Rotational Properties of QM Vector Operators

QM $\vec{T}$-vectors: Selection Rules

refs. Sakurai, Sec. 3.10; Landau & Lifshitz "QM", ¶29

1) A QM "$\vec{T}$-vector" is any 3D Hermitian vector operator obeying the following commutation rule w.r.t. ∡ momentum $\vec{J}$...

$$\boxed{[J_\alpha, T_\beta] = i\hbar\, \epsilon_{\alpha\beta\gamma} T_\gamma}, \quad \epsilon_{\alpha\beta\gamma} = \begin{cases} 0, \text{unless } \alpha\beta\gamma \text{ all different;} \\ +1, \text{ when } \alpha\beta\gamma = \text{even perm}^{\underline{n}} \text{ of } 123; \\ -1, \text{ when } \alpha\beta\gamma = \text{odd perm}^{\underline{n}} \text{ of } 123. \end{cases} \tag{1}$$

We shall set $\hbar = 1$ for convenience. Note: $\vec{J}$ itself is a $\vec{T}$-vector. Also, $\vec{r}$ & $\vec{p}$ are $\vec{T}$-vectors w.r.t. orbital ∡ momentum $\vec{L}$. We shall now show that any QM vector operator $\vec{V}$ is a $\vec{T}$-vector w.r.t. $\vec{J}$ (so long as $\vec{V}$ & $\vec{J}$ inhabit the same space); this constitutes a definition of $\vec{V}$ by its behavior under rotations, not unlike the classical definition of a vector field.

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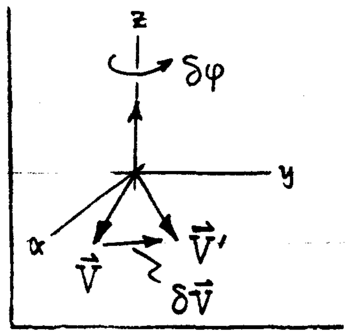
2) Rotate $\vec{V}$ by $\delta\varphi$ about z-axis. Specify z-direction by unit vector $\hat{n}$. Change in $\vec{V}$ given by...



→ $$\delta\vec{V} = \vec{V}' - \vec{V} = \delta\varphi(\hat{n} \times \vec{V}). \tag{2}$$

The individual components of $\vec{V}$ must transform like any Hermitian operator Q under the rotation operator R, i.e.

$R^\dagger = R^{-1}$, for rtns

$$\psi \to R\psi \Rightarrow \langle\psi|Q|\psi\rangle \to \langle R\psi|Q|R\psi\rangle = \langle\psi|R^\dagger Q R|\psi\rangle,$$

so// $$Q \to Q' = R^{-1} Q R, \quad \text{with: } R = 1 - i\,\delta\varphi(\hat{n}\cdot\vec{J});$$

→ and// $$\delta Q = Q' - Q = \cdots = i\,\delta\varphi\,[\hat{n}\cdot\vec{J}, Q], \text{ to 1st order in } \delta\varphi. \tag{3}$$

Now apply Eqs. (2) & (3) to a given component of $\vec{V}$, say V_x. Get...

$$\delta V_x = \delta\varphi \underbrace{(\hat{n}\times\vec{V})_x}_{(-)V_y} = i\,\delta\varphi\,[\underbrace{\hat{n}\cdot\vec{J}}_{J_z}, V_x]$$

by Eq. (2) by Eq. (3)

$$\Rightarrow \; (-)V_y = i\,[J_z, V_x], \quad \text{or} \quad [J_z, V_x] = i\,V_y. \tag{4}$$

This is just one of the commutation relations in Eq. (1); the others are proved similarly. So, indeed <u>any QM $\vec{V}$-operator is a $\vec{T}$-vector w.r.t. the ∡ momentum operator of its own space</u>.

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3) Since <u>all</u> vector operators in QM are $\vec{T}$-vectors, it is worth studying them to find their most general properties. E.g. if $\vec{A}$ & $\vec{B}$ are $\vec{T}$-vectors, it is easy to show that...

$$[\vec{J}, \vec{A}\cdot\vec{B}] = 0 \Rightarrow \vec{A}\cdot\vec{B} \text{ is a rotation-invariant scalar.} \tag{5}$$

Question: what would this look like if $\vec{A}$ or $\vec{B}$ were a pseudovector?

