

Basic and useful formulas of Angular momentum algebra

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I. BASIC PROPERTIES OF 3J-SYMBOL

The relation between the Clebsch-Gordan's coefficient is

$$C_{j_1 m_1, j_2 m_2}^{j_3 m_3} = \langle j_1 m_1 : j_2 m_2 | j_3 m_3 \rangle = (-)^{-j_1+j_2-m_3} \hat{j}_3 \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix} \quad (1)$$

where $\hat{j} = \sqrt{2j+1}$

3j-symbol has a property as

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \quad (2)$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-)^{-j_1-j_2-j_3} \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} \quad (3)$$

$$= (-)^{-j_1-j_2-j_3} \begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix} \quad (4)$$

$$= (-)^{-j_1-j_2-j_3} \begin{pmatrix} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{pmatrix} \quad (5)$$

Note that this relation is correct for both the integer and half-integer j 's.

3j-symbol has the orthogonality shown as below

$$\sum_{j_3 m_3} \hat{j}_3^2 \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m'_1 & m'_2 & m_3 \end{pmatrix} = \delta_{m_1 m'_1} \delta_{m_2 m'_2} \quad (6)$$

$$\sum_{m_1 m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j'_3 \\ m_1 & m_2 & m'_3 \end{pmatrix} = \hat{j}_3^{-2} \delta_{j_3 j'_3} \delta_{m_3 m'_3} \delta(j_1, j_2, j_3) \quad (7)$$

where $\delta(j_1, j_2, j_3) = 1$ if j_1, j_2, j_3 satisfy the triangular condition.

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A. 3j-symbol and 6j-symbol

$$\sum_{\mu_1 \mu_2 \mu_3} (-1)^{l_1+l_2+l_3+\mu_1+\mu_2+\mu_3} \begin{pmatrix} j_1 & l_2 & l_3 \\ m_1 & \mu_2 & -\mu_3 \end{pmatrix} \begin{pmatrix} l_1 & j_2 & l_3 \\ -\mu_1 & m_2 & \mu_3 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & j_3 \\ \mu_1 & -\mu_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \left\{ \begin{matrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{matrix} \right\} \quad (8)$$

$$\sum_{\mu_3} (-1)^{l_1+l_2+l_3+\mu_1+\mu_2+\mu_3} \begin{pmatrix} j_1 & l_2 & l_3 \\ m_1 & \mu_2 & -\mu_3 \end{pmatrix} \begin{pmatrix} l_1 & j_2 & l_3 \\ -\mu_1 & m_2 & \mu_3 \end{pmatrix} = \sum_{j_3 m_3} \hat{j}_3^2 \begin{pmatrix} l_1 & l_2 & j_3 \\ \mu_1 & -\mu_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \left\{ \begin{matrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{matrix} \right\} \quad (9)$$

1. Useful formula

$$\begin{aligned} \begin{pmatrix} L & l' & l \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} j & j' & L \\ l' & l & \frac{1}{2} \end{matrix} \right\} &= (-1)^{j+j'} \left\{ 1 + (-1)^{L+l+l'} \right\} \begin{pmatrix} j & j' & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} l' & \frac{1}{2} & j' \\ 0 & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} l & \frac{1}{2} & j \\ 0 & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \\ &= \frac{-1}{\widehat{l}l'} \left\{ \frac{1 + (-1)^{L+l+l'}}{2} \right\} \begin{pmatrix} j & j' & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \\ &= \frac{(-1)^{j+j'}}{\widehat{l}l'\widehat{L}} \left\{ \frac{1 + (-1)^{L+l+l'}}{2} \right\} \langle j1/2; j' - 1/2 | L0 \rangle \end{aligned} \quad (10)$$

$$\begin{aligned} \begin{pmatrix} \lambda & l' & l'' \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} \lambda & l' & l'' \\ l & 1 & L \end{matrix} \right\} &= \sum_{\mu} (-1)^{l+1+L+\mu} \begin{pmatrix} \lambda & 1 & L \\ 0 & \mu & -\mu \end{pmatrix} \begin{pmatrix} l & l' & L \\ -\mu & 0 & \mu \end{pmatrix} \begin{pmatrix} l & 1 & l'' \\ \mu & -\mu & 0 \end{pmatrix} \\ &= (-1)^{L+l+1} \begin{pmatrix} \lambda & 1 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & 1 & l'' \\ 0 & 0 & 0 \end{pmatrix} \\ &\quad + (-1)^{L+l} \left\{ 1 + (-1)^{\lambda+l'+l''} \right\} \begin{pmatrix} \lambda & 1 & L \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} l & l' & L \\ -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} l & 1 & l'' \\ 1 & -1 & 0 \end{pmatrix} \end{aligned} \quad (11)$$

$$+ (-1)^{L+l} \left\{ 1 + (-1)^{\lambda+l'+l''} \right\} \begin{pmatrix} \lambda & 1 & L \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} l & l' & L \\ -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} l & 1 & l'' \\ 1 & -1 & 0 \end{pmatrix} \quad (12)$$

