Tensor Operators and Wigner-Eckart Theorem

I. SCALAR AND VECTOR OPERATORS

Under a roatation, a state vector is transformed as:

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

Operators may be classified according to how their expectation value is affected by the rotation.

- *scalar operators* are those operators whose expectation value w.r.t. to an arbitrary state is not affected by rotation, i.e., $\langle\alpha'|\hat{A}|\alpha'\rangle = \langle\alpha|\hat{A}|\alpha\rangle$. This can only be true if

  $$\hat{\mathcal{D}}^\dagger(R)\,\hat{A}\,\hat{\mathcal{D}}(R) = \hat{A}$$

  Since $\hat{\mathcal{D}}(R) = e^{-i\hat{\mathbf{J}}\cdot\hat{\mathbf{n}}\phi/\hbar}$, the above condition is equivalent to

  $$[\hat{A}, \hat{\mathbf{J}}] = 0$$

  Examples of scalar operators are: $\hat{J}^2$, $\hat{r}$, $\hat{p}^2$, $\mathbf{r}\cdot\mathbf{p}$.

- *vector* operators are those operators whose expectation value w.r.t. to an arbitrary state transforms like a ordinary vector under rotation. For a vector operator $\hat{\mathbf{V}} = (\hat{V}_x, \hat{V}_y, \hat{V}_z)$,

  $$\hat{\mathcal{D}}^\dagger(R)\,\hat{V}_i\,\hat{\mathcal{D}}(R) = \sum_{i,j} R_{ij}\hat{V}_j$$

  where R_{ij} form the 3×3 matrix representing the rotation. By considering an infinitesimally small rotation, one can show that the above consition is equivalent to the following commutation relation:

  $$[\hat{V}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{V}_k$$

  Examples of vector operators include $\hat{\mathbf{r}}$, $\hat{\mathbf{p}}$, $\hat{\mathbf{J}}$.

II. MATRIX ELEMENTS OF VECTOR OPERATOR

Consider a vector operator $\hat{\mathbf{V}} = (\hat{V}_x, \hat{V}_y, \hat{V}_z)$. We may define

$$\hat{V}_\pm \equiv \hat{V}_x \pm i\hat{V}_y$$

The following comutation relations can be easily proved:

$$[\hat{J}_+, \hat{V}_+] = 0\,,\ [\hat{J}_+, \hat{V}_-] = 2\hbar\hat{V}_z\,,\ [\hat{J}_-, \hat{V}_+] = -2\hbar\hat{V}_z\,,\ [\hat{J}_-, \hat{V}_-] = 0\,,\ [\hat{J}_z, \hat{V}_+] = \hbar\hat{V}_+\,,\ [\hat{J}_-, \hat{V}_-] = -\hbar\hat{V}_-$$

Consider a complete set of ket states $|\alpha, j, m\rangle$. Here the j's and m's denote the usual angular momentum eigenstates and the α's are nonangular quantum numbers, such as those for radial states. We shall evaluate matrix elements of $\hat{\mathbf{V}}$ w.r.t. these states.

From the commutation relations between $\hat{\mathbf{V}}$ and $\hat{\mathbf{J}}$, one can show the following:

$$\begin{aligned}
\langle\alpha', j', m'|\hat{V}_z|\alpha, j, m\rangle &\propto \delta_{m',m} \\
\langle\alpha', j', m'|\hat{V}_+|\alpha, j, m\rangle &\propto \delta_{m',m+1} \\
\langle\alpha', j', m'|\hat{V}_-|\alpha, j, m\rangle &\propto \delta_{m',m-1}
\end{aligned}$$

Hence we have the m-selection rules:

- For transitions induced by $\hat{V}_z$, $\Delta m = m' - m = 0$
- For transitions induced by $\hat{V}_\pm$, $\Delta m = m' - m = \pm 1$

