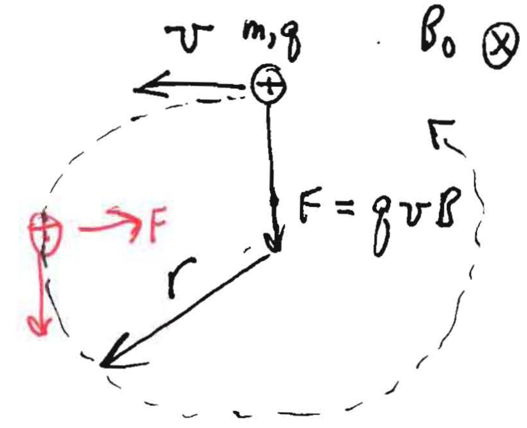
CS138 | 2001-40

ICR



$(v \perp B)$

$$F_{OUT} = \frac{mv^2}{r} = qvB = F_{IN}$$

BUT $\omega = \frac{v}{r}$

$$m\omega = qB$$

$$\boxed{\omega_c = \frac{qB}{m}} \qquad \boxed{\nu_c = \frac{\omega_c}{2\pi} = \frac{qB}{2\pi m}}$$

(S.I. UNITS)

e.g. @ 7.0 TESLA (300 MHz ^1H NMR)

$$\nu_c = \frac{(1.6\times10^{-19})(7)}{(2\pi)(1\ Da)(1.66\times10^{-27}\ kg/Da)} = 1.1\times10^{8} \cong 100\ MHz$$

↑ H^+

$\nu_{LARMOR} \neq \nu_c$ (PROVES PROTON IS A COMPOSITE PARTICLE (MADE UP OF QUARKS)

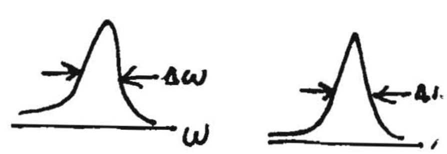
FOR "CHEMICAL" IONS @ 7 TESLA

18 Da ⟷ 1000 Da

4.3 MHz ⟷ 120 KHz

RESOLVING POWER

$$\omega_c = \frac{qB}{m}$$



$$\frac{d\omega_c}{dm} = -\frac{qB}{m^2} = -\frac{\omega_c}{m}$$

$$\boxed{\frac{\omega_c}{\Delta\omega_c} = -\frac{m}{\Delta m}}$$

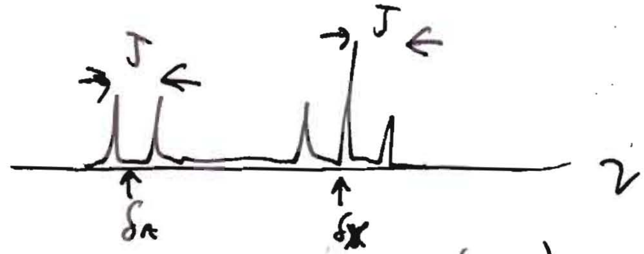
MASS RESOLVING POWER IS SAME AS FREQUENCY RESOLVING POWER

IF TIME-DOMAIN SIGNAL LASTS FOR 1 sec THEN $\frac{\omega}{\Delta\omega} = \frac{\nu}{\Delta\nu}$ (ν ← 4.3×10^6 FOR H_2O^+ @ 7 T; $\Delta\nu$ ≈ 1 Hz) = 4,300,000 FOR H_2O^+