B. 3j-symbol and 9j-symbol

$$\begin{aligned}
& \sum_{JM} \hat{J}^2 \begin{pmatrix} J & j_{32} & j_{33} \\ M & m_{32} & m_{33} \end{pmatrix} \begin{pmatrix} j_{11} & j_{21} & J \\ m_{11} & m_{21} & M \end{pmatrix} \left\{ \begin{matrix} j_{11} & j_{12} & j_{13} \\ j_{21} & j_{22} & j_{23} \\ J & j_{32} & j_{33} \end{matrix} \right\} \\
&= \sum_{m_{12}m_{13}m_{22}m_{23}} \begin{pmatrix} j_{11} & j_{12} & j_{13} \\ m_{11} & \mathbf{m}_{12} & \mathbf{m}_{13} \end{pmatrix} \begin{pmatrix} j_{21} & j_{22} & j_{23} \\ m_{21} & \mathbf{m}_{22} & \mathbf{m}_{23} \end{pmatrix} \begin{pmatrix} j_{12} & j_{22} & j_{32} \\ \mathbf{m}_{12} & \mathbf{m}_{22} & m_{32} \end{pmatrix} \begin{pmatrix} j_{13} & j_{23} & j_{33} \\ \mathbf{m}_{13} & \mathbf{m}_{23} & m_{33} \end{pmatrix}
\end{aligned} \tag{13}$$

$$\begin{aligned}
& \sum_{JM,J'M'} \hat{J}^2 \hat{J}'^2 \begin{pmatrix} J & J' & j_{33} \\ M & M' & m_{33} \end{pmatrix} \begin{pmatrix} j_{11} & j_{21} & J \\ m_{11} & m_{21} & M \end{pmatrix} \begin{pmatrix} j_{12} & j_{22} & J' \\ m_{12} & m_{22} & M' \end{pmatrix} \left\{ \begin{matrix} j_{11} & j_{12} & j_{13} \\ j_{21} & j_{22} & j_{23} \\ J & J' & j_{33} \end{matrix} \right\} \\
&= \sum_{m_{13}m_{23}} \begin{pmatrix} j_{11} & j_{12} & j_{13} \\ m_{11} & m_{12} & \mathbf{m}_{13} \end{pmatrix} \begin{pmatrix} j_{21} & j_{22} & j_{23} \\ m_{21} & m_{22} & \mathbf{m}_{23} \end{pmatrix} \begin{pmatrix} j_{13} & j_{23} & j_{33} \\ \mathbf{m}_{13} & \mathbf{m}_{23} & m_{33} \end{pmatrix}
\end{aligned} \tag{14}$$

C. Special properties of 3j-symbol

$$\begin{pmatrix} j & j & 0 \\ m & -m & 0 \end{pmatrix} = \frac{(-)^{j-m}}{\hat{j}} \tag{15}$$

$$\sum_m (-)^m \begin{pmatrix} j & j & L \\ m & -m & M \end{pmatrix} = (-)^j \hat{j} \delta_{L0} \delta_{M0} \tag{16}$$

$$\frac{1 + (-)^{l+l'+L}}{2} \sqrt{l(l+1)} \begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix} = \frac{l'(l'+1) - l(l+1) - L(L+1)}{2\sqrt{L(L+1)}} \begin{pmatrix} l' & l & L \\ 0 & 0 & 0 \end{pmatrix} \quad \text{If } L \neq 0. \tag{17}$$

$$\begin{pmatrix} 1 & l & l'' \\ 0 & 0 & 0 \end{pmatrix} = \delta_{l'',l+1} (-)^{l+1} \hat{l}''^{-1} \sqrt{\frac{l+1}{2l+1}} + \delta_{l'',l-1} (-)^l \hat{l}''^{-1} \sqrt{\frac{l}{2l+1}} \tag{18}$$

