QM I
Phys 651

Lecture #20

①

Parity operator. Symmetric potentials and parity.

Inversion or parity operation $\Rightarrow$ reflection in space about the origin

$$\hat{P}|\vec{r}\rangle = |-\vec{r}\rangle$$

parity operator

$$\langle \vec{r}|\hat{P}^+ = \langle -\vec{r}|$$

$$\hat{P}\psi(\vec{r}) = \psi(-\vec{r})$$

- $\hat{P}$ is Hermitian $\Rightarrow$

$$\langle \varphi|\hat{P}\psi\rangle = \int d^3r\, \varphi^*(\vec{r})\hat{P}\psi(\vec{r}) =$$

$$= \int d^3r\, \varphi^*(\vec{r})\,\psi(-\vec{r}) =$$

$$= \int d^3r\, \varphi^*(-\vec{r})\,\psi(\vec{r}) =$$

$$= \int d^3r\, \left[\hat{P}\varphi(\vec{r})\right]^*\psi(\vec{r})$$

$$\hat{P}^+ = \hat{P} \Leftarrow \langle \varphi|\hat{P}^+|\psi\rangle \Rightarrow \hat{P}^+ = \hat{P}$$

- $\hat{P}^2 = \hat{I} \Rightarrow \hat{P} = \hat{P}^{-1}$
- $\hat{P}^{+} = \hat{P}^{-1} \Rightarrow$ unitary
- Eigenvalues are ± 1

$$\hat{P}\Psi_+(\vec{r}) = \Psi_+(-\vec{r}) = \Psi_+(\vec{r}) \leftarrow \text{even function}$$
$$\hat{P}\Psi_-(\vec{r}) = \Psi_-(-\vec{r}) = -\Psi_-(\vec{r}) \leftarrow \text{odd function}$$

So, the eigenfunctions of $\hat{P}$ have definite parity they are either even or odd

- $|\Psi_+\rangle, |\Psi_-\rangle$ are orthogonal (since $\hat{P}$ is Hermitian and $|\Psi_+\rangle, |\Psi_-\rangle$ correspond to different eigenvalues

$$\langle\Psi_+|\Psi_-\rangle = \int d^3r\, \Psi_+^*(\vec{r})\Psi_-(\vec{r}) =$$
$$= \int d^3r\, \Psi_+^*(-\vec{r})\Psi_-(-\vec{r}) =$$
$$= -\int d^3r\, \Psi_+^*(\vec{r})\Psi_-(\vec{r}) = -\langle\Psi_+|\Psi_-\rangle \Rightarrow = 0$$

- For any function $\Psi(\vec{r})$ we can construct even function $\Psi_+(\vec{r}) = \frac{1}{2}[\Psi(\vec{r}) + \Psi(-\vec{r})]$ and odd function $\Psi_-(\vec{r}) = \frac{1}{2}[\Psi(\vec{r}) - \Psi(-\vec{r})]$

- Since $\hat{P}^2 = \hat{I} \Rightarrow \hat{P}^n = \begin{cases} \hat{P} & \text{when } n \text{ is odd} \\ \hat{I} & \text{when } n \text{ is even} \end{cases}$

$$\hat{P}^n = \underbrace{\hat{P}\hat{P}\ldots\hat{P}}_{n \text{ times}} = \underbrace{\hat{I}\hat{I}\ldots}_{\frac{n}{2} \text{ times if } n \text{ is even}} = \hat{I}$$

or

$$= \underbrace{\hat{I}\hat{I}\ldots}_{\frac{n-1}{2} \text{ times if } n \text{ is odd}}\hat{P} = \hat{P}$$

Even and odd operators

$\hat{A}$ is even if $\hat{P}\hat{A}\hat{P} = \hat{A}$

$\hat{A}$ is odd if $\hat{P}\hat{A}\hat{P} = -\hat{A}$

For even operators $\Rightarrow [\hat{A}, \hat{P}] = [\hat{P}\hat{A}\hat{P}, \hat{P}] =$

$$= \hat{P}[\hat{P}\hat{A}, \hat{P}] = \hat{P}\underbrace{[\hat{P}, \hat{P}]}_{=0}\hat{A} + \hat{P}\hat{A}\underbrace{[\hat{P}, \hat{P}]}_{=0} = 0$$

So, $\hat{A}$, $\hat{P}$ commute

For odd operators $\Rightarrow \hat{A}\hat{P} = -\hat{P}\hat{A}\underbrace{\hat{P}\hat{P}}_{=\hat{I}} = -\hat{P}\hat{A}$

$\Downarrow$

$\hat{A}$, $\hat{P}$ anti-commute

<u>Example</u> What is the parity of the position and momentum operators?

