Phys 5701   3 Dec 2020

OUR LAST CLASS TOGETHER!

Vectors, Tensors, & Wigner Eckart thm

What is a vector? V_i, $i = 1,2,3$ (x,y,z)

$$V_i \longrightarrow V_i' = \sum_j R_{ij} V_j \quad \leftarrow$$

"A vector is something that transforms like a vector"

For QM: Demand same for expectation values for vector operator

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$$|\alpha\rangle \longrightarrow |\alpha\rangle_R = \mathcal{D}(R)|\alpha\rangle$$

$${}_R\langle\alpha|V_i|\alpha\rangle_R = \boxed{\langle\alpha|\mathcal{D}^\dagger(R)\, V_i\, \mathcal{D}(R)|\alpha\rangle = \sum_j R_{ij} \langle\alpha|V_j|\alpha\rangle}$$

$$\mathcal{D}^\dagger(R)\, V_i\, \mathcal{D}(R) = \sum_j R_{ij} V_j \quad \leftarrow$$

Consider R = Infinitesimal rotation about $\hat{z}$

$$D(R) = 1 - \frac{i}{\hbar}\varepsilon J_z \qquad \varepsilon = \text{Rotation angle}$$

$$R = \begin{bmatrix} 1 & -\varepsilon & 0 \\ \varepsilon & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

uouze (3.4)

$$\left[1 + \frac{i}{\hbar}\varepsilon J_z\right]\begin{bmatrix} V_x \\ V_y \\ V_z \end{bmatrix}\left[1 - \frac{i}{\hbar}\varepsilon J_z\right] = R\begin{bmatrix} V_x \\ V_y \\ V_z \end{bmatrix}.$$

$$V_x - \frac{i}{\hbar}\varepsilon\,[V_x, J_z] = V_x - \varepsilon V_y$$

$$\Longleftrightarrow \quad [V_x, J_z] = -i\hbar V_y$$

$$V_y - \frac{i}{\hbar}\varepsilon\,[V_y, J_z] = \varepsilon V_x + V_y$$

$$\Longleftrightarrow \quad [V_y, J_z] = +i\hbar V_x$$

$$V_z - \frac{i}{\hbar}\varepsilon\,[V_z, J_z] = V_z$$

$$\Longleftrightarrow \quad [V_z, J_z] = 0$$

THREE EQUATIONS for "z" rotation.

Generalize this

NINE EQUATIONS!

$$\boxed{[V_i, J_j] = i\hbar \sum_k \varepsilon_{ijk} V_k}$$

Defines Vector Operator in QM!

Example: $\vec{J}$ is a vector!!

i.e. $[J_i, J_j] = i\hbar \varepsilon_{ijk} J_k$

Example: $\vec{x}$ is a vector!!

$[x, L_z] = [x, xp_y - yp_x]$

$= \cancel{[x, xp_y]} - [x, yp_x]$

$= -y[x, p_x] = -i\hbar y$ ✓

$[y, L_z] = [y, xp_y - yp_x]$

$= [y, xp_y] = +i\hbar x$ ✓

$[z, L_z] = [z, xp_y - yp_x] = 0$ ✓

Example: $\vec{p}$ is a vector!!

Cartesian Tensor: Generalization of vector.

$$V_i \to V_i' = \sum_j R_{ij} V_j$$

$$T_{ij} \to T_{ij}' = \sum_k \sum_l R_{ik} R_{jl} T_{kl}$$

e.g. $T_{ij} = U_i V_j$ "Dyad"

"2nd Rank Cartesian Tensor"

$$T_{ijk\ldots} \to T'_{ijk\ldots} = \sum_{i'} \sum_{j'} \sum_{k'} \cdots R_{ii'} R_{jj'} R_{kk'} \cdots T_{i'j'k'\ldots}$$

"N^{TH} Rank Tensor"

$$U_i V_j = \overset{①}{\frac{1}{3} \vec{U} \cdot \vec{V} \delta_{ij}} + \frac{1}{2}(U_i V_j - U_j V_i)^{②}$$

$$+ \left[\frac{1}{2}(U_i V_j + U_j V_i) - \frac{1}{3} \vec{U} \cdot \vec{V} \delta_{ij} \right]^{③}$$

① Transforms like a "Rank 0" tensor

② $U_i V_j - U_j V_i = \varepsilon_{ijk} (\vec{U} \times \vec{V})_k$

Transforms like a "Rank 1" tensor

③ Symmetric! Traceless!