$$(-)^L \hat{L} \begin{pmatrix} L+1 & 1 & L \\ -q & q & 0 \end{pmatrix} = (-)^L \hat{L} \begin{pmatrix} L+1 & L & 1 \\ -q & 0 & q \end{pmatrix} = \begin{cases} (q = \pm 1) & (-)^L \hat{L} \begin{pmatrix} L+1 & L & 1 \\ -1 & 0 & 1 \end{pmatrix} = \sqrt{\frac{L+2}{2(2L+3)}} \\ (q = 0) & (-)^L \hat{L} \begin{pmatrix} L+1 & L & 1 \\ 0 & 0 & 0 \end{pmatrix} = -\sqrt{\frac{L+1}{2L+3}} \end{cases} \tag{19}$$

$$(-)^L \hat{L} \begin{pmatrix} L-1 & 1 & L \\ -q & q & 0 \end{pmatrix} = (-)^L \hat{L} \begin{pmatrix} L & L-1 & 1 \\ 0 & -q & q \end{pmatrix} = \begin{cases} (q = \pm 1) & (-)^L \hat{L} \begin{pmatrix} L & L-1 & 1 \\ 0 & -1 & 1 \end{pmatrix} = \sqrt{\frac{L-1}{2(2L-1)}} \\ (q = 0) & (-)^L \hat{L} \begin{pmatrix} L & L-1 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \sqrt{\frac{L}{2L-1}} \end{cases} \tag{20}$$

D. Special properties of 6j-symbol

$$\left\{ \begin{matrix} 1 & l'' & l \\ l & 1 & 1 \end{matrix} \right\} = \delta_{l'', l+1} \widehat{l}^{-1} \frac{l}{\sqrt{6l(l+1)}} - \delta_{l'', l-1} \widehat{l}^{-1} \frac{l+1}{\sqrt{6l(l+1)}} \quad (21)$$

$$\left\{ \begin{matrix} l & l & 1 \\ 1/2 & 1/2 & j \end{matrix} \right\} = (-)^{j+l+1/2} \frac{j(j+1) - l(l+1) - 3/4}{\widehat{l} \sqrt{6l(l+1)}} \quad (22)$$

$$\left\{ \begin{matrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & 0 \end{matrix} \right\} = \frac{(-)^{j_1+j_2+j_3}}{\widehat{j_1} \widehat{j_2}} \delta_{j_1 j_5} \delta_{j_2 j_4} \quad (23)$$

$$\sum_j (-)^{j+j'+j''} \widehat{j}^2 \left\{ \begin{matrix} j_1 & j_2 & j' \\ j_3 & j_4 & j \end{matrix} \right\} \left\{ \begin{matrix} j_1 & j_3 & j'' \\ j_2 & j_4 & j \end{matrix} \right\} = \left\{ \begin{matrix} j_1 & j_2 & j' \\ j_4 & j_3 & j'' \end{matrix} \right\} \quad (24)$$

$$\sum_j \widehat{j}^2 \left\{ \begin{matrix} j_1 & j_2 & j' \\ j_3 & j_4 & j \end{matrix} \right\} \left\{ \begin{matrix} j_1 & j_2 & j'' \\ j_3 & j_4 & j \end{matrix} \right\} = \frac{\delta_{j' j''}}{\widehat{j}^2} \delta(j_1, j_2, j') \delta(j_3, j_4, j'') \quad (25)$$

1. 6j-symbol and 9j-symbol in special case

$$\left\{ \begin{matrix} a & b & c \\ d & e & f \\ g & h & 0 \end{matrix} \right\} = \delta_{cf} \delta_{gh} \frac{(-)^{b+c+d+g}}{\sqrt{(2c+1)(2g+1)}} \left\{ \begin{matrix} a & b & c \\ e & d & g \end{matrix} \right\} \quad (26)$$

$$\left\{ \begin{matrix} j & 1 & \lambda \\ j' & 1 & \lambda' \\ J & 0 & L \end{matrix} \right\} = - \frac{(-)^{j+\lambda'+L}}{\sqrt{3}} \frac{\delta_{J,L}}{\widehat{L}} \left\{ \begin{matrix} j & \lambda & 1 \\ \lambda' & j' & L \end{matrix} \right\} \quad (27)$$

$$\left\{ \begin{matrix} j & \frac{1}{2} & l \\ j & \frac{1}{2} & l \\ J & 1 & 0 \end{matrix} \right\} = \delta_{J,1} \left\{ \begin{matrix} j & \frac{1}{2} & l \\ j & \frac{1}{2} & l \\ 1 & 1 & 0 \end{matrix} \right\} \quad (28)$$

$$\left\{ \begin{matrix} a & b & c \\ d & e & c \\ g & g & 1 \end{matrix} \right\} = \frac{a(a+1) + e(e+1) - d(d+1) - b(b+1)}{2\sqrt{c(c+1)g(g+1)}} \left\{ \begin{matrix} a & b & c \\ d & e & c \\ g & g & 0 \end{matrix} \right\} \quad (29)$$

$$= (-)^{b+c+d+g} \frac{a(a+1) + e(e+1) - d(d+1) - b(b+1)}{2\sqrt{c(c+1)(2c+1)g(g+1)(2g+1)}} \left\{ \begin{matrix} a & b & c \\ e & d & g \end{matrix} \right\} \quad (30)$$

