TENSOR OPERATORS & THE WIGNER-ECKART THEOREM

In this section we shall be interested in the behaviour of quantum operators under rotations. Before we do this, let's consider a classification of classical objects under rotations.

- a scalar is an object that remains unchanged under rotations, an example being the length² of a vector, $A^2 = \vec{A}\cdot\vec{A}$.

- a vector is an object that, e.g. when expressed in a cartesian basis transforms as

$$A_i \longrightarrow \sum_j R_{ij} A_j$$

where $\underline{\underline{R}}$ is the rotation matrix, e.g.

$$\underline{\underline{R}}_z(\phi) = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

- a rank two tensor is an object that transforms as

$$T_{ij} \longrightarrow \sum_{i'j'} R_{ii'} R_{jj'} T_{i'j'}$$

- a rank q tensor is an object that transforms as

$$\underbrace{T_{ijk\ldots}}_{q \text{ indices}} \longrightarrow \sum_{i'j'\ldots} R_{ii'} R_{jj'} R_{kk'} \cdots \underbrace{T_{i'j'k'\ldots}}_{q \text{ indices}}$$

Now in fact a cartesian basis is not the best for transformations under rotation, since it is reducible. For example, consider the tensor formed from two vectors:

$$T_{ij} = A_i B_j \qquad \text{which is described by } 9 \text{ numbers}$$

now consider expressing this tensor in the following way:

$$T_{ij} = \underbrace{\frac{1}{3}\vec{A}\cdot\vec{B}\,\delta_{ij}}_{\substack{\text{scalar} \\ \text{one component} \\ \text{"}\ell=0\text{" ?}}} + \underbrace{\frac{1}{2}(A_i B_j - A_j B_i)}_{\substack{\text{vector } \epsilon_{ijk}(\vec{A}\times\vec{B})_k \\ \text{three components} \\ \text{"}\ell=1\text{" ?}}} + \underbrace{\left[\frac{1}{2}(A_i B_j + A_j B_i) - \frac{1}{3}\vec{A}\cdot\vec{B}\,\delta_{ij}\right]}_{\substack{\text{symmetric tensor} \\ \text{five components} \\ \text{"}\ell=2\text{" ?}}}$$

$(9 = 1+3+5\ \checkmark)$

A more useful basis are irreducible spherical tensors - an example being furnished by the spherical harmonic functions:

for a vector $\vec{A}$, a spherical tensor of rank k is given by

$$T_q^{(k)} = f(|\vec{A}|)\, Y_k^q(\hat{A})$$

e.g. • a scalar : $T_0^{(0)} = f(|\vec{A}|)\, Y_0^0(\hat{A}) = f(|\vec{A}|)\frac{1}{\sqrt{4\pi}}$

• a (spherical) vector : $T_q^{(1)} = f(|\vec{A}|)\, Y_1^q(\hat{A})$

$$= f(|\vec{A}|) \begin{cases} \sqrt{\frac{3}{4\pi}}\cos\theta_A = \sqrt{\frac{3}{4\pi}}\frac{A_z}{|\vec{A}|} \\ \mp\sqrt{\frac{3}{8\pi}}\, e^{\pm i\phi_A}\cdot \sin\theta_A = \mp\sqrt{\frac{3}{4\pi}}\left(\frac{A_x \pm i A_y}{\sqrt{2}\,|\vec{A}|}\right) \end{cases}$$

• a rank-two spherical tensor : $T_q^{(2)} = f(|\vec{A}|)\, Y_2^q(\hat{A})$

e.g. $T_0^{(2)} = f(|\vec{A}|)\frac{1}{2}\sqrt{\frac{5}{4\pi}}\left(3\cos^2\theta_A - 1\right)$

$$= f(|\vec{A}|)\sqrt{\frac{5}{16\pi}}\left(3\frac{A_z^2}{|\vec{A}|^2} - 1\right)$$

which is irreducible (contains no scalar or vector piece).

