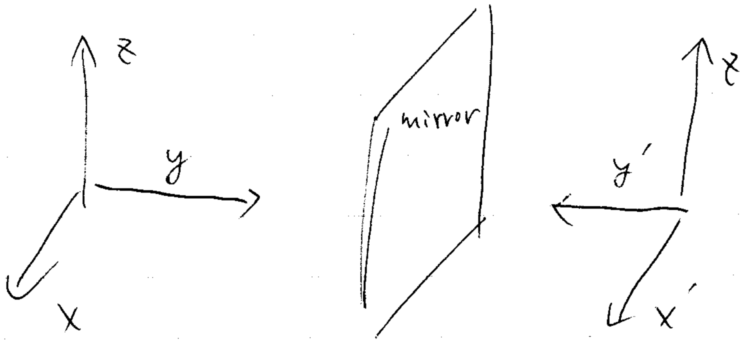
* Parity with a mirror.



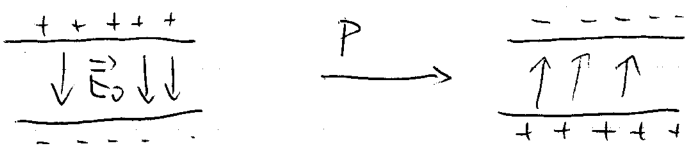
$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \underbrace{\begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix}}_{\substack{\det = -1 \\ \text{is an improper} \\ \text{rotation}}} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \underbrace{\begin{pmatrix} -1 & & 0 \\ & 1 & \\ 0 & & -1 \end{pmatrix}}_{\substack{\det = +1 \\ \text{is a proper rotation}}} \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix} = \begin{pmatrix} \cos\pi & 0 & -\sin\pi \\ 0 & 1 & 0 \\ \sin\pi & 0 & \cos\pi \end{pmatrix} P \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

* This part is the usual 3D rotation.

* You may think it easy to create a system that does not conserve parity simply placing it in an external field $\vec{E}_0$

$$H = \frac{p^2}{2m} + V(r) - \underbrace{q\,\vec{r}\cdot\vec{E}_0}$$ the last term seems to break parity.

However, if you include the saure into the system, parity is restored.



$$\vec{E}_0 \rightarrow -\vec{E}_0$$

* Parity in 1-D system

$$H = \frac{p^2}{2m} + V(r), \qquad [H, \pi] = 0 \quad \text{iff} \quad V(x) = V(-x)$$

$\Rightarrow$ $\boxed{\text{Bound states must also be the eigenstates of parity !!}}$

namely, $\quad \psi_n(x) = \pm\psi_n(-x)$

For example, in S.H.O. $\quad V(x) = \frac{m\omega^2}{2}x^2 \quad \Rightarrow \quad \psi_n(x) = (-1)^n \psi_n(-x)$

$n = 0, 1, 2, \ldots$

$\pi^2 = 1. \Rightarrow$ eigenvalues $p = \pm 1$

The Hilbert space is decomposed into two subspace

$$\mathcal{E} = \mathcal{E}_{even} \oplus \mathcal{E}_{odd}$$

denoted as $|n,+\rangle \quad |n,-\rangle$

and we can define the projection operator

$$P_\pm = \frac{1}{2}(1 \pm \pi)$$

$$\begin{cases} ① \ \mathbb{1} = P_+ + P_- \\ ② \ P_\pm^2 = \frac{1}{4}(1+\pi^2 \pm 2\pi) = P_\pm \\ ③ \ P_+P_- = P_-P_+ = 0 \end{cases}$$

For any 1D Wave function

$$(P_+\psi)(x) = \frac{1}{2}[\psi(x) + \psi(-x)] \quad \text{with } p=+1$$

$$(P_-\psi)(x) = \frac{1}{2}[\psi(x) - \psi(-x)] \quad p=-1$$

☆ Matrix elements of the Hamiltonian :

$$\langle n'p'|H|np\rangle = \langle n'p'|\pi^+ H \pi|np\rangle$$
$$= p'p \langle n'p'|H|np\rangle \neq 0 \quad \text{unless } p'p=1$$
$$\Rightarrow p=p'$$

In many cases, parity saves you lot of effort.

$$\langle n'p'|H|np\rangle \longrightarrow \left(\begin{array}{c|c} \text{even} & 0 \\ \hline 0 & \text{odd} \end{array}\right)$$

computer time to diagonalize a $(N\times N)$ matrix $\propto N^3$

$$\text{Time :} \quad N^3 \longrightarrow 2\left(\frac{N}{2}\right)^3 = \frac{1}{4}N^3$$

A simple step speed up the computation by factor 4 !

In 3D problem

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\, Y_{\ell m}(\theta,\phi)$$

which is relevant to electric dipole transition.

$$\langle n'\ell'm' | \hat{r} | n\ell m \rangle$$

since $|\vec{r}| = |-\vec{r}| \Rightarrow R_{n\ell}$ is not affected by parity

under parity

$$|\vec{r}| \to |\vec{r}|, \quad \theta \to \pi - \theta, \quad \phi \to \phi + \pi$$

$\Rightarrow \Pi Y_{\ell m} = (-1)^{\ell} Y_{\ell m}$ (simply read from the expression of $Y_{\ell m}$)

$\Rightarrow \Pi |n\ell m\rangle = (-1)^{\ell} |n\ell m\rangle$

$$\langle n'\ell'm' | \hat{r} | n\ell m\rangle = \langle n'\ell'm' | -\Pi^{+} \hat{r}\, \Pi | n\ell m\rangle = (-)(-)^{\ell'+\ell} \langle n'\ell'm' | \hat{r} | n\ell m\rangle$$

$\Rightarrow \Delta\ell =$ odd ~~for~~ nonzero dipole transition

$\Rightarrow$ Laporte's rule

Wigner-Eckart theorem $\Rightarrow \Delta\ell = 0, \pm 1$

(since $\vec{r}$ is a vector ($\ell=1$))

$\Rightarrow$ selection rule $\Delta\ell = \pm 1$

★ 2 other ways to see the $(-1)^{\ell}$ factor

① $|r|^{\ell} Y_{\ell m}$ = homogeneous polynomial in the Cartesian coordinates x, y, z of degree ℓ

e.g. $rY_1^0 = \sqrt{\frac{3}{4\pi}}\, z, \quad rY_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\,(x \pm iy)$

$- - - - \quad \Rightarrow (-1)^{\ell}$

② since $[L_{\pm}, \Pi] = 0$ we can just look at the $|n\ell 0\rangle$ state

$$Y_{\ell}^{0} = \sqrt{\frac{2\ell+1}{4\pi}}\, P_{\ell}^{0}(\cos\theta), \quad P_{\ell}(\cos\theta) = \frac{(-1)^{\ell}}{2^{\ell}\ell!}\left(\frac{d}{d\cos\theta}\right)^{\ell} \sin^{2\ell}\theta$$

$\theta \to \pi - \theta \quad \Rightarrow (-1)^{\ell}$

(There is no ϕ)