II. SPHERICAL HARMONICS

The most important and often used formula of the spherical harmonics is

$$Y_{lm_l}(\hat{\mathbf{r}})Y_{l'm'_l}^*(\hat{\mathbf{r}}) = \sum_{LM} (-)^{m'_l} \frac{\widehat{l'l'}\widehat{L}}{\sqrt{4\pi}} \begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l' & L & l \\ -m'_l & M & m_l \end{pmatrix} Y_{LM}^*(\hat{\mathbf{r}}) \quad (31)$$

$$= \sum_{LM} \langle l' || Y_L || l \rangle (-)^{l'-m'_l} \begin{pmatrix} l' & L & l \\ -m'_l & M & m_l \end{pmatrix} Y_{LM}^*(\hat{\mathbf{r}}) \quad (32)$$

$$\sum_{m_l} Y_{lm_l}(\hat{\mathbf{r}})Y_{lm_l}^*(\hat{\mathbf{r}}') = \frac{2l+1}{4\pi} P_l(\cos \theta) \quad \text{where } \theta \text{ is the relative angle between } \hat{\mathbf{r}} \text{ and } \hat{\mathbf{r}}'. \quad (33)$$

In case $\hat{\mathbf{r}} = \hat{\mathbf{r}}'$,

$$\sum_{m_l} Y_{lm_l}(\hat{\mathbf{r}})Y_{lm_l}^*(\hat{\mathbf{r}}) = \frac{\widehat{l}^2}{4\pi} P_l(1) = \frac{2l+1}{4\pi} \quad (34)$$

A. Spin-function: $S = \frac{1}{2}$

The spin function $\chi_{\frac{1}{2}m_s}(\sigma)$ satisfies the following properties,

$$\sum_{m_s} \chi_{\frac{1}{2}m_s}(\sigma')\chi_{\frac{1}{2}m_s}^\dagger(\sigma) = \delta_{\sigma\sigma'}, \quad \sum_{\sigma} \chi_{\frac{1}{2}m_s}^\dagger(\sigma)\chi_{\frac{1}{2}m'_s}(\sigma) = \delta_{m_sm'_s} \quad (35)$$

$$\chi_{\frac{1}{2}m_s}(\sigma)\chi_{\frac{1}{2}m'_s}^\dagger(\sigma') = \frac{1}{2}\delta_{m_sm'_s}\langle\sigma|\sigma'\rangle + \frac{1}{2}(-)^{\frac{1}{2}-m'_s} \left\langle \frac{1}{2} || \sigma || \frac{1}{2} \right\rangle \sum_{\mu} \begin{pmatrix} \frac{1}{2} & 1 & \frac{1}{2} \\ -m'_s & \mu & m_s \end{pmatrix} (-)^{\mu} \langle \sigma | \sigma_{-\mu} | \sigma' \rangle \quad (36)$$

$$\text{where } \left\langle \frac{1}{2} || \sigma || \frac{1}{2} \right\rangle = \sqrt{6} \quad (37)$$

B. Spin-spherical harmonics

Coupling with the spin wave function, the so-called spin-spherical harmonics is defined by

$$\mathcal{Y}_{lm}(\hat{\mathbf{r}}\sigma) = \sum_{m_l, m_s} \langle lm_l : \frac{1}{2}m_s | jm \rangle \chi_{\frac{1}{2}m_s}(\sigma) Y_{lm_l}(\hat{\mathbf{r}}) \quad (38)$$

$$\mathcal{Y}_{lm}^*(\hat{\mathbf{r}}\sigma) = (-)^{l+1/2+j+m} \mathcal{Y}_{l-j-m}(\hat{\mathbf{r}}\sigma) \quad (39)$$

