Tensor Operators

Vectors and tensors are defined by how they transform under rotation

Classical case: Momentum for example -

$$\vec{p} = (p_x, p_y, p_z)$$

Under the rotation $\vec{\theta}$, each component transforms:

$$p_i' = \sum_j R_{ij} p_j$$

$R(\vec{\theta})$: rotational Matrix turning original vector $\vec{p}$ into rotated vector $\overrightarrow{p'}$, $R^T = R^{-1}$

The component *i* of the transformed vector is the linear combination of the original components.

Rotational Matrices on three-dimensional space form group SO(3) (special orthogonal group). Simple example for rotation by angle θ around the x-axis: $R = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}$

Vector operators in QM: A set of three operators that behave in a similar way under rotations.

$$\mathbf{V}_i \quad i = 1,..,3$$

The same rotation as before in QM is expressed through the unitary operator $U(\vec{\theta}) = e^{-i\vec{\theta}\cdot\vec{\mathrm{J}}/\hbar}$

$$|\Psi> \xrightarrow{Rotation} |\Psi'> = U(\vec{\theta})|\Psi>$$

$$\langle\varphi'|\mathbf{V}_i|\Psi'\rangle = \langle\varphi|U^\dagger(\vec{\theta})\mathbf{V}_i U(\vec{\theta})|\Psi\rangle$$

Instead of taking this as the matrix element of $\mathbf{V}_i$ between the rotated wave functions, we can also interpret it as the matrix element of the rotated operator $\mathbf{V}_i' = U^\dagger(\vec{\theta})\mathbf{V_i}U(\vec{\theta})$ between the original wave functions. Now we can define a set of three operators as a vector operator if the following is true:

$$U^\dagger(\vec{\theta})\mathbf{V}_i U(\vec{\theta}) = \sum_j R_{ij}(\vec{\theta})\mathbf{V}_j$$

for all possible rotations. I.e., $\vec{\mathbf{V}}$ is a vector operator.

Replace $\vec{\theta} \to -\vec{\theta}$ (different way of expressing the same relationship, needed later)

$$R \to R^T \,;\; U^\dagger \to U \quad \text{and} \quad U \to U^\dagger$$

$$\Rightarrow U(\vec{\theta})\mathbf{V}_i U^\dagger(\vec{\theta}) = \sum_j R_{ji}(\vec{\theta})\mathbf{V}_j$$

Infinitesimal rotation around x-axis: $x \rightarrow x' = x; y \rightarrow y' = y - z\delta\theta; z \rightarrow z' = z + y\delta\theta$

$$R = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -\delta\theta \\ 0 & \delta\theta & 1 \end{bmatrix};\ R_{ij} = \delta_{ij} + \epsilon_{i1j} \cdot \delta\theta\ ;\ U = e^{-i\delta\theta J_x/\hbar}$$

Since $\delta\theta$ is small one can expand:

$$U = e^{-i\delta\theta J_x/h} = \mathbb{1} - \frac{i}{\hbar}\delta\theta \cdot \mathbf{J_x}$$

$$U^\dagger(\vec{\theta})\mathbf{V}_i U(\vec{\theta}) = \left(\mathbb{1} + \frac{i}{\hbar}\delta\theta \cdot \mathbf{J}_x\right)\mathbf{V}_i\left(\mathbb{1} - \frac{i}{\hbar}\delta\theta \cdot \mathbf{J}_x\right) = \mathbf{V}_i + \epsilon_{i1j} \cdot \delta\theta \cdot \mathbf{V}_j$$

$$\left(\mathbb{1} + \frac{i}{\hbar}\delta\theta \cdot \mathbf{J}_x\right)\mathbf{V}_i\left(\mathbb{1} - \frac{i}{\hbar}\delta\theta \cdot \mathbf{J}_x\right) = \mathbf{V}_i + \frac{i}{\hbar} \cdot \delta\theta(\mathbf{J}_x\mathbf{V}_i - \mathbf{V}_i\mathbf{J}_x) = \mathbf{V}_i + \frac{i}{\hbar} \cdot \delta\theta[\mathbf{J_x}, \mathbf{V}_i] = \mathbf{V}_i + \frac{1}{i\hbar}\delta\theta[\mathbf{V}_i, \mathbf{J}_x]$$

