Parity

ASTR 300B

Parity is the behavior of a wavefunction under the inversion of the coordinate system

CARTESIAN

$x \to -x$
$y \to -y$
$z \to -z$

SPHERICAL

$r \to r$
$\theta \to \pi - \theta$
$\phi \to \phi + \pi$
$(\vec{r} \to -\vec{r})$

In atoms, e^- wavefunctions have the form

$$\psi \sim R_{n\ell}(r)\, Y_{\ell m_\ell}(\theta, \phi)$$ ← $Y_{\ell\ell}(\theta,\phi) \sim \sin^{\ell}(\theta)\, e^{i\ell\phi}$

$R_{n\ell}(r)$ is unaffected by inversion because $r \to r$ and it is symmetric about the origin. The parity depends then on how $Y_{\ell m_\ell}(\theta,\phi)$ transforms

Consider the situation $m_\ell = \ell$ so that we have $Y_{\ell\ell}(\theta,\phi)$ Then

$$\hat{P}\, Y_{\ell\ell}(\theta,\phi) = Y_{\ell\ell}(\pi-\theta, \phi+\pi) = e^{i\ell\phi} e^{i\ell\pi} \sin^{\ell}(\theta)$$ ← because $\sin(\pi-\theta) = \sin\theta$

$$= e^{i\ell\pi}\, Y_{\ell\ell}(\theta,\phi) = (-1)^{\ell}\, Y_{\ell\ell}$$

$\vec{L} = \vec{r} \times \vec{p}$
$\hat{P}\vec{L} = -\vec{r} \times -\vec{p} = \vec{L}$

Since angular momentum operators do NOT change sign under Parity transformations, we can use the lowering operator to prove this is true for $Y_{\ell m_\ell}$:

$$\hat{P}(\hat{L}_- Y_{\ell\ell}) = (-1)^{\ell}\, \hat{L}_- Y_{\ell\ell} = (-1)^{\ell}\, Y_{\ell m_\ell}$$

Parity depends on $(-1)^{\ell}$ for each e^-.

Parity in Term Symbols

$$^{2S+1}L_J^{\,o \text{ or } e}$$

o or e ← lowercase

"odd" or "even" Parity

The parity of a spectroscopic term is calculated by taking the products of the valence e⁻ $(-1)^{\ell}$

$$\prod_i (-1)^{\ell_i}$$

If this product $= +1 \Rightarrow$ "even"

$= -1 \Rightarrow$ "odd"

Example $\ell_1 = 1$ and $\ell_2 = 1$ $(1s^2 2s^2)\, 2p^2$ Neutral Carbon

$$\prod_i (-1)^{\ell_i} = (-1)^1 \cdot (-1)^1 = +1$$

So the ground state terms for CI

$$^3P^e_{0,1,2}\,,\quad ^1D^e_2\,,\quad ^1S^e_0$$

NOTE: Most of the time, if Parity is even, the "e" superscript is left off. Odd parity is only shown then.

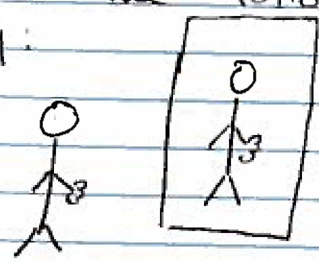
Multipole Radiation

Electromagnetic radiation can be expressed as a series expansion of different electric/magnetic "multipoles"

- electric monopole ← generates NO RADIATION (CHARGE CONSERVATION)
- electric dipole ← highest order multipole that generates radiation
- magnetic dipole
- electric quadrupole
- magnetic quadrupole
- octupoles etc.

