PHYS 4410

Quantum Mechanics 2

Spring 2023

Lecture 14

Rotational symmetry

February 22

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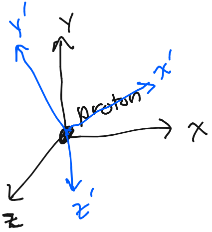


e.g. hydrogen atom Hamiltonian

$$H = \frac{\vec{p}\cdot\vec{p}}{2m} + \underbrace{V(r)}_{r=\sqrt{x^2+y^2+z^2}}$$

(central force)

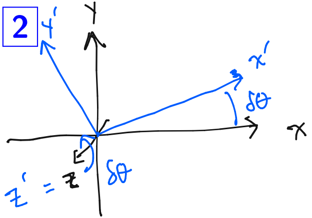
Rotational symmetry: problem (H) looks same in (x,y,z) or (x',y',z') coords.

$$\text{e.g. } r = \sqrt{x^2+y^2+z^2} = \sqrt{x'^2+y'^2+z'^2}$$

High level goals:

- what's the rotation symmetry group? (generated by angular momentum)
- non-commutative (non-Abelian) group (symmetry-enforced degeneracy H)

$\boxed{2}$



$$x' = x\cos(\delta\theta) + \sin(\delta\theta)\,y \approx x + \delta\theta\cdot y$$

$$y' = \cos(\delta\theta)\,y - \sin(\delta\theta)\,x \approx y - \delta\theta\cdot x$$

$$z' = z$$

If $|\delta\theta| \ll 1$

What operator takes $\psi(x,y,z) \to \psi(x',y',z')$?

$$\psi(x,y,z) \xrightarrow{?} \psi(x+\delta\theta\cdot y,\ y-\delta\theta\cdot x,\ z)$$

$\delta\theta$ small...

$$\approx \psi(x,y,z) + \delta\theta\cdot \underbrace{\left[y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right]}_{y\cdot\frac{i}{\hbar}p_x \,-\, x\cdot\frac{i}{\hbar}p_y}\psi(x,y,z) + \cdots$$

But $-i\hbar\frac{\partial}{\partial x} = p_x$

$-i\hbar\frac{\partial}{\partial y} = p_y$

$$= -\frac{i}{\hbar}(xp_y - yp_x)$$

$$= -\frac{i}{\hbar}L_z \quad \text{(z-angular momentum)}$$

$\boxed{3}$ There are 3 independent generators of rotation:

$L_x = yp_z - zp_y$

$L_y = zp_x - xp_z$

$L_z = xp_y - yp_x$

Claim: all rotation unitary transform... of the form:

$$\underbrace{e^{i\alpha L_x/\hbar}\, e^{i\beta L_y/\hbar}\, e^{i\gamma L_x/\hbar}\, e^{i\delta L_z/\hbar}}_{\text{order of multiplication important: (non-commutative)}} \cdots$$

$U_1 U_2 \neq U_2 U_1$

Example: $U_1 = e^{i\alpha L_x/\hbar}$, $U_2 = e^{i\beta L_y/\hbar}$, $\alpha, \beta \ll 1$

$U_1 \approx 1 + \frac{i\alpha}{\hbar} L_x$ [Taylor expand exponential].

$U_1 U_2 \overset{?}{=} U_2 U_1$

$U_1 U_2 U_1^{-1} \overset{?}{=} U_2$

$U_1 U_2 U_1^{-1} U_2^{-1} = 1$?

$\left(1 + \frac{i\alpha}{\hbar} L_x\right) \cdots \left[1 - \frac{i\alpha}{\hbar} L_x\right] \cdots$

$= 1 - \frac{\alpha\beta}{\hbar^2} L_x L_y + \frac{\alpha\beta}{\hbar^2} L_y L_x + \cdots \overset{?}{=} 1$

$L_x L_y - L_y L_x = [L_x, L_y] = i\hbar L_z$

4 Since: $[L_x, L_y] = i\hbar L_z$
$[L_y, L_z] = i\hbar L_x$
$[L_z, L_x] = i\hbar L_y$

rotation group is not commutative (non-Abelian group).

QM: $[H, U(\text{rotation})] = 0$; $[H, L_x] = 0$, $[H, L_y] = 0$, $[H, L_z] = 0$.

diagonalize simult...

$$L_z = \left(\begin{array}{cc|cc} 0 & & & \\ & -\hbar & & \\ \hline & & 2\hbar & 0 \\ & & 0 & \hbar \end{array}\right) \qquad L_x = \left(\begin{array}{cc|cc} a & b & 0 & 0 \\ c & d & 0 & 0 \\ \hline 0 & 0 & e & f \\ 0 & 0 & g & h \end{array}\right)$$

$E_1 = E_2$ $\quad E_3 = E_4$ $\quad \dots$

$$H = \left(\begin{array}{cc|cc} E_1 & & & \\ & E_2 & & \\ \hline & & E_3 & 0 \\ & & 0 & E_4 \end{array}\right)$$

Lec 15: blocks are called irreducible represent.

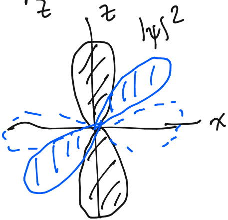
Know that $[H, L_x] = 0$?

$$[H, L_x] = \left(\begin{array}{c|cc} & & \\ \hline & \cancel{e(E_3 - E_3)} & f(E_3 - E_4) \\ & g(E_4 - E_3) & \cancel{h(E_4 - E_4)} = 0 \end{array}\right)$$

this matrix $= 0$ only if $E_3 = E_4$.

5 Example: $\psi(x,y,z) = z \cdot f(r)$ is e-function of H

p_z - orbital:



Rotated ψ must also be e-function

$$\psi(x,y,z) = \begin{cases} x\,f(r) & 90^\circ \text{ rot.} \\ (\cos\theta\, z + \sin\theta\, x)\, f(r) & \theta \text{ rot.} \end{cases}$$

for any θ, this must be eigenfunction.

... or, $\psi(x,y,z) = (\cos\alpha\, z + \sin\alpha \cdot y)\, f(r)$ ...

End:

$$H \begin{pmatrix} x f(r) \\ y f(r) \\ z f(r) \end{pmatrix} = \begin{pmatrix} E & 0 & 0 \\ 0 & E & 0 \\ 0 & 0 & E \end{pmatrix} \begin{pmatrix} x f(r) \\ y f(r) \\ z f(r) \end{pmatrix}.$$

3-fold degeneracy = p-orbitals $(l=1)$.

$\boxed{6}$ lec 15: Irreps classified by

$$\vec{L}^2 = L_x^2 + L_y^2 + L_z^2 = \hbar^2 \ell(\ell+1)$$

orbital: $\ell = 0, 1, 2, 3, \dots$

3-dim irrep: $\begin{pmatrix} xf \\ yf \\ zf \end{pmatrix}$ is $\ell = 1$.

Here $L_z = \begin{bmatrix} \hbar & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\hbar \end{bmatrix}$ (after basis rotation):

$$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \frac{x+iy}{\sqrt{2}} f \ ; \quad \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = zf \ ; \quad \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \frac{x-iy}{\sqrt{2}} f.$$

eigenfunctions / irreps of rotation:

$\{Y_{\ell m}$, fixed ℓ, $m = -\ell, -\ell+1, \dots, \ell\}$ irreps of rotation.

rotation symmetry: $H Y_{\ell m} = E_\ell Y_{\ell m}$.