$$\begin{aligned} \mathcal{Y}_{lm}(\hat{\mathbf{r}}\sigma)\mathcal{Y}_{l'j'm'}^*(\hat{\mathbf{r}}\sigma') &= \frac{1}{2}\langle\sigma|\sigma'\rangle \sum_{LM} \langle l'j' || Y_L || lj \rangle (-)^{j'-m'} \begin{pmatrix} j' & L & j \\ -m' & M & m \end{pmatrix} Y_{LM}^*(\hat{\mathbf{r}}) \\ &+ \frac{1}{2}\langle\sigma|\sigma|\sigma'\rangle \cdot \sum_{L, JM_J} \langle l'j' || \mathbf{Y}_{JL} \cdot \boldsymbol{\sigma} || lj \rangle (-)^{j'-m'} \begin{pmatrix} j' & J & j \\ -m' & M_J & m \end{pmatrix} \mathbf{Y}_{JLM_J}^*(\hat{\mathbf{r}}) \end{aligned} \quad (40)$$

$$\begin{aligned} &= \frac{1}{2}\langle\sigma|\sigma'\rangle \sum_{LM} \langle l'j' || Y_L || lj \rangle (-)^{j'-m'} \begin{pmatrix} j' & L & j \\ -m' & M & m \end{pmatrix} Y_{LM}^*(\hat{\mathbf{r}}) \\ &+ \frac{1}{2} \sum_{L, JM_J, \mu} \langle l'j' || \mathbf{Y}_{JL} \cdot \boldsymbol{\sigma} || lj \rangle (-)^{j'-m'} \begin{pmatrix} j' & J & j \\ -m' & M_J & m \end{pmatrix} \\ &\quad \times \widehat{J}(-)^{J-M_J} \begin{pmatrix} J & L & 1 \\ -M_J & M & \mu \end{pmatrix} (-)^{\mu} \langle \sigma | \sigma_{-\mu} | \sigma' \rangle Y_{LM}^* \end{aligned} \quad (41)$$

C. Special application of the sphrical harmonics

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_l i^l j_l(kr) \sum_m Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}) \quad (42)$$

$$\delta(\mathbf{r}_1 - \mathbf{r}_2) = \frac{\delta(r_1 - r_2)}{r_1^2} \sum_m Y_{lm}^*(\hat{\mathbf{r}}_1) Y_{lm}(\hat{\mathbf{r}}_2) \quad (43)$$

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_l \frac{r_{<}^l}{r_{>}^{l+1}} P_l(\cos \theta) \quad (44)$$

$$= \sum_l \frac{r_{<}^l}{r_{>}^{l+1}} \frac{4\pi}{2l+1} \sum_m Y_{lm}^*(\hat{\mathbf{r}}_1) Y_{lm}(\hat{\mathbf{r}}_2) \quad (45)$$

$$\frac{e^{-\alpha|\mathbf{r}_1 - \mathbf{r}_2|}}{\alpha|\mathbf{r}_1 - \mathbf{r}_2|} = -4\pi \sum_l j_l(i\alpha r_{<}) h_l^{(1)}(i\alpha r_{>}) \sum_m Y_{lm}^*(\hat{\mathbf{r}}_1) Y_{lm}(\hat{\mathbf{r}}_2) \quad (46)$$

D. Matrix element of the angular momentum operator

$$\langle j'm' | J_\mu | jm \rangle = \delta_{j'j} (-)^{-j+1-m'} \hat{j} \sqrt{j(j+1)} \begin{pmatrix} j' & 1 & j \\ m' & -\mu & -m \end{pmatrix} \quad (47)$$

$$\leftrightarrow J_\mu Y_{jm} = \delta_{j'j} (-)^{-j+1-m'} \hat{j} \sqrt{j(j+1)} \begin{pmatrix} j' & 1 & j \\ m' & -\mu & -m \end{pmatrix} Y_{j'm'} \quad (48)$$

$$\langle \frac{1}{2}m'_s | \sigma_\mu | \frac{1}{2}m_s \rangle = (-)^{\frac{1}{2}-m'_s} \sqrt{6} \begin{pmatrix} \frac{1}{2} & 1 & \frac{1}{2} \\ m'_s & -\mu & -m_s \end{pmatrix} \quad (49)$$

$$\langle \frac{1}{2}m'_s | S_\mu | \frac{1}{2}m_s \rangle = (-)^{\frac{1}{2}-m'_s} \sqrt{\frac{3}{2}} \begin{pmatrix} \frac{1}{2} & 1 & \frac{1}{2} \\ m'_s & -\mu & -m_s \end{pmatrix} \quad (50)$$

where σ_μ is the Pauli's matrix, $S_\mu = \frac{1}{2}\sigma_\mu$.