Another item to study is the so-called "<u>selection rules</u>" on matrix elements of T-vectors. In what follows, we shall prove the very general rule...

$$\boxed{\langle \alpha j m | \vec{T} | \alpha' j' m' \rangle \equiv 0, \text{ unless } \begin{cases} j' = j, \text{ or } j\pm1; \\ m' = m, \text{ or } m\pm1. \end{cases}} \left\{ \begin{array}{l} \text{Dipole} \\ \text{Selection} \\ \text{Rules} \end{array} \right. \tag{6}$$

Here j & m are the eigenvalues of $\vec{J}^2$ & J_z for the system ∡ momentum, and we have added a new quantum # α to denote all other relevant system eigenvalues (e.g. energy, fugacity, etc.). Eq. (6) -- known as the "dipole selection rules" -- shows, among other things, that a quantum system which interacts via a vector coupling can <u>only</u> make transitions which change j by 0 or 1 unit of ∡ momentum (i.e. $0\cdot\hbar$ or $1\cdot\hbar$).

4) Once we have proven Eq. (6), all that will remain regarding matrix elements of $\vec{T}$-vectors is to find out what the 9 non-zero elements are -- for the cases $j' = j, j\pm 1$ and $m' = m, m\pm 1$. We'll do this later.

Selection Rules on m

Since: $[J_z, T_z] = 0$, then: $\langle \alpha j m | J_z T_z | \alpha' j' m' \rangle = \langle \alpha j m | T_z J_z | \alpha' j' m' \rangle$, (operate to left; operate to right)

and/ $(m - m') \langle \alpha j m | T_z | \alpha' j' m' \rangle = 0$,

$$\Rightarrow \langle \alpha j m | T_z | \alpha' j' m' \rangle = 0, \text{ unless } m' = m. \tag{7}$$

Next, consider the commutator involving: $T^{\pm} = T_x \pm i T_y$ ...

$$\rightarrow [J_z, T^{\pm}] = \underbrace{[J_z, T_x]}_{= +iT_y} \pm i \underbrace{[J_z, T_y]}_{-iT_x} = \pm T^{\pm},$$

So/ $\langle \alpha j m | J_z T^{\pm} | \alpha' j' m' \rangle - \langle \alpha j m | T^{\pm} J_z | \alpha' j' m' \rangle = \pm \langle \alpha j m | T^{\pm} | \alpha' j' m' \rangle$,

and/ $[m - (m' \pm 1)] \langle \alpha j m | T^{\pm} | \alpha' j' m' \rangle = 0$,

$$\Rightarrow \langle \alpha j m | T^{\pm} | \alpha' j' m' \rangle = 0, \text{ unless } m' = m \pm 1. \tag{8}$$

Since: $T_x = \frac{1}{2}(T^+ + T^-)$, $T_y = \frac{1}{2i}(T^+ - T^-)$, indeed their matrix elements vanish unless $m' = m \pm 1$. Altogether, we have -- as advertised

$$\langle \alpha j m | \vec{T} | \alpha' j' m' \rangle = 0, \text{ unless } \begin{cases} m' = m & (T_z \text{ elt non-zero}), \\ m' = m \pm 1 & ((T_x \mp i T_y) \text{ elt non-zero}). \end{cases} \tag{9}$$

These selection rules on m fix the polarization of the "fields" involved in $|\alpha' j' m'\rangle \to |\alpha j m\rangle$: $\Delta m = 0$ (z-axis) $\Rightarrow$ linear, $\Delta m = \pm 1$ (xy-plane) $\Rightarrow$ circular.

5) The j-selection rules are harder to get. Following is a sketch of a tedious proof from Condon & Shortley, p. 60.

Selection Rules on j

The proof relies on fiddling with the commutator...

$$\vec{C} = [\vec{J}^2, [\vec{J}^2, \vec{T}]] = \vec{J}^4 \vec{T} - 2\vec{J}^2 \vec{T} \vec{J}^2 + \vec{T} \vec{J}^4. \tag{10}$$

This is the straightforward expansion of $\vec{C}$. Alternatively, expand $[\vec{J}^2, \vec{T}]$ first, and use the identities...

$$\left.\begin{aligned} [\vec{J}^2, \vec{T}] &= i(\vec{T}\times\vec{J} - \vec{J}\times\vec{T}) \\ \vec{T}\times\vec{J} + \vec{J}\times\vec{T} &= 2i\vec{T} \end{aligned}\right\} [\vec{J}^2, \vec{T}] = -2i(\vec{J}\times\vec{T} - i\vec{T})$$

so, $$\vec{C} = -2i \underbrace{[\vec{J}^2, \vec{J}\times\vec{T}]}_{=\, 2i(\vec{J}^2\vec{T} - (\vec{J}\cdot\vec{T})\vec{J})} - 2[\vec{J}^2, T]$$

or, $$\vec{C} = 2(\vec{J}^2\vec{T} + \vec{T}\vec{J}^2) - 4(\vec{J}\cdot\vec{T})\vec{J} \tag{11}$$

