ROTATIONS in QM

$R(\hat{n},\theta)$ = rotation by θ around $\hat{n}$

Symmetries have structure of a group:

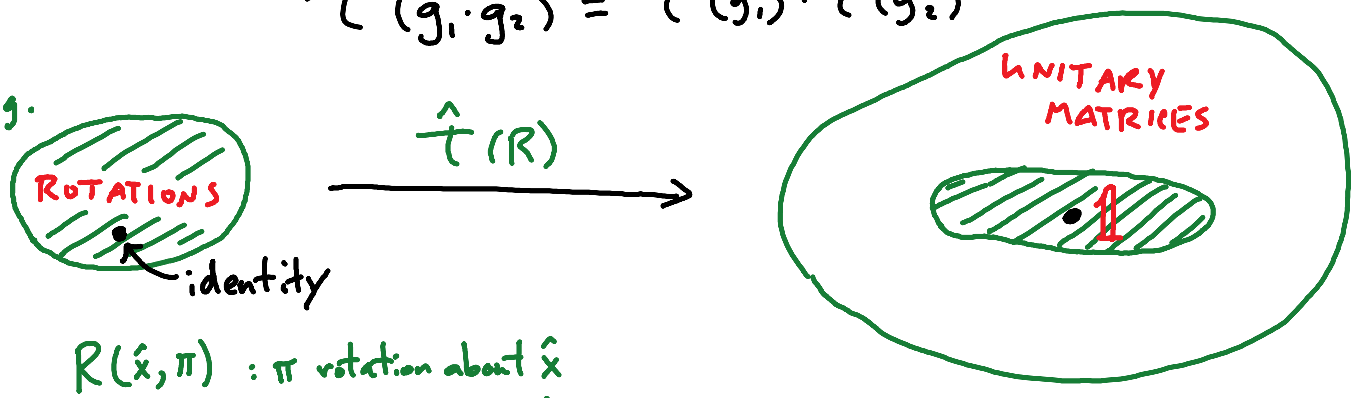
$g_1 \cdot g_2$ = combined operation of doing g_2 then g_1

associative, have identity, inverses

Action of symmetry g on a QM Hilbert space via unitary operator $\hat{\mathcal{T}}(g)$. Must satisfy

$$\hat{\mathcal{T}}(g_1 \cdot g_2) = \hat{\mathcal{T}}(g_1)\cdot\hat{\mathcal{T}}(g_2)$$

e.g.



e.g: $R(\hat{x},\pi)$: π rotation about $\hat{x}$

$R(\hat{y},\pi)$: π rotation about $\hat{y}$

Have: $R(\hat{x},\pi)R(\hat{y},\pi) = R(\hat{z},\pi)$

So: $\hat{\mathcal{T}}(R(\hat{z},\pi)) = \hat{\mathcal{T}}(R(\hat{x},\pi))\cdot\hat{\mathcal{T}}(R(\hat{y},\pi))$

operator for combined rotation is equal to product of operators for the individual rotations.

any rotation: product of infinitesimal rotations

* $\hat{\mathcal{T}}(R)$ completely determined once we say what $\hat{\mathcal{T}}$ is for infinitesimal rotations about x, y, z axes *

define: $\hat{\mathcal{T}}(R(\hat{x},\varepsilon)) = \mathbb{1} - \varepsilon\frac{i}{\hbar}\hat{J}_x + \dots$

$\hat{\mathcal{T}}(R(\hat{y},\varepsilon)) = \mathbb{1} - \varepsilon\frac{i}{\hbar}\hat{J}_y + \dots$

$\hat{\mathcal{T}}(R(\hat{z},\varepsilon)) = \mathbb{1} - \varepsilon\frac{i}{\hbar}\hat{J}_z + \dots$

these hermitian ops. are the ANGULAR MOMENTUM operators

then, for general rotation: $\hat{\mathcal{T}}(R(\hat{n},\theta)) = e^{-\frac{i}{\hbar}\theta(n_x\hat{J}_x + n_y\hat{J}_y + n_z\hat{J}_z)}$

Action of rotations on Hilbert space determined by how $\hat{J}_x, \hat{J}_y, \hat{J}_z$ are represented.

Multiplication rule for infinitesimal rotation implies:

$$[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z$$
$$[\hat{J}_y, \hat{J}_z] = i\hbar \hat{J}_x$$
$$[\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y$$

← e.g. do $\hat{x}$ rotation by ε_1
$\hat{y}$ rotation by ε_2
$\hat{x}$ rotation by $-\varepsilon_1$
$\hat{y}$ rotation by $-\varepsilon_2$
gives $\hat{z}$ rotation by $2\varepsilon_1 \cdot \varepsilon_2$

Solutions of these constraints give the possible ways rotations can act on a quantum system.

example: can have 2D Hilbertspace with

J_x, J_y, J_z represented by 2×2 matrices

in basis of J_z eigenstates:

$$J_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad J_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad J_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

usually call operators $\hat{S}_x, \hat{S}_y, \hat{S}_z$, matrices = Pauli matrices

Have: $\underbrace{J_x^2 + J_y^2 + J_z^2}_{\equiv}= \frac{3\hbar^2}{4}\mathbb{1}$: all states in this space have $J^2 = \frac{3\hbar^2}{4}$

TOTAL ANGULAR MOMENTUM OPERATOR J^2

J_i eigenvalues are $\pm\frac{1}{2}\hbar$ → we call such a system SPIN $\frac{1}{2}$