From $[\hat{J}_+, \hat{V}_+] = 0$, we have

$$\langle \alpha, j, m+2|\hat{J}_+\hat{V}_+|\alpha, j, m\rangle = \langle \alpha, j, m+2|\hat{V}_+\hat{J}_+|\alpha, j, m\rangle$$

Inserting the identity operator

$$\hat{\mathbf{1}} = \sum_{\alpha'}\sum_{j'}\sum_{m'} |\alpha', j', m'\rangle\langle \alpha', j', m'|$$

on both sides in between $\hat{J}_+$ and $\hat{V}_+$, we have

$$\langle \alpha, j, m+2|\hat{J}_+|\alpha, j, m+1\rangle \, \langle \alpha, j, m+1|\hat{V}_+|\alpha, j, m\rangle = \langle \alpha, j, m+2|\hat{V}_+|\alpha, j, m+1\rangle \, \langle \alpha, j, m+1|\hat{J}_+|\alpha, j, m\rangle$$

or

$$\frac{\langle \alpha, j, m+1|\hat{V}_+|\alpha, j, m\rangle}{\langle \alpha, j, m+1|\hat{J}_+|\alpha, j, m\rangle} = \frac{\langle \alpha, j, m+2|\hat{V}_+|\alpha, j, m+1\rangle}{\langle \alpha, j, m+2|\hat{J}_+|\alpha, j, m+1\rangle} = k_+(\alpha, j)$$

Clearly, the ratio k_+ is independent of m. Therefore, we conclude:

$$\langle \alpha, j, m+1|\hat{V}_+|\alpha, j, m\rangle = k_+(\alpha, j) \, \langle \alpha, j, m+1|\hat{J}_+|\alpha, j, m\rangle$$

Since if $m+1$ in $\langle \alpha, j, m+1|$ is changed to other values, both sides will be zero, we can simply replace it by m', i.e.,

$$\langle \alpha, j, m'|\hat{V}_+|\alpha, j, m\rangle = k_+(\alpha, j) \, \langle \alpha, j, m'|\hat{J}_+|\alpha, j, m\rangle \tag{1}$$

Similarly, from $[\hat{J}_-, \hat{V}_-] = 0$, we can derive

$$\langle \alpha, j, m'|\hat{V}_-|\alpha, j, m\rangle = k_-(\alpha, j) \, \langle \alpha, j, m'|\hat{J}_-|\alpha, j, m\rangle \tag{2}$$

Again, k_- is a constant independent of m.

From $[\hat{J}_-, \hat{V}_+] = -2\hbar\hat{V}_z$, we have

$$\begin{aligned}
-2\langle \alpha, j, m|\hat{V}_z|\alpha, j, m\rangle &= \langle \alpha, j, m|(\hat{J}_-\hat{V}_+ - \hat{V}_+\hat{J}_-|\alpha, j, m\rangle \\
&= \sqrt{j(j+1) - m(m+1)} \, \langle \alpha, j, m+1|\hat{V}_+|\alpha, j, m\rangle - \sqrt{j(j+1) - m(m-1)} \, \langle \alpha, j, m|\hat{V}_+|\alpha, j, m-1\rangle \\
&= \sqrt{j(j+1) - m(m+1)} \; k_+(\alpha, j) \, \langle \alpha, j, m+1|\hat{J}_+|\alpha, j, m\rangle \\
&\quad -\sqrt{j(j+1) - m(m-1)} \; k_+(\alpha, j) \, \langle \alpha, j, m|\hat{J}_+|\alpha, j, m-1\rangle \\
&= \sqrt{j(j+1) - m(m+1)} \; k_+(\alpha, j) \, \hbar\sqrt{j(j+1) - m(m+1)} \\
&\quad -\sqrt{j(j+1) - m(m-1)} \; k_+(\alpha, j) \, \hbar\sqrt{j(j+1) - m(m-1)} \\
&= -2m\hbar k_+(\alpha, j)
\end{aligned}$$

Hence

$$\langle \alpha, j, m|\hat{V}_z|\alpha, j, m\rangle = m\hbar k_+(\alpha, j) = k_+(\alpha, j) \, \langle \alpha, j, m|\hat{J}_z|\alpha, j, m\rangle \tag{3}$$