III. VECTOR SPHERICAL HARMONICS

A. Spherical coordinate system

First of all, the spherical unit vector is defined as

$$\mathbf{e}_0 = \mathbf{e}_z \quad (51)$$

$$\mathbf{e}_{\pm 1} = \mp \frac{1}{\sqrt{2}} (\mathbf{e}_x \pm i\mathbf{e}_y) \quad (52)$$

$$(53)$$

These vectors are associated a radial unit vector $\hat{\mathbf{r}} = \frac{\mathbf{r}}{r}$ as

$$\begin{aligned} \hat{\mathbf{r}} &= \frac{\mathbf{r}}{r} \\ &= \sum_{\mu=0,\pm 1} \mathbf{e}_\mu^* \sqrt{\frac{4\pi}{3}} Y_{1\mu} \end{aligned} \quad (54)$$

The spherical unit vector has some properties

$$\mathbf{e}_\mu^* = (-)^{\mu} \mathbf{e}_{-\mu}, \quad \mathbf{e}_\mu^* \cdot \mathbf{e}_\nu = \delta_{\mu\nu} \quad (55)$$

$$\mathbf{e}_\mu \times \mathbf{e}_\nu = i\sqrt{2} \langle 1\mu : 1\nu | 1\mu + \nu \rangle \mathbf{e}_{\mu+\nu} \quad (56)$$

$$= i\sqrt{6} \begin{pmatrix} 1 & 1 & 1 \\ \mu & \nu & -\mu - \nu \end{pmatrix} \mathbf{e}_{-\mu-\nu}^* \quad (57)$$

A vector $\mathbf{A}$ is represented by using the spherical unit vector $\mathbf{e}_\mu$ as

$$\mathbf{A} = \sum_{i=x,y,z} A_i \mathbf{e}_i = \sum_{\mu=0,\pm 1} A_\mu \mathbf{e}_\mu^*, \quad A_\mu = \mathbf{e}_\mu \cdot \mathbf{A} \quad (58)$$

Inner product and vector product are described as

$$\mathbf{A} \cdot \mathbf{B} = \sum_{\mu} (-)^{\mu} A_\mu B_{-\mu} \quad (59)$$

$$\mathbf{A} \times \mathbf{B} = \sum_{\mu\nu} (-)^{\mu+\nu} i\sqrt{6} \begin{pmatrix} 1 & 1 & 1 \\ -\mu & -\nu & \mu + \nu \end{pmatrix} A_\mu B_\nu \mathbf{e}_{\mu+\nu}^* \quad (60)$$

$$(\mathbf{A} \times \mathbf{B})_\lambda = \mathbf{e}_\lambda \cdot (\mathbf{A} \times \mathbf{B}) \quad (61)$$

$$= \sum_{\mu\nu} (-)^{\lambda} i\sqrt{6} \begin{pmatrix} 1 & 1 & 1 \\ -\mu & -\nu & \lambda \end{pmatrix} A_\mu B_\nu \quad (62)$$

B. Vector spherical harmonics

The vector spherical harmonics is a kind of the spherical harmonics coupled with the spherical unit vector as

$$\mathbf{Y}_{L\lambda M}(\hat{\mathbf{r}}) = \sum_{m_\lambda, q} \langle \lambda m_\lambda : 1q | LM \rangle \mathbf{e}_q Y_{\lambda m_\lambda}(\hat{\mathbf{r}}) \quad (63)$$

$$= \sum_{m_\lambda, q} (-)^{-\lambda+1-M} \hat{L} \begin{pmatrix} \lambda & 1 & L \\ m_\lambda & q & -M \end{pmatrix} \mathbf{e}_q Y_{\lambda m_\lambda}(\hat{\mathbf{r}}) \quad (64)$$

$$\mathbf{Y}_{L\lambda M}^*(\hat{\mathbf{r}}) = (-)^{L+\lambda+1+M} \mathbf{Y}_{L\lambda-M}(\hat{\mathbf{r}}) \quad (65)$$

In case $M = 0, \lambda = L \pm 1$, the vector spherical harmonics is represented as

$$\mathbf{Y}_{L\lambda 0}(\hat{\mathbf{r}}) = \sum_q (-)^L \hat{L} \begin{pmatrix} \lambda & 1 & L \\ -q & q & 0 \end{pmatrix} \mathbf{e}_q Y_{\lambda-q}(\hat{\mathbf{r}}) \quad (66)$$

$$= (-)^L \hat{L} \begin{pmatrix} \lambda & 1 & L \\ -1 & 1 & 0 \end{pmatrix} (\mathbf{e}_{+1} Y_{\lambda-1}(\hat{\mathbf{r}}) + \mathbf{e}_{-1} Y_{\lambda+1}(\hat{\mathbf{r}})) + (-)^L \hat{L} \begin{pmatrix} \lambda & 1 & L \\ 0 & 0 & 0 \end{pmatrix} \mathbf{e}_0 Y_{\lambda 0}(\hat{\mathbf{r}}) \quad (67)$$