More solutions: SPIN j $\quad j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ dimension $2j+1$

J_x, J_y, J_z are $(2j+1)\times(2j+1)$ matrices with

$$J^2 = \hbar^2 j(j+1)\cdot \mathbb{1}$$

- each has eigenvalues: $-\hbar j, -\hbar(j-1), \ldots, \hbar(j-1), \hbar j$
- label J_z basis by m, $m = -j, -j+1, \ldots, j$

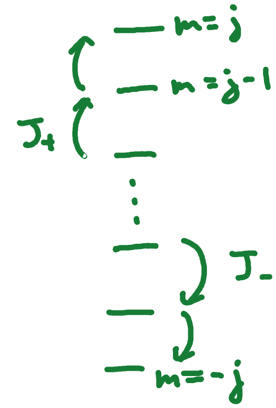
$$J_z|m\rangle = \hbar m|m\rangle$$

J_+

$$\underbrace{(J_x + iJ_y)}_{J_+}|m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}\;|m+1\rangle$$

$$\underbrace{(J_x - iJ_y)}_{J_-}|m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\;|m-1\rangle$$

J_-



★ Key result: for any system, can divide states into groups of J^2 eigenstates which each transform under rotations as a spin j system ★

$\hbar^2 j(j+1)$ are the only possible values of J^2

$\hbar \cdot m$, $m = -j \ldots j$ are the only possible values of J_x, J_y, J_z for spin j.

For any quantum system on which 3D rotations act:

- Hilbert space splits into groups of states that can be rotated into one another.
- In each group, can choose basis of J_z eigenstates, J_z eigenvalues are $\hbar$ times $-J, -J+1, \ldots, J$ where $J = 0, \frac{1}{2}, 1, \ldots$ (total # in the group is $2J+1$).

Call J_z eigenstates $|M\rangle$ Let $J_\pm = J_x \pm i J_y$

$$J_z|M\rangle = \hbar|M\rangle \qquad J_\pm|M\rangle = \hbar\sqrt{J(J+1) - M(M\pm1)}\,|M\rangle$$

- All states in such a group have same total angular momentum: J^2 eigenvalue $\hbar^2 J(J+1)$

simple examples:

spin $\frac{1}{2}$ particle

$|\uparrow\rangle = |J=\frac{1}{2}\ \ M=\frac{1}{2}\rangle$

J_- $\downarrow$ $\quad$ $\uparrow$ J_+

$|\downarrow\rangle = |J=\frac{1}{2}\ \ M=-\frac{1}{2}\rangle$

Js are the same as the S operators

spin 1 particle:

$|1\rangle$

J_- $\downarrow$ $\quad$ $\uparrow$ J_+

$|0\rangle$

J_- $\downarrow$ $\quad$ $\uparrow$ J_+

$|-1\rangle$

Example: Hydrogen atom:

Approximation: particle in Coulomb potential

$$H = \frac{\vec{P}^2}{2m} + V(\vec{x}) \qquad V = \frac{-e^2}{4\pi\varepsilon_0} \cdot \frac{1}{|\vec{x}|}$$

Gives time indep Schrodinger eqn:

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + V(\vec{x})\psi = E\psi$$

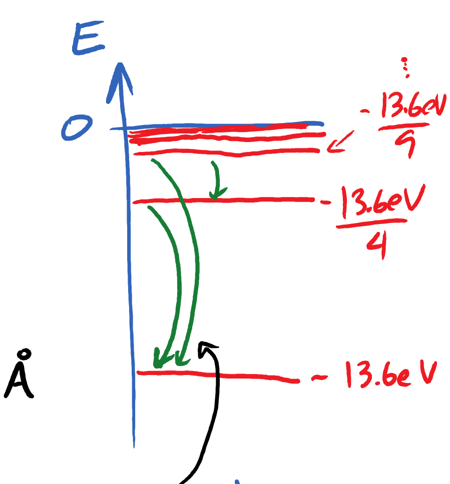
Solve via spherical coordinates, separation of variables.

Get: eigenstates $|\psi_{n\ell m}\rangle$ with $E = \frac{-13.6\text{eV}}{n^2}$ $\quad n = 1, 2, \ldots$

or: $|n\ \ell\ m\rangle$ $\quad \ell = 0, 1, \ldots, n-1$

$\frac{m}{2\hbar}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2$ $\quad m = -\ell, -\ell+1, \ldots, \ell$

★ $1 + 3 + \ldots + (2n-1) = n^2$
states w. energy E_n ★



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

$$R_{n,\ell}(r) = e^{-\frac{r}{n \cdot a}} P_{n,\ell}(r) \qquad a = \frac{4\pi\varepsilon_0\hbar}{me^2} \approx 0.529\text{Å}$$

polynomial degree $n-1$ $\qquad$ Bohr radius

experiment: measure emission spectra

$Y_{\ell,m}(\theta, \phi)$ spherical harmonics. (Griffiths 4.1.2)

light w. freq $hf = E_n - E_m$

★ real expt. gives groups of closely separated frequencies near these ★

ℓ and m quantum numbers for H atom relate to eigenvalues of angular momentum

$|n\, \ell\, m\rangle$ states $\rightarrow$ states with fixed n, ℓ form a group with $J = \ell$ $(m = -\ell \ldots \ell)$