SPIN MAGNETIC MOMENT

CHEM 2430

L **associated with an e⁻ has magnetic moment** $\frac{-e}{2m_e}\boldsymbol{L}$

Would anticipate that spin has the magnetic moment $-\frac{e}{2m_e}\boldsymbol{S}$

Actually it is $\boldsymbol{m}_s = -g_e \frac{e}{2me}\boldsymbol{S}$

Dirac predicted $g_e = 2$

Now known that $g_e \approx 2.0023$

The α and β levels of an unpaired electron are split in a magnetic field

ESR detects transitions between these levels

Nuclei can also have non-zero spin

$$m_I = g_N\left(\frac{e}{2m_p}\right)I = \gamma I$$

Basis of NMR spectroscopy

$$^{1}H, \quad \gamma = 267 Mhz/T$$

$$^{13}C, \quad \gamma = 67.3 Mhz/T$$

These all have I=1/2

$$^{15}N, \quad \gamma = -27.1 Mhz/T$$

$$E = -\gamma \hbar B m_I$$

$$h\upsilon = |\Delta E| = |\gamma| \hbar B |\Delta m_I| = |\gamma| \hbar B$$

What makes the NMR so useful is that the external B field perturbs the electronic wavefunction, so the net B field at a nucleus depends on the external field and that due to the electrons.

$$B_{eff} = (1 - \sigma_i) B$$

shielding constant

In addition the spins on adjacent nuclei interact

Ladder operator for Spin

$$\hat{S}_+ = \hat{S}_x + i\hat{S}_y$$

$$\hat{S}_- = \hat{S}_x - i\hat{S}_y$$

$$\hat{S}_+\hat{S}_- = \hat{S}_x{}^2 + \hat{S}_y{}^2 + i\left[\hat{S}_y, \hat{S}_x\right] \quad = \hat{S}^2 - \hat{S}_z{}^2 + \hbar\hat{S}_z$$

$$\hat{S}_-\hat{S}_+ = \hat{S}^2 - \hat{S}_z{}^2 - \hbar\hat{S}_z$$

$$\hat{S}_+\beta = \hbar\alpha, \quad \hat{S}_+\alpha = 0$$

$$\hat{S}_-\alpha = \hbar\beta, \quad \hat{S}_-\beta = 0$$

$$\hat{S}_x\beta = \frac{1}{2}\hbar\alpha$$

$$\hat{S}_y\beta = \frac{-1}{2}i\hbar\alpha$$

$$\hat{S}_x\alpha = \frac{1}{2}\hbar\beta$$

$$\hat{S}_y\alpha = \frac{1}{2}i\hbar\beta$$