Therefore

$$\mathbf{e}_x \cdot \mathbf{Y}_{L\lambda 0}(\hat{\mathbf{r}}) = \frac{1}{\sqrt{2}} (\mathbf{e}_{-1}^* - \mathbf{e}_{+1}^*) \cdot \mathbf{Y}_{L\lambda 0}(\hat{\mathbf{r}}) \quad (68)$$

$$= \frac{1}{\sqrt{2}} (-)^L \hat{L} \begin{pmatrix} \lambda & 1 & L \\ -1 & 1 & 0 \end{pmatrix} (Y_{\lambda+1}(\hat{\mathbf{r}}) - Y_{\lambda-1}(\hat{\mathbf{r}})) \quad (69)$$

$$= \begin{cases} (\lambda = L+1) & \frac{1}{2} \sqrt{\frac{L+2}{2L+3}} (Y_{\lambda+1}(\hat{\mathbf{r}}) - Y_{\lambda-1}(\hat{\mathbf{r}})) \\ (\lambda = L-1) & \frac{1}{2} \sqrt{\frac{L-1}{2L-1}} (Y_{\lambda+1}(\hat{\mathbf{r}}) - Y_{\lambda-1}(\hat{\mathbf{r}})) \end{cases} \quad (70)$$

$$\mathbf{e}_z \cdot \mathbf{Y}_{L\lambda 0}(\hat{\mathbf{r}}) = \mathbf{e}_0 \cdot \mathbf{Y}_{L\lambda 0}(\hat{\mathbf{r}}) = (-)^L \hat{L} \begin{pmatrix} \lambda & 1 & L \\ 0 & 0 & 0 \end{pmatrix} Y_{\lambda 0}(\hat{\mathbf{r}}) \quad (71)$$

$$= \begin{cases} (\lambda = L+1) & -\sqrt{\frac{L+1}{2L+3}} Y_{\lambda 0}(\hat{\mathbf{r}}) \\ (\lambda = L-1) & \sqrt{\frac{L}{2L-1}} Y_{\lambda 0}(\hat{\mathbf{r}}) \end{cases} \quad (72)$$

$$\begin{aligned} & \mathbf{Y}_{L\lambda M}(\hat{\mathbf{r}}) \cdot \mathbf{Y}_{L'\lambda' M'}(\hat{\mathbf{r}}) \\ &= \sum_{L'' M''} (-)^{L+\lambda} \frac{\hat{L} \hat{L}' \hat{\lambda} \hat{\lambda}' \hat{L}''}{\sqrt{4\pi}} \begin{pmatrix} \lambda & \lambda' & L'' \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} L & L' & L'' \\ \lambda' & \lambda & 1 \end{matrix} \right\} \begin{pmatrix} L & L' & L'' \\ M & M' & M'' \end{pmatrix} Y_{L'' M''}^*(\hat{\mathbf{r}}) \end{aligned} \quad (73)$$

$$\begin{aligned} & Y_{l' m'_l}^*(\hat{\mathbf{r}}) Y_{l'' m''_l}(\hat{\mathbf{r}}) \\ &= \sum_{L J M_J} (-)^{J+L} \frac{\hat{l} \hat{l}' \hat{l}'' \hat{L} \hat{J}}{\sqrt{4\pi}} \begin{pmatrix} l'' & l' & L \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} 1 & L & J \\ l' & l & l'' \end{matrix} \right\} (-)^{m'_l} \begin{pmatrix} l' & J & l \\ -m'_l & M_J & m_l \end{pmatrix} \mathbf{Y}_{J L M_J}^*(\hat{\mathbf{r}}) \end{aligned} \quad (74)$$

$$\mathbf{J} Y_{jm} = \sum_{\mu} \mathbf{e}_{\mu}^* J_{\mu} Y_{jm} = \sum_{\mu, m'} (-)^{-j+1-m} \hat{j} \sqrt{j(j+1)} \begin{pmatrix} j & 1 & j \\ m' & \mu & -m \end{pmatrix} \mathbf{e}_{\mu} Y_{jm'} = \sqrt{j(j+1)} \mathbf{Y}_{jjm} \quad (75)$$