By equating LHS and RHS

$$[\mathbf{V}_i, \mathbf{J}_1] = i\hbar\epsilon_{i1j}\mathbf{V}_j$$

This is like the commutation relationship of angular momentum components. i.e.,

$$[\mathbf{J}_i, \mathbf{J}_k] = i\hbar\epsilon_{ikj}\mathbf{J_j}$$

This leads to alternative definition of vector operator: Any operator that commutes with $\mathbf{J}_k$ like a component of the angular momentum: $[\mathbf{V}_i, \mathbf{J}_k] = i\hbar\epsilon_{ikj}\mathbf{V}_j$

Vector operators are just one example of a whole class of "cartesian tensor operators of rank *n*". For a vector operator like $\vec{p}$ the rank is 1. The space of all such Cartesian vectors form a irreducible representation of SO(3) (the set of all possible orthogonal 3x3 matrices, i.e. all rotations).

Rank-0 tensors : scalar (invariant under rotation – a trivial representation)

Rank-1 cartesian tensors: smallest irreducible representation

Rank-2 cartesian tensors (energy-momentum tensor in special relativity and E&M; stress tensor or inertia tensor in classical mechanics): Reducible representation since you cannot connect all tensor components to each other via rotations. E.g., the 2nd rank tensor made up of the unit matrix times some constant is invariant under rotations and therefore a scalar; the asymmetric part of a tensor really transforms like a vector etc.

While Cartesian tensor operators in quantum mechanics transform like their classical counterparts under rotation, we can also define spherical tensors that follow the eigenvectors of the total angular momentum in their behavior under rotations.

How does |*j*,*m*> behave under rotation? See Shankar p. 328 ff – since all components of the angular momentum operator have a block diagonal form, mixing only states with the same *j*, we can conclude that all rotations are also block diagonal (as power series in the **J**'s). In fact, each set of 2*j*+1 eigenstates for fixed *j* form an irreducible presentation of the same group *O*(3) – see below. For a given fixed *j*, the rotation operator $U(\vec{\theta}) = e^{-i\vec{\theta}\cdot\vec{\mathbf{J}}/\hbar}$ can therefore be represented by a (2j+1)x(2j+1) matrix with matrix elements $D^j_{mm'}$ such that the rotated version of some eigenstate |*j*,*m*> is a linear superposition of other eigenstates:

$$U(\vec{\theta})|j,m\rangle = \sum_{m'} D^j_{mm'}\,(\vec{\theta})|j,m'\rangle$$

We can now define a spherical tensor of rank *k* ($k = 0,1,2, \ldots$) as a collection of operators T_k^q

$$-k \leq q \leq k \text{ in integer steps}$$

such that

$$U(\vec{\theta})T_k^q U^\dagger(\vec{\theta}) = \sum_{q'} D^k_{qq'}\,(\vec{\theta})T_k^{q'}$$

Important note: Watch out for the ordering of the rotational operators!

Why is it irreducible representation?

In $e^{-i\vec{\theta}\cdot\vec{\mathbf{J}}/\hbar}$, $\vec{\theta}\cdot\vec{\mathbf{J}} = \frac{\theta_x - i\theta_y}{2}\mathbf{J}_+ + \frac{\theta_x + i\theta_y}{2}\mathbf{J}_- + \theta_z\mathbf{J_z}$

Where $\mathbf{J}_+ = \mathbf{J_x} + i\mathbf{J_y}$ and $\mathbf{J}_- = \mathbf{J_x} - i\mathbf{J_y}$. So, starting with |*j*,*j*>, I can always find rotations that mix in lower values of *m*. Repeat until I cover all possible values.

Again, there is an alternative way to define tensor operators: Their commutators with the components of J should behave the same as applying those components of J to the corresponding eigenfunctions |*j*,*m*>:

$$[\mathbf{J}_+, T_k^q] = C^+_{kq} T_k^{q+1}$$

$$[\mathbf{J}_-, T_k^q] = C^-_{kq} T_k^{q-1}$$

$$[\mathbf{J_z}, T_k^q] = \hbar q T_k^q$$

We also notate $\mathbf{J_z} = \mathbf{J}_0$. The constants $C^\pm_{kq}$ are given in Shankar; e.g. $\mathbf{J}_+|j,m\rangle = C^+_{jm}|j,m+1\rangle$ etc.