We can ask how these objects transform under rotations - even though we are working "classically" we can borrow the mathematics of quantum mechanics:

an eigenstate of angle : $|\theta',\phi'\rangle = \mathcal{D}(R)\,|\theta,\phi\rangle$

an eigenstate of l,m : $|l,m\rangle_R = \mathcal{D}(R)\,|l,m\rangle = \sum_{m'} \langle l,m'|\mathcal{D}(R)|l,m\rangle\, |l,m'\rangle$

$$= \sum_{m'} \mathcal{D}^{(l)}_{m'm}(R)\, |l,m'\rangle$$

considering the inverse rotation $\mathcal{D}(R^{-1})\,|l,m\rangle = \sum_{m'} \mathcal{D}^{(l)}_{m'm}(R^{-1})\, |l,m'\rangle$

contract with $\langle\theta,\phi|$: $\langle\theta,\phi|\mathcal{D}(R^{-1})|l,m\rangle = \sum_{m'} \mathcal{D}^{(l)}_{m'm}(R^{-1})\,\langle\theta,\phi|l,m'\rangle$

$$\langle\theta',\phi'|l,m\rangle$$

$$Y_l^m(\theta',\phi') = \sum_{m'} \mathcal{D}^{(l)}_{m'm}(R^{-1})\, Y_l^{m'}(\theta,\phi)$$

$$= \sum_{m'} \mathcal{D}^{(l)*}_{mm'}(R)\, Y_l^{m'}(\theta,\phi) \quad \left(\begin{array}{c}\text{unitarity} \\ \text{of } \mathcal{D}\end{array}\right)$$

so mathematically the spherical harmonics transform as

$$Y_\ell^m(\hat{A}') = \sum_{m'} D^{(\ell)*}_{mm'}(R_{\hat{A}\to\hat{A}'})\, Y_\ell^{m'}(\hat{A})$$

we will extrapolate & state that all spherical tensors transform in this way:

$$\boxed{T_q^{(k)} = \sum_{q'=-k}^{k} D^{(k)*}_{qq'}(R)\, T_{q'}^{(k)}}$$

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* Operators in quantum mechanics :

- we can call a 'vector operator' one whose expectation value transforms like a vector under rotations, ie.

$$\langle A_i\rangle \xrightarrow{R} \sum_j R_{ij}\langle A_j\rangle \qquad \text{(returning briefly to cartesian components)}$$

How is this manifested quantum mechanically?

$$\langle\alpha|A_i|\alpha\rangle \xrightarrow{R} {}_R\langle\alpha|A_i|\alpha\rangle_R = \langle\alpha|D^\dagger(R)\,A_i\,D(R)|\alpha\rangle \qquad \left(\text{since } |\alpha\rangle_R = D(R)|\alpha\rangle\right)$$

$$= \sum_j R_{ij}\langle\alpha|A_j|\alpha\rangle$$

Since this must be true for abitrary states $|\alpha\rangle \Rightarrow \underline{D^\dagger(R)A_iD(R) = R_{ij}A_j}$

now recall that rotation operators can be parameterised as

$$D(R) = \exp\left[-\tfrac{i}{\hbar}\hat{n}\cdot\vec{J}\phi\right] \xrightarrow{\text{infinite-simal}} 1 - \tfrac{i}{\hbar}\hat{n}\cdot\vec{J}\,\delta\phi$$

$$\text{so } D^\dagger(R)A_iD(R) = \left(1+\tfrac{i}{\hbar}\hat{n}\cdot\vec{J}\,\delta\phi\right)A_i\left(1-\tfrac{i}{\hbar}\hat{n}\cdot\vec{J}\,\delta\phi\right)$$

$$= A_i - \tfrac{i}{\hbar}\sum_j \hat{n}_j\,[A_i, J_j]\,\delta\phi$$

$$\text{e.g. } \hat{n} = \hat{z} \qquad \rightarrow A_i - \tfrac{i}{\hbar}\delta\phi\cdot[A_i, J_z]$$

$$\sum_j R_{ij}A_j \quad\rightarrow \begin{bmatrix} 1 & -\delta\phi & 0 \\ \delta\phi & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} A_x \\ A_y \\ A_z \end{bmatrix} = \begin{bmatrix} A_x - \delta\phi A_y \\ A_y + \delta\phi A_x \\ A_z \end{bmatrix}$$

for these to agree we require $\underline{[A_i, J_j] = i\epsilon_{ijk}\hbar A_k}$

