Lecture 27, More on Tensor operators, Friday, Nov. 11

Direct (or tensor) product of spherical tensors:

If $X^{(k_1)}_{q_1}$ and $Z^{(k_2)}_{q_2}$ are spherical tensors of ranks k_1 and k_2 respectively, one can construct spherical tensors of ranks $k = k_1+k_2, k_1+k_2-1, ..., |k_1-k_2|$ by making the following product,

$$T^{(k)}_q = \sum_{q_1 q_2} \langle q_1 q_2 | kq \rangle X^{(k_1)}_{q_1} Z^{(k_2)}_{q_2} \tag{96}$$

where $\langle q_1 q_2 | kq \rangle$ is the Clebsch-Gordan coefficients to couple representations k_1 and k_2 to representation k.

Example, consider a rank-1 tensor operator $S^{(1)}$ which is a spin operator with,

$$\begin{aligned} S_\pm &= \mp(S_x \pm iS_y) \\ S_0 &= S_z \end{aligned} \tag{97}$$

which forms a 3D representation of SO(3). Consider another rank-1 tensor operator $r^{(1)}$ which is a position operator with,

$$\begin{aligned} r_\pm &= \mp(x \pm iy) \sim Y_{1\pm1} \\ r_0 &= S_z \sim Y_{10} \end{aligned} \tag{98}$$

which forms also a 3D representation of SO(3).

Since $3\times3 = 1+3+5$, let us consider first the scalar operator from the tensor product: Using the following CG coefficient (in the form of $\langle m_1 m_2 | jm \rangle$)

$$\langle 1-1|00\rangle = \frac{1}{\sqrt{3}}; \quad \langle 00|00\rangle = -\frac{1}{\sqrt{3}}; \quad \langle -11|00\rangle = \frac{1}{\sqrt{3}} \tag{99}$$

we have

$$(r^{(1)} \otimes S^{(1)})^{(0)} = (r_{+1}S_{-1} - r_0 S_0 + r_{-1}S_{+1})/\sqrt{3} = -\frac{\vec{r}\cdot\vec{S}}{\sqrt{3}} \tag{100}$$

For coupling to a rank-1 operator, we use the following CG coefficients,

$$\begin{aligned} \langle 10|11\rangle &= \frac{1}{\sqrt{2}}; \quad \langle 01|11\rangle = -\frac{1}{\sqrt{2}} \\ \langle 1-1|10\rangle &= \frac{1}{\sqrt{2}}; \quad \langle -11|10\rangle = -\frac{1}{\sqrt{2}} \\ \langle 0-1|1-1\rangle &= \frac{1}{\sqrt{2}}; \quad \langle -10|1-1\rangle = -\frac{1}{\sqrt{2}} \end{aligned} \tag{101}$$

We have then,

$$\begin{aligned}(r^{(1)} \otimes S^{(1)})_1^{(1)} &= (r_{+1}S_0 - r_0 S_{+1})/\sqrt{2} \\ (r^{(1)} \otimes S^{(1)})_0^{(1)} &= (r_{+1}S_{-1} - r_{-1}S_{+1})/\sqrt{2} \\ (r^{(1)} \otimes S^{(1)})_{-1}^{(1)} &= (r_0 S_{-1} - r_{-1}S_0)/\sqrt{2} \end{aligned} \tag{102}$$

Finally, for coupling to a rank-2 operator, we use the following CG coefficients,

$$\begin{aligned}\langle 11|22\rangle &= 1; \quad \langle -1-1|2-2\rangle = 1, \\ \langle \pm 10|2\pm 1\rangle &= 1/\sqrt{2}; \quad \langle 0\pm 1|2\pm 1\rangle = 1/\sqrt{2} \\ \langle 1-1|20\rangle &= 1/\sqrt{6}; \quad \langle 00|20\rangle = \sqrt{2/3}; \quad \langle -11|20\rangle = 1/\sqrt{6} \end{aligned} \tag{103}$$

We find,

$$\begin{aligned}(r^{(1)} \otimes S^{(1)})_{\pm 2}^{(2)} &= r_{\pm 1}S_{\pm 1} \\ (r^{(1)} \otimes S^{(1)})_{\pm 1}^{(2)} &= (r_{\pm 1}S_0 + r_0 S_{\pm 1})/\sqrt{2} \\ (r^{(1)} \otimes S^{(1)})_0^{(2)} &= (r_1 S_{-1} + 2r_0 S_0 + r_{-1}S_1)/\sqrt{6} \end{aligned} \tag{104}$$

Matrix elements of Tensor Operators:

Introducing spherical tensor operators is to simplify calculations of their matrix elements. In fact, the matrix element of a tensor operator, $\langle j'm'|T_q^{(k)}|jm\rangle$ is non-vanishing only when $m' = q + m$ and $|j - j'| \le k \le j + j'$. To see this, let us introduce the famous Wigner-Eckart theorem.