Consider the position operator $\hat{\vec{R}}$ $\Rightarrow$

$\hat{\vec{R}}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle$

Apply $\hat{P}$ $\Rightarrow$ $\hat{P}\hat{\vec{R}}|\vec{r}\rangle = \vec{r}\underbrace{\hat{P}|\vec{r}\rangle}_{=|-\vec{r}\rangle} =$

$= \vec{r}\,|-\vec{r}\rangle$

If apply $\hat{P}$ first:

$\hat{P}|\vec{r}\rangle = |-\vec{r}\rangle$; now apply $\hat{\vec{R}}$ $\Rightarrow$

$\hat{\vec{R}}\hat{P}|\vec{r}\rangle = \hat{\vec{R}}|-\vec{r}\rangle = -\vec{r}\,|-\vec{r}\rangle$

$\Downarrow$

$\hat{P}\hat{\vec{R}} = -\hat{\vec{R}}\hat{P}$ → anti-commute $\Rightarrow$ $\hat{\vec{R}}$ is odd

Similarly, $\hat{\vec{P}}$ is odd

- For even operators $\hat{A}$ $\Rightarrow$ $\hat{P}\hat{A}^n\hat{P} = \hat{A}^n$
  odd $\Rightarrow$ $\hat{P}\hat{A}^n\hat{P} = (-1)^n\hat{A}^n$

Why do we care about parity? $\Rightarrow$ can simplify calculations

Consider symmetric (or <u>even</u>) potentials

$V(x) = V(-x)$ $\Rightarrow$ in this case, the Hamiltonian $H(x) = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{\substack{P \text{ is odd,} \\ \text{but } P^2 \text{ is even}}} + V(x)$ is also even,

i.e. $H(-x) = H(x)$

$\Downarrow$

H and $\mathcal{P}$ commute! $\Rightarrow$ share an eigenbasis.

- Consider nondegenerate spectrum

In the case of <u>bound states</u> (discrete spectrum) in 1D

Since $\hat{\mathcal{P}}$ has eigenstates of <u>definite</u> parity $\Rightarrow$ the bound states (eigenstates of H) also have definite parity; i.e. they are either even or odd

$V(-x) = V(x) \Rightarrow \psi(-x) = \pm\psi(x)$

So, for any symmetric 1D potential $\Rightarrow$ have two families of solutions $\begin{matrix} \nearrow \text{even} \\ \searrow \text{odd} \end{matrix}$

- Degenerate spectrum

In this case the eigenfunctions do not have definite parity

$\Uparrow$

See Sakurai pp. 256 – 258 ← red ~~book~~ for discussion
274 – 276 ← gray (newest) edition

Parity – selection rule

Consider $|\alpha\rangle, |\beta\rangle$ ⇐ eigenstates of parity operator

$$\mathcal{P}|\alpha\rangle = \varepsilon_\alpha |\alpha\rangle, \quad \mathcal{P}|\beta\rangle = \varepsilon_\beta |\beta\rangle,$$

$$\varepsilon_\alpha, \varepsilon_\beta = \pm 1$$

Then $\langle \beta | \vec{R} | \alpha \rangle = \underbrace{\langle \beta | \mathcal{P}^{-1}}_{= \varepsilon_\beta \langle \beta |} \underbrace{\mathcal{P} \vec{R} \mathcal{P}^{-1}}_{= -\vec{R}} \underbrace{\mathcal{P} |\alpha\rangle}_{= \varepsilon_\alpha |\alpha\rangle}$

↑ position operator

(since $\vec{R}$ is an odd operator)

$$= -\varepsilon_\alpha \varepsilon_\beta \langle \beta | \vec{R} | \alpha \rangle$$

$\Downarrow$

$\langle \beta | \vec{R} | \alpha \rangle = 0$ unless $\varepsilon_\alpha = -\varepsilon_\beta$ ⟹

$\langle \beta | \vec{R} | \alpha \rangle \neq 0$ only if $|\alpha\rangle, |\beta\rangle$ have opposite parity

$$\int \psi_\beta^* \vec{R} \psi_\alpha \, d\vec{r} = 0$$ ⇐ if ψ_α, ψ_β are of the same parity

↑ selection rule ⟹ used a lot in optics!