$\Rightarrow$ to be a vector operator must satisfy this ↗.

vector operator : $[A_i, J_j] = i\epsilon_{ijk}\hbar A_k$

e.g. $\vec{A} = \vec{J}$ – trivially this a vector operator.

e.g. $\vec{A} = \vec{p}$ in the case of a single spinless particle : $\vec{J} = \vec{L} = \vec{r}\times\vec{p}$

$$[A_i, J_j] = [p_i, (\vec{r}\times\vec{p})_j] = [p_i, \epsilon_{jlm} r_l p_m] = \epsilon_{jlm} p_m [p_i, r_l]$$

$$= \epsilon_{jlm}\, p_m (-1) i\hbar \delta_{il} = -i\hbar\, \epsilon_{jim} p_m = i\hbar \epsilon_{ijk} p_k$$

$\Rightarrow$ the momentum is a vector operator

e.g. $\vec{A} = \vec{r}$ in the case of a particle with spin : $\vec{J} = \vec{L} + \vec{S}$

$$[A_i, J_j] = [r_i, (\vec{r}\times\vec{p})_j + S_j] = \epsilon_{jlm} r_l [r_i, p_m] + \cancel{[r_i, S_j]}^{\,0}$$

$$= i\hbar \epsilon_{jli} r_l = i\hbar \epsilon_{ijk} r_k$$ $\Rightarrow$ position is a vector operator.

e.g. particle in a background electric field $\vec{E}$ (uniform for simplicity)

$\vec{A} = \vec{E}$: $[A_i, J_j] = [E_i, J_j] = 0$ $\Rightarrow$ $\vec{E}$ is <u>not</u> a vector <u>operator</u>.

just a set of numbers

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we can generalize $D^\dagger(R) A_i D(R) = \sum_j R_{ij} A_j$ for a vector operator

to $D^\dagger(R) T_q^{(k)} D(R) = \sum_{q'=-k}^{k} D_{qq'}^{(k)*}(R)\, T_{q'}^{(k)}$ for a spherical tensor operator

and from this we can obtain the condition

$$[\hat{n}\cdot\vec{J}, T_q^{(k)}] = \sum_{q'} T_{q'}^{(k)} \langle kq' | \hat{n}\cdot\vec{J} | kq\rangle$$

* Products of spherical tensors are spherical tensors :

if $X^{(k_1)}_{q_1}$ & $Z^{(k_2)}_{q_2}$ are spherical tensors then so is $T^{(k)}_q$, where

$$T^{(k)}_q \equiv \sum_{q_1 q_2} \langle k_1 q_1 ; k_2 q_2 | [k_1 k_2] kq \rangle X^{(k_1)}_{q_1} Z^{(k_2)}_{q_2}$$

the proof is straightforward, we need to show that $D^\dagger(R)\, T^{(k)}_q D(R) = \sum_{q'} D^{(k)*}_{qq'}(R)\, T^{(k)}_{q'}$

given that $D^\dagger(R)\, X^{(k_1)}_{q_1} D(R) = \sum_{q_1'} D^{(k_1)*}_{q_1 q_1'}(R)\, X^{(k_1)}_{q_1'}$ & similar for Z

$$D^\dagger(R)\, T^{(k)}_q D(R) = \sum_{q_1 q_2} \langle k_1 q_1 ; k_2 q_2 | [k_1 k_2] kq \rangle D^\dagger(R) X^{(k_1)}_{q_1} \overbrace{D(R) D^\dagger(R)}^{=1} Z^{(k_2)}_{q_2} D(R)$$

$$= \sum_{q_1 q_2} \langle k_1 q_1 ; k_2 q_2 | [k_1 k_2] kq \rangle \sum_{q_1' q_2'} D^{(k_1)*}_{q_1 q_1'}(R)\, X^{(k_1)}_{q_1'}\, D^{(k_2)*}_{q_2 q_2'} Z^{(k_2)}_{q_2'}$$