Similarly, from $[\hat{J}_+, \hat{V}_-] = 2\hbar\hat{V}_z$, we can derive

$$\langle \alpha, j, m|\hat{V}_z|\alpha, j, m\rangle = m\hbar k_-(\alpha, j) = k_-(\alpha, j) \, \langle \alpha, j, m|\hat{J}_z|\alpha, j, m\rangle \tag{4}$$

Therefore, we have

$$k_+(\alpha, j) = k_-(\alpha, j) \equiv k(\alpha, j)$$

Furthermore, from Eqs. (1), (2) and (3), we have

$$\langle \alpha, j, m'|\hat{V}_i|\alpha, j, m\rangle = k(\alpha, j) \, \langle \alpha, j, m'|\hat{J}_i|\alpha, j, m\rangle$$

or we may write

$$\langle \alpha, j, m'|\hat{\mathbf{V}}|\alpha, j, m\rangle = k(\alpha, j) \, \langle \alpha, j, m'|\hat{\mathbf{J}}|\alpha, j, m\rangle \tag{5}$$

The equation is a manifestation of the Wigner-Echart theorem (to be discussed later) for the vector operator. It tells us that, for given α and j, we only need to calculate one (non-zero) matrix element of $\hat{V}_i$ to obtain $k(\alpha, j)$, then all other matrix elements $\hat{V}_j$ will be obtained automatically.

We may go further to obtain $k(\alpha, j)$. To this end, we calculate $\langle \alpha, j, m|\hat{\mathbf{V}} \cdot \hat{\mathbf{J}}|\alpha, j, m\rangle$. Inserting the identity operator

$$\hat{\mathbf{1}} = \sum_{m'} |\alpha, j, m'\rangle\langle\alpha, j, m'|$$

between $\hat{\mathbf{V}}$ and $\hat{\mathbf{J}}$. (We restrict ourselves in the subspace defined by the given α and j, hence we do not sum over these two quantum numbers.) Using Eq. (5), we have

$$\langle \alpha, j, m|\hat{\mathbf{V}} \cdot \hat{\mathbf{J}}|\alpha, j, m\rangle = k(\alpha, j)\, \langle \alpha, j, m|\hat{\mathbf{J}} \cdot \hat{\mathbf{J}}|\alpha, j, m\rangle = k(\alpha, j)\, j(j+1)\hbar^2$$

Therefore,

$$k(\alpha, j) = \frac{\langle \alpha, j, m|\hat{\mathbf{V}} \cdot \hat{\mathbf{J}}|\alpha, j, m\rangle}{j(j+1)\hbar^2}$$

Since $\hat{\mathbf{V}} \cdot \hat{\mathbf{J}}$ is a scalar operator (it commutes with $\hat{\mathbf{J}}$), the expectation value $\langle \alpha, j, m|\hat{\mathbf{V}} \cdot \hat{\mathbf{J}}|\alpha, j, m\rangle$ must be m-independent. Sometimes people write this as

$$\langle \alpha, j, m|\hat{\mathbf{V}} \cdot \hat{\mathbf{J}}|\alpha, j, m\rangle = \langle \hat{\mathbf{V}} \cdot \hat{\mathbf{J}}\rangle_{\alpha,j}$$

then we have

$$\hat{\mathbf{V}} = \frac{\langle \hat{\mathbf{V}} \cdot \hat{\mathbf{J}}\rangle_{\alpha,j}}{j(j+1)\hbar^2}\, \hat{\mathbf{J}}$$

III. TENSOR OPERATORS

A tensor is a generalization of a such a vector to an object with more than one suffix, such as, for example, $\hat{T}_{ij}$ or $\hat{T}_{ijk}$ (having 9 and 27 components respectively in three dimensions) with the requirement that these components mix among themselves under rotation by each individual suffix following the vector rule, for example

$$\hat{T}_{ijk} \longrightarrow \sum_{i'}\sum_{j'}\sum_{k'} \hat{T}_{i'j'k'}$$

The number of suffix is the rank of the tensor. Such tensors are called Cartesian tensors.

