C}=\text{CH}_2$	4.6 – 5.0	100–160
	$\begin{array}{c} \text{R}_2\text{C}=\text{C}-\text{H} \\ \\ \text{R} \end{array}$	5.2 – 5.7	