$$= \sum_{\substack{q_1 q_2 \\ q_1' q_2'}} \langle k_1 q_1 ; k_2 q_2 | [k_1 k_2] kq \rangle \sum_{\bar{k} \bar{q} \bar{q}'} \langle [k_1 k_2] \bar{k} \bar{q} | k_1 q_1 ; k_2 q_2 \rangle^* \langle [k_1 k_2] \bar{k} \bar{q}' | k_1 q_1' ; k_2 q_2' \rangle^* \times D^{(\bar{k})*}_{\bar{q}\bar{q}'}(R)\, X^{(k_1)}_{q_1'} Z^{(k_2)}_{q_2'}$$

$$= \sum_{\substack{\bar{k}\bar{q}\bar{q}' \\ q_1' q_2'}} \left(\sum_{q_1 q_2} \langle [k_1 k_2] kq | k_1 q_1 ; k_2 q_2 \rangle \langle k_1 q_1 ; k_2 q_2 | [k_1 k_2] \bar{k} \bar{q} \rangle \right) \times \langle [k_1 k_2] \bar{k} \bar{q}' | k_1 q_1' ; k_2 q_2' \rangle D^{(\bar{k})*}_{\bar{q}\bar{q}'}(R)\, X^{(k_1)}_{q_1'} Z^{(k_2)}_{q_2'}$$

$$= \sum_{\bar{q}'} \left(\sum_{q_1' q_2'} \langle k_1 q_1' ; k_2 q_2' | [k_1 k_2] k \bar{q}' \rangle X^{(k_1)}_{q_1'} Z^{(k_2)}_{q_2'} \right) D^{(k)*}_{q \bar{q}'}(R)$$

$$= \sum_{\bar{q}'} T^{(k)}_{\bar{q}'} D^{(k)*}_{q\bar{q}'}(R) \qquad \underline{\text{QED}}.$$

So we can always form new spherical tensor operators by taking Clebsch-Gordan weighted products of existing tensor operators.

e.g. $k_1 = 1$; $k_2 = 1$ $\longrightarrow$ $T^{(0)}_0 = \langle 1{+}1 ; 1{-}1 | [11] 00 \rangle X_{+1} Y_{-1} + \langle 10 ; 10 | [11] 00 \rangle X_0 Y_0 + \langle 1{-}1 ; 1{+}1 | [11] 00 \rangle X_{-1} Y_{+1}$

$$= \frac{1}{\sqrt{3}} (X_{+1} Y_{-1} - X_0 Y_0 + X_{-1} Y_{+1}) = -\frac{1}{\sqrt{3}} \vec{X} \cdot \vec{Y} \quad \text{"scalar"}$$

$$T^{(1)}_{+1} = \langle 1{+}1 ; 10 | [11] 1{+}1 \rangle X_{+1} Y_0 + \langle 10 ; 1{+}1 | [11] 1{+}1 \rangle X_0 Y_{+1}$$

$$= \frac{1}{\sqrt{2}} (X_{+1} Y_0 - X_0 Y_{+1}) = \frac{1}{\sqrt{2}} \left(\frac{X_x + i X_y}{\sqrt{2}} Y_z - X_z \frac{Y_x + i Y_y}{\sqrt{2}} \right)$$

n.b. $\vec{X} \times \vec{Y} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ X_x & X_y & X_z \\ Y_x & Y_y & Y_z \end{vmatrix} \Rightarrow (\vec{X} \times \vec{Y})_{x+iy} \propto T^{(1)}_{+1}$ "spherical vector"

* Matrix elements of spherical tensors — the WIGNER-ECKART theorem

All this hard work will have a pay-off when we consider the matrix elements of spherical tensors w.r.t angular momentum eigenstates:

$$\langle \alpha' j' m' | T_q^{(k)} | \alpha j m \rangle$$ where α encodes all state information except the rotational properties.