Example for a Spherical tensor of rank 1: take any vector operator and make it into a spherical tensor -

$$\vec{V} \to V_1^q$$

$$V_1^0 = V_z$$

$$V_1^{+1} = \frac{1}{\sqrt{2}}(-V_x - iV_y)$$

$$V_1^{-1} = \frac{1}{\sqrt{2}}(V_x - iV_y)$$

These three $(V_1^0, V_1^{+1}, V_1^{-1})$ form a spherical tensor of rank 1. Also $-\mathbf{J}_+, \mathbf{J}_{0,}\mathbf{J}_-$ itself is a spherical tensor of rank 1.

To verify check the various commutators, e.g.

$$[\mathbf{J_z}, V_1^0] = [\mathbf{J}_z, V_z] = 0 = \hbar q T_1^q$$

$[\mathbf{J_z}, V_1^1] = -\frac{1}{\sqrt{2}}[\mathbf{J_z}, V_x] - \frac{i}{\sqrt{2}}[\mathbf{J_z}, V_y] = -\frac{i\hbar}{\sqrt{2}}V_y + \frac{i}{\sqrt{2}}i\hbar V_x = \frac{\hbar}{\sqrt{2}}(-V_x - iV_y) = \hbar V_1^1$ etc.

Now we can find out something very important about the matrix elements of any tensor operator. Lets apply T_k^q on some state vector $|\alpha, j, m\rangle$ (α describes all other quantum numbers not having to do with angular momentum). If we rotate the resulting state, we find the following:

$$U(\vec{\theta})T_k^q|\alpha, j, m\rangle = U(\vec{\theta})T_k^q U^\dagger(\vec{\theta})U(\vec{\theta})|\alpha, j, m\rangle = \sum_{q'} D_{qq'}^k \; T_k^{q'} \sum_{m'} D_{mm'}^j \; |\alpha, j, m'\rangle$$

The LHS separates $U(\vec{\theta})T_k^q U^\dagger(\vec{\theta})$ which is the operator rotated and $U(\vec{\theta})|\alpha, j, m\rangle$, the wave function rotated. In other words, the rotation looks like a simultaneous rotation of TWO angular momentum eigenstates that are combined:

$$|k, q\rangle \otimes |j, m\rangle$$

We know that such a product state can be written as a sum of "total angular momentum states" |J,M> with $|j - k| \leq J \leq j + k$ and $m + q = M$, with coefficients given by the Clebsch-Gordan coefficients. Similarly, we can conclude that for any matrix element of the tensor operator between two angular momentum eigenstates,

$$\langle \alpha', j', m' | T_k^q | \alpha, j, m \rangle$$

we must have

$$m + q = m'$$

$$|j - k| \leq j' \leq j + k$$

This yields important selection rules; e.g., transitions between states induced by a vector operator (like dipole moment for electromagnetic dipole radiation) requires that $|j - 1| \leq j' \leq j + 1$ since it is a spherical tensor of rank 1. In particular, transitions like 0 -> 0 (from an orbital angular momentum s state to another s state) are forbidden. Similarly, expectation values for any tensor rank 1 for a given wave function (where $j' = j$) can only be non-zero if the wave function contains at least j = ½ (1/2 < j' < 3/2) and tensors of rank 2 (like the quadrupole moment) require j ≥ 1.

Putting everything together, we can express any matrix element of such an operator in terms of the invariant matrix element $\langle \alpha', j' || T_k || \alpha, j \rangle$ which depends only on the total angular momenta, the rank of the tensor and the radial quantum numbers, and a Clebsch-Gordan coefficient which expresses the dependence on the magnetic quantum numbers *m*, *m'* and *q*:

$\left\langle \alpha', j', m' \middle| T_k^q \middle| \alpha, j, m \right\rangle = \langle \alpha, j' || T_k || \alpha, j \rangle \cdot \langle j', m' | k, q, j, m \rangle$ (Wigner-Eckart theorem)

Where $\langle j', m' | k, q, j, m \rangle$ is the Clebsch-Gordan coefficient. Once you determine the matrix element for any **one** (allowed) combination of *m*, *m'* and *q*, you can extract the invariant matrix element

$$\langle \alpha', j' || T_k || \alpha, j \rangle = \left\langle \alpha', j', m' \middle| T_k^q \middle| \alpha, j, m \right\rangle / \langle j', m' | k, q, j, m \rangle$$

and can then proceed to calculate any other matrix element for different *m*, *m'* and *q*. This allows you to arrive at pretty powerful theoretical conclusions about a system even if you know nothing more than its total angular momentum.