2nd Rank Cartesian tensor decomposes into

$$\underset{2\cdot 0+1}{1} + \underset{2\cdot 1+1}{3} + \underset{2\cdot 2+1}{5} \qquad \vec{L}\ ??$$

$\Rightarrow$ Spherical Irreducible Tensor associate with Y_ℓ^m ("θ", "ϕ")

i.e. $$T_q^{(k)} = Y_{\ell=k}^{m=q}(\vec{V})$$

<u>Examples</u>: MQM 3e (3.459) (3.460)

$$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta = \frac{1}{r}\left(\frac{3}{4\pi}\right)^{1/2} z$$

$$\Rightarrow\ T_0^{(1)} = \left(\frac{3}{4\pi}\right)^{1/2} V_z$$

$\Rightarrow$ $$\boxed{\begin{aligned}[][J_z, T_q^{(k)}] &= \hbar q\, T_q^{(k)} \\ [J_\pm, T_q^{(k)}] &= \hbar\left[(k\mp q)(k\pm q+1)\right]^{1/2} T_{q\pm1}^{(k)}\end{aligned}}$$

Defines Irreducible Spherical Tensor Operator.

Matrix Elements of $T_q^{(k)}$

i.e. $\langle \alpha' j' m' | T_q^{(k)} | \alpha j m \rangle$

One simple result right away:

$$[J_z, T_q^{(k)}] - \hbar q T_q^{(k)} = \underbrace{J_z T_q^{(k)} - T_q^{(k)} J_z - \hbar q T_q^{(k)}}_{=0}$$

$$\Leftrightarrow \; [m'\hbar - m\hbar - \hbar q] \langle \alpha' j' m' | T_q^{(k)} | \alpha j m \rangle = 0$$

i.e. $\boxed{\langle \alpha' j' m' | T_q^{(k)} | \alpha j m \rangle = 0 \quad \text{unless} \quad m' = m + q}$.

Theorem

$$\langle \alpha' j' m' | T_q^{(k)} | \alpha j m \rangle = \underbrace{\langle j k ; m q | j k ; j' m' \rangle}_{=0 \text{ unless } m+q=m'}$$

$$\times \frac{1}{\sqrt{2j'+1}} \langle \alpha' j' \| T_q^{(k)} \| \alpha j \rangle$$

Wigner Eckart theorem

Example: MQM 3e Prob 3.45

Find the matrix element

$$e\langle \alpha j m' | (x^2 - y^2) | \alpha j\, m=j \rangle$$

in terms of Quadrupole Moment

$$Q \equiv e \langle \alpha j, m=j | (3z^2 - r^2) | \alpha j, m=j \rangle$$

↳ Show that both operators are related to the same $T_q^{(k)}$

then apply Wigner-Eckart thm

First consider $3z^2 - r^2 = r^2(\underbrace{3\cos^2\theta - 1}_{P_2(\cos\theta)})$

↳ $Y_2^0(\theta,\phi) = \left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta - 1)$

i.e. $Q = e\left(\frac{16\pi}{5}\right)^{1/2} \langle \alpha j j | Y_2^0 r^2 | \alpha j j \rangle$

$$= e\left(\frac{16\pi}{5}\right)^{1/2} \langle \alpha j j | T_0^{(2)} | \alpha j j \rangle$$

Try $Y_2^{\pm 2}(\theta,\phi) = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta \, e^{\pm 2i\phi}$

with $x = r\sin\theta\cos\phi$

$y = r\sin\theta\sin\phi$

$\Leftrightarrow r^2 Y_2^{\pm 2}(\theta,\phi) = \left(\frac{15}{32\pi}\right)^{1/2}$

$\times \left[r^2\sin^2\theta\cos(2\phi) \pm i r^2 \sin^2\theta \sin(2\phi)\right]$

$r^2\sin^2\theta\,(\cos^2\phi - \sin^2\phi)$ $\quad$ $2r^2\sin^2\theta\sin\phi\cos\phi$

$= x^2 - y^2$ $\quad$ $= 2xy$

$\Leftrightarrow x^2 - y^2 = \left(\dots\right)^{1/2} r^2 \left[Y_2^{+2}(\theta,\phi) + Y_2^{-2}(\theta,\phi)\right]$

$T_{+2}^{(2)}$ $\quad$ $T_{-2}^{(2)}$