Equating Eqs. (10) & (11), you get the Unbelievable Identity...

$$\boxed{\vec{J}^4\vec{T} - 2\vec{J}^2\vec{T}\vec{J}^2 + \vec{T}\vec{J}^4 = 2(\vec{J}^2\vec{T} + \vec{T}\vec{J}^2) - 4\vec{J}(\vec{J}\cdot\vec{T})}. \tag{12}$$

This actually has physical content -- we shall get the j-selection rules from it, and also the basis of the so-called Vector Model.

Operate on both sides of Eq. (12) with $\langle \alpha j m | \quad | \alpha' j' m' \rangle$. Note that since $(\vec{J}\cdot\vec{T})$ commutes with $\vec{J}$, its matrix elements can be non-zero only when they are diagonal with $\vec{J}^2$ & J_z, so: $\langle \alpha j m | \vec{J}(\vec{J}\cdot\vec{T}) | \alpha' j' m' \rangle = 0$, when $j' \neq j$. For the case $j' \neq j$, then, Eq. (12) gives...

$$\rightarrow \{ [j(j+1)]^2 - 2j(j+1)j'(j'+1) + [j'(j'+1)]^2 \} \langle \alpha j m | \vec{T} | \alpha' j' m' \rangle =$$

$$2\{ j(j+1) + j'(j'+1) \} \langle \alpha j m | T | \alpha' j' m' \rangle, \quad \underline{j' \neq j}. \tag{13}$$

The LHS { } = $[j(j+1) - j'(j'+1)]^2$. After some arithmetic, find...

$$[(j+j'+1)^2 - 1][(j-j')^2 - 1] \langle \alpha j m | \vec{T} | \alpha' j' m' \rangle = 0, \quad j' \neq j;$$

$$\Rightarrow \langle \alpha j m | \vec{T} | \alpha' j' m' \rangle = 0, \text{ unless } j' = j \pm 1 \ (\text{when } j' \neq j). \tag{14}$$

For the case of $j' = j$, $\langle \alpha j m | \text{Eq. (12)} | \alpha' j' m' \rangle$ shows that the LHS vanishes identically, so that we get...

$$2 \cdot [j(j+1) + j(j+1)] \langle \alpha j m | \vec{T} | \alpha' j m' \rangle = 4 \underbrace{\langle \alpha j m | \vec{J} (\vec{J} \cdot \vec{T}) | \alpha' j m' \rangle}$$

$$= \sum_{\alpha'' j'' m''} \underbrace{\langle \alpha j m | \vec{J} | \alpha'' j'' m'' \rangle}_{\Rightarrow \delta_{\alpha\alpha''} \delta_{jj''}} \underbrace{\langle \alpha'' j'' m'' | (\vec{J} \cdot \vec{T}) | \alpha' j m' \rangle}_{\Rightarrow \delta_{j''j} \delta_{m''m'}}$$ by completeness of eigenfcns $|\alpha j m\rangle$

$$= \langle \alpha j m | \vec{J} | \alpha j m' \rangle \langle \alpha j m' | (\vec{J} \cdot \vec{T}) | \alpha' j m' \rangle, \text{ with } m' = m, m \pm 1;$$

so//

$$\left. \begin{array}{l} \boxed{j(j+1) \langle \alpha j m | \vec{T} | \alpha' j m' \rangle = \langle \alpha j m | \vec{J} | \alpha j m' \rangle \langle \alpha j m' | \vec{J} \cdot T | \alpha' j m' \rangle}; \\ \Rightarrow \langle \alpha j m | \vec{T} | \alpha' j' m' \rangle \ \underline{\text{can}} \text{ (but need not) be non-zero for } j' = j. \end{array} \right\} \tag{15}$$

Eqs (14) & (15) together give the j-selection rule: $\langle \alpha j m | \vec{T} | \alpha' j' m' \rangle = 0$, unless $j' = j$, or $j \pm 1$. With the m-selection rule of Eq. (9), we now have verified the claim made in Eq. (6), namely that all $\langle \alpha j m | \vec{T} | \alpha' j' m' \rangle = 0$, except for the "dipole selection rules": $j' = j, j \pm 1$ and $m' = m, m \pm 1$.