Wigner-Eckart theorem: The m dependence of the matrix element is entirely in the CG coefficients,

$$\langle \alpha' j' m'|T_q^{(k)}|\alpha jm\rangle = \langle mq|jm'\rangle \frac{\langle \alpha' j'||T^{(k)}||\alpha j\rangle}{\sqrt{2j+1}} \tag{105}$$

where the double-bar matrix element is just a notation for a quantity which depends only on j, j' and k, but not on the magnetic quantum numbers. α and α' are labels which have nothing to do with the SO(3) group. From the selection rules for the CG coefficients, we know that the matrix element is non-vanishing only when $m' = q + m$ and $|j - j'| \le k \le j + j'$.

Here is a heuristic way to think about the Wigner-Eckart theorem. Consider two vectors $\vec{a}$ and $\vec{b}$. If we know the product of the two vectors at one specific angle, we can calculate the product at any other angles:

$$\vec{a} \cdot \vec{b} = ab\cos\theta \tag{106}$$

where ab is like a reduced matrix element which depends on physics and $\cos\theta$ depending on the geometry.

Example: the matrix element of scalar operator $T_0^{(0)}$,

$$\langle j'm'|T_0^{(0)}|jm\rangle = \delta_{jj'}\delta_{mm'}\frac{\langle j'||T^{(0)}||j\rangle}{\sqrt{2j+1}} \tag{107}$$

which is non-vanishing only if the initial and final states have the same quantum numbers. For example, the matrix element r^2 (which is a rank-0 tensor operator) between $l = 1$ and $l = 2$ states in the hydrogen atom must vanish. So does $\vec{r}\cdot\vec{s}$, or any other scalar operator.

Another exmaple: the matrix element of electric dipole operator $\vec{d} = e\vec{r}$,

$$\langle j'm'|d_q^{(1)}|jm\rangle = \langle jm1q|j'm'\rangle\frac{\langle j'||d^{(1)}||j\rangle}{\sqrt{2j+1}} \tag{108}$$

which is non-vanishing only if $|j - j'| \le 1$ [there is no transition from $j = 0$ to $j' = 0$, however.] This is just the selection rule for dipole transitions of the electrons in atoms. The selection rule from parity conservation will be discussed later.

Quadrupole momentum of a system is defined as the matrix element of the sperical tensor of rank-2 Y_{2m}, or in cartesian coordinate, the traceless symmetric tensor

$$\hat{Q}_{ij} = 3x_ix_j - r^2\ . \tag{109}$$

More specifically, the quadrupole moment of a quantum state with total angular momentum j is the matrix element of $Q_{33} \sim Y_{20}$ in the state with maximum magnetic quantum number $j = m$

$$Q = e\langle\alpha jm = j|\hat{Q}_{33}|jm = j\rangle\ . \tag{110}$$

Clearly, a spin-1/2 particle cannot have non-vanishing quadrupole moment because coupling of 1/2 and 1/2 cannot produce 2. However, for a spin-1 particle, one can have a non-vanishing quadrupole moment. For example, the deuteron which is a bound state of a proton and a neutron has spin 1, and the system has a quadrupole moment 0.2859 e$\cdot$fm^2. For this reason, we say the deuteron is not spherically symmetric. Knowing Q, we can calculate the matrix element of $\hat{Q}_{33}$ in any other state. For example,

$$\langle 10|\hat{Q}_{33}|10\rangle = \frac{\langle 1020|10\rangle}{\langle 1120|11\rangle}Q$$

$$= \frac{-\sqrt{2/5}}{\sqrt{1/10}} Q = -2Q \qquad (111)$$

However, the deuteron cannot have an electric dipole momentum because of time-reversal symmetry as will be discussed later.