If $\hat{\mathbf{U}}$ and $\hat{\mathbf{V}}$ are two vectors, then we can construct a rank 2 Cartesian tensor whose elements are given by

$$T_{ij} = U_i V_j$$

The problem with this tensor is that it is reducible. That is to say, combinations of the elements can be arranged in sets such that rotations operate only within these sets. To study the rotation properties, it is more convenient to work with irreducible spherical tensors.

A spherical tensor of rank k has $(2k+1)$ elements labelled as

$$T_q^{(k)}\,, \quad q = -k, -k+1, ..., k$$

(Scalars and vectors can be regarded as rank 0 and 1 tensors, respectively.) A spherical tensor is defined through its properties under rotation:

$$\hat{\mathcal{D}}(R)\, T_q^{(k)}\, \hat{\mathcal{D}}^\dagger(R) = \sum_{q'=-k}^{k} \mathcal{D}_{q'q}^{(k)}(R)\, T_{q'}^{(k)}$$

where $\mathcal{D}_{q'q}^{(k)}(R) = \langle k, q'|\hat{\mathcal{D}}(R)|k, q\rangle$ is the matrix element of the rotation operator. Again, using an infinitesimal rotation, one can show that the above is equivalent to the following commutation relations:

$$[\hat{J}_z, T_q^{(k)}] = q\hbar\, T_q^{(k)}\,, \quad [\hat{J}_\pm, T_q^{(k)}] = \hbar\sqrt{(k \mp q)(k \pm q + 1)}\; T_{q\pm 1}^{(k)}$$

One can show that for a vector operator, if we define

$$\hat{V}_z = T_0^{(1)}\,, \quad -\frac{\hat{V}_+}{\sqrt{2}} = T_{+1}^{(1)}\,, \quad \frac{\hat{V}_-}{\sqrt{2}} = T_{-1}^{(1)}$$

then the above commutation relation is satisfied. Hence a vector operator can be regarded as a spherical tensor with rank 1.

Given two spherical tensors $X_{q_1}^{(k_1)}$ and $Z_{q_2}^{(k_2)}$ with ranks k_1 and k_2, respectively, one can construct

$$T_q^{(k)} = \sum_{q_1=-k_1}^{k_1} \sum_{q_2=-k_2}^{k_2} C_{k_1 k_2; q_1 q_2}^{kq} \, X_{q_1}^{(k_1)} \, Z_{q_2}^{(k_2)}$$

which is a spherical tensor with rank k. Here $C_{k_1 k_2; q_1 q_2}^{kq}$ are the C-G coefficients.

IV. WIGNER-ECKART THEOREM FOR SPHERICAL TENSORS

First, it can be readily shown

$$\langle \alpha', j', m' | T_q^{(k)} | \alpha, j, m \rangle \propto \delta_{m', m+q}$$

which is the selection rule for spherical tensors.

The Wigner-Eckart Theorem states that the matrix elements of tensor operators w.r.t. angular-momentum eigenstates satisfy:

$$\langle \alpha', j', m' | T_q^{(k)} | \alpha, j, m \rangle = C_{jk;mq}^{j'm'} \, \frac{\langle \alpha', j' || T^{(k)} || \alpha, j \rangle}{\sqrt{2j+1}}$$

The denominator $\sqrt{2j+1}$ is the conventional normalization of the double-bar matrix element. The proof of this theorem is given in Sakurai.

The basic point of the WignerEckart theorem is that *the angular dependence of these matrix elements can be factored out, and it is given by the Clebsch-Gordan coefficients.* To evaluate $\langle \alpha', j', m' | T_q^{(k)} | \alpha, j, m \rangle$ with various combinations of m, m' and q (for a given set of α, α', j and j'), it is sufficient to know just of the them; all others can be related through the C-G coefficients!