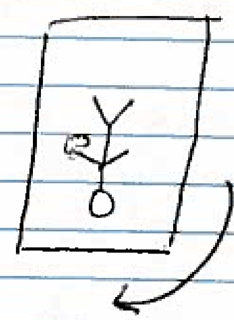
Different multipoles have different behavior with Parity:

CONSIDER the following model to think about Parity:



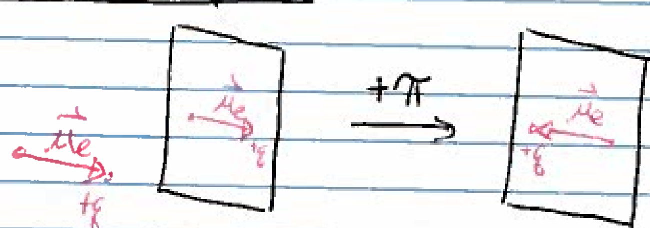
① LOOK IN A MIRROR
This transforms
$z \to -z$

②



Rotate MIRROR by $+\pi$
transforms $x \to -x$
$y \to -y$

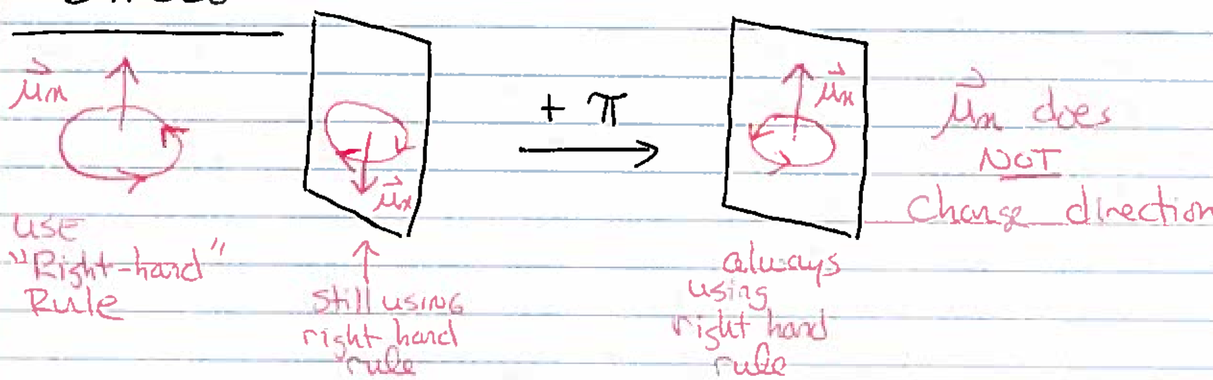
Electric Dipole



$\vec{\mu}_e$ changes direction!

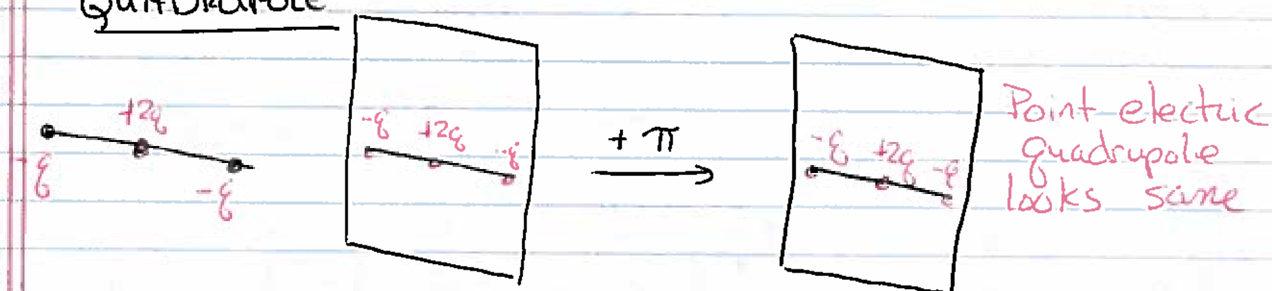
PARITY of electric dipole transitions CHANGES

MAGNETIC DIPOLE



PARITY of MAGNETIC DIPOLE transitions DOES NOT CHANGE

ELECTRIC QUADRUPOLE



PARITY of Electic Quadrupole transitions DOES NOT CHANGE