Since $[J_z, T_q^{(k)}] = \sum_{q'} \langle kq' | J_z | kq \rangle T_{q'}^{(k)} = \hbar q \, T_q^{(k)}$

$$\Rightarrow 0 = \langle \alpha' j' m' | \left([J_z, T_q^{(k)}] - \hbar q T_q^{(k)} \right) | \alpha j m \rangle$$

$$= \langle \alpha' j' m' | \left(m' \hbar T_q^{(k)} - T_q^{(k)} m\hbar - q\hbar T_q^{(k)} \right) | \alpha j m \rangle$$

$$= \hbar (m' - m - q) \langle \alpha' j' m' | T_q^{(k)} | \alpha j m \rangle \qquad \Rightarrow \underline{m' = m + q}$$

the "Wigner-Eckart" theorem can be written

$$\boxed{\langle \alpha' j' m' | T_q^{(k)} | \alpha j m \rangle = \langle jm ; kq | [jk] j' m' \rangle \cdot \left[\frac{\langle \alpha' j' \| T^{(k)} \| \alpha j \rangle}{\sqrt{2j+1}} \right]_{\underline{m' = m+q}}}$$

notice that all the (m, m', q) dependence is encoded in a Clebsch-Gordan coefficient, with the dynamics hidden in the matrix element $\langle \alpha j' \| T^{(k)} \| \alpha j \rangle$.

(proofs of the theorem can be found in all advanced quantum mechanics books)

Application:

* tensor of rank-zero (a scalar): $T_0^{(0)} = S$

$$\Rightarrow \langle \alpha' j' m' | S | \alpha j m \rangle = \delta_{jj'} \delta_{mm'} \frac{\langle \alpha' j \| S \| \alpha j \rangle}{\sqrt{2j+1}}$$

so scalars (as expected) cannot change (j, m) values

* tensor of rank-one (a vector): $T_q^{(1)} = V_q \qquad (q = \pm 1, 0)$

clearly $\Delta m = m' - m = q = (\pm 1, 0)$
& $\Delta j = j' - j = \begin{Bmatrix} \pm \\ 0 \end{Bmatrix}$ } so a vector operator can change j by one unit.

* static electric multipole moments. Consider the energy response of a quantum system of charged particles to the application of an external electric field $\vec{E} = -\vec{\nabla}\phi$.

eg a particle of charge q in quantum state α, to first order undergoes an energy shift of

$$E = q\int d^3\vec{x}\ \psi_\alpha^*(\vec{x}) \cdot \phi(\vec{x}) \cdot \psi_\alpha(\vec{x}).$$

away from the sources of the electric field, $\nabla^2\phi(\vec{x}) = 0$ & $\phi(\vec{x})$ may be expanded in solutions of Laplace's eqn:

$$\phi(\vec{x}) = \sum_{k=0}^{\infty}\sum_{q=-k}^{k} A_{kq}\cdot\Big[\underbrace{r^k Y_k^q(\theta,\phi)}_{\text{spherical tensor operator.}}\Big]$$

$$\Rightarrow E = q\int d^3\vec{x}\ \rho(\vec{x})\ \phi(\vec{x}) = \sum_{kq} A_{kq} \underbrace{\int d^3\vec{x}\ \rho(x)\, r^k Y_k^q(\theta,\phi)}_{\text{electric } 2^k\text{-pole moment}}$$

e.g. $k=0 \rightarrow$ charge
$k=1 \rightarrow$ electric dipole moment
$k=2 \rightarrow$ electric quadrupole moment.
$\vdots$

e.g. there must be a P-wave (or higher) component in $\psi_\alpha(\vec{x})$ in order to have a quadrupole moment:

$$\langle \alpha l m | T_0^{(2)} | \alpha l m\rangle = \underbrace{\langle lm; 20 | lm\rangle}_{\substack{=0 \quad l=0 \\ \neq 0 \quad l=1 \\ \neq 0 \quad l=2 \\ \vdots}} \cdot \frac{\langle \alpha l \| T^{(2)} \| \alpha l\rangle}{\sqrt{2l+1}}$$