i.e. MASS RESOLVING POWER = # OF CYCLOTRON ORBITS DURING TIME-DOMAIN DATA ACQUISITION PERIOD

C4130 POST-MIDTERM #2

NMR PARAMETERS



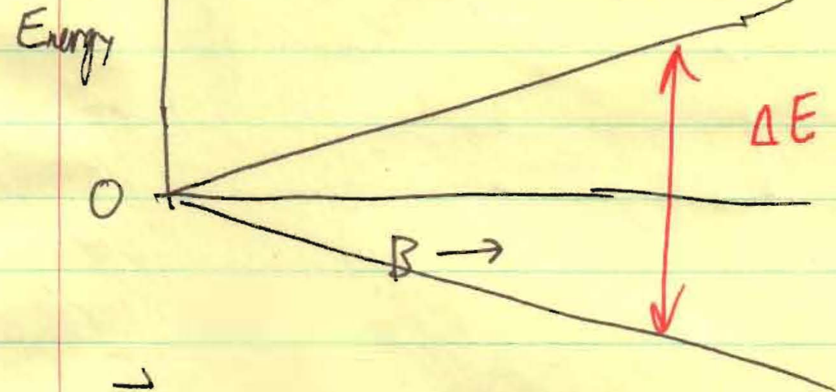
- PEAK AREA → # OF NUCLEI OF THAT TYPE (MRI)
- δ (i.e., ω_0) → BOND TYPE + PROXIMITY TO π-electrons ($\delta_x, \delta_y, \delta_z$)
- J → DIHEDRAL ANGLE (THROUGH-BOND COUPLING)

- T_1, T_2 → INTER- + INTRA-MOLECULAR DISTANCES (MRI)
- D → THROUGH SPACE COUPLING
- LINESHAPE (SOLIDS) → SPATIAL ORDERING

Origin of spin:

# protons	(protons + neutrons)	Nuclear spin	Examples
even	even	0	^{12}C, ^{16}O, ^{32}S
odd	even	1, 2, 3	^{14}N, ^{2}H
even or odd	odd	$\frac{1}{2}, \frac{3}{2}, \frac{5}{2}$	^{1}H, ^{13}C, ^{15}N, ^{31}P, ^{19}F, ^{35}Cl, ^{23}Na, ^{17}O

E-levels (spin = $\frac{1}{2}$)



ENERGY = $-\mu \cdot B = -\mu_z B_0$

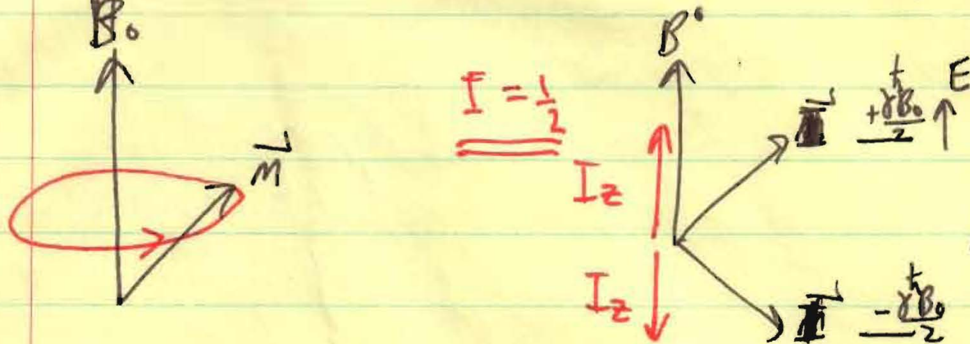
MAGNETIC MOMENT → $\vec{\mu} = \gamma \frac{h}{2\pi} \vec{I}$ ← ANGULAR MOMENTUM; γ = MAGNETOGYRIC RATIO

$$\Delta E = \gamma \frac{h}{2\pi} B_0 = h\nu = h\frac{\omega}{2\pi} = \hbar\omega$$

$$\hbar = \frac{h}{2\pi}$$

$$\nu_0 = \frac{\gamma B_0}{2\pi}$$

$$\omega_0 = \gamma B_0$$



$$\frac{N_{up}}{N_{down}} = e^{-\Delta E/kT}$$

HOMEWORK VERIFY — See handout pp. 4-5, p. 6

Classical — magnet (dipole) ← no mag monopole yet — can point anywhere, + be detected at any angle

Q.M. — spin can point anywhere, but can be observed only with z-component "up" or "down"

For Spin = I = $\frac{1}{2}$; I_z eigenvalues are $\hbar/2$, $-\frac{\hbar}{2}$