C. Gradient formula

$$\nabla Y_{lm} f_l(r) = \left[\hat{\mathbf{r}} \frac{\partial}{\partial r} - i \frac{\hat{\mathbf{r}} \times \mathbf{l}}{r} \right] Y_{lm} f_l(r) \quad (76)$$

$$= \sum_{\eta=l\pm1} (-)^l \hat{\eta} \begin{pmatrix} 1 & l & \eta \\ 0 & 0 & 0 \end{pmatrix} \mathbf{Y}_{l\eta m} \left[\frac{\partial}{\partial r} - \hat{l} \sqrt{6l(l+1)} \left\{ \begin{matrix} 1 & \eta & l \\ l & 1 & 1 \end{matrix} \right\} \frac{1}{r} \right] f_l(r) \quad (77)$$

Note that

$$(-)^l \hat{\eta} \begin{pmatrix} 1 & l & \eta \\ 0 & 0 & 0 \end{pmatrix} = -\delta_{\eta,l+1} \sqrt{\frac{l+1}{2l+1}} + \delta_{\eta,l-1} \sqrt{\frac{l}{2l+1}} = \frac{(-)^{\frac{1}{2}(\eta-l+1)}}{\hat{l}} \sqrt{\frac{\eta+l+1}{2}} \quad (78)$$

$$\hat{l} \sqrt{6l(l+1)} \left\{ \begin{matrix} 1 & \eta & l \\ l & 1 & 1 \end{matrix} \right\} = \delta_{\eta,l+1} l - \delta_{\eta,l-1} (l+1) = (-)^{\frac{1}{2}(l+1-\eta)} \frac{3l+1-\eta}{2} \quad (79)$$

Therefore finally one can get

$$\vec{\nabla} Y_{lm} f_l(r) = \sum_{\eta=l\pm1} \frac{(-)^{\frac{1}{2}(\eta-l+1)}}{\hat{l}} \sqrt{\frac{\eta+l+1}{2}} \mathbf{Y}_{l\eta m} \left[\frac{\vec{\partial}}{\partial r} - (-)^{\frac{1}{2}(l+1-\eta)} \left(\frac{3l+1-\eta}{2} \right) \frac{1}{r} \right] f_l(r) \quad (80)$$

1. special case of the gradient formula

As an application of the gradient formula...

$$\begin{aligned} \nabla e^{+i\mathbf{k}\mathbf{r}} &= 4\pi \sum_{lm} i^l Y_{lm}^*(\hat{\mathbf{k}}) \nabla Y_{lm}(\hat{\mathbf{r}}) j_l(kr) \\ &= 4\pi \sum_{lm} i^l Y_{lm}^*(\hat{\mathbf{k}}) \left[-\sqrt{\frac{l+1}{2l+1}} \mathbf{Y}_{l+1m}(\hat{\mathbf{r}}) \left(\frac{\partial j_l(kr)}{\partial r} - \frac{l}{r} j_l(kr) \right) \right. \\ &\quad \left. + \sqrt{\frac{l}{2l+1}} \mathbf{Y}_{l-1m}(\hat{\mathbf{r}}) \left(\frac{\partial j_l(kr)}{\partial r} + \frac{l+1}{r} j_l(kr) \right) \right] \end{aligned} \quad (81)$$

(Using the recursion formula of the spherical Bessel function,)

$$= 4\pi k \sum_{lm} i^l Y_{lm}^*(\hat{\mathbf{k}}) \left[\sqrt{\frac{l+1}{2l+1}} \mathbf{Y}_{l+1m}(\hat{\mathbf{r}}) j_{l+1}(kr) + \sqrt{\frac{l}{2l+1}} \mathbf{Y}_{l-1m}(\hat{\mathbf{r}}) j_{l-1}(kr) \right] \quad (82)$$

Where the recursion formula of the spherical Bessel function is given by

$$\left(\frac{\partial}{\partial r} - \frac{l}{r} \right) j_l(kr) = -k j_{l+1}(kr) \quad (83)$$

$$\left(\frac{\partial}{\partial r} + \frac{l+1}{r} \right) j_l(kr) = k j_{l-1}(kr) \quad (84)$$

By applying the following formula to Eq.(82)

$$\begin{aligned} \sum_m Y_{lm}^*(\hat{\mathbf{k}}) \mathbf{Y}_{l+1m}(\hat{\mathbf{r}}) &= \sum_{m,n,q} Y_{lm}^*(\hat{\mathbf{k}}) \left[(-)^{-l-m} \sqrt{2l+1} \begin{pmatrix} l+1 & 1 & l \\ n & q & -m \end{pmatrix} e_q Y_{l+1,n}(\hat{\mathbf{r}}) \right] \\ &= \sum_n (-)^{n+1} \sqrt{\frac{2l+1}{2l+3}} \left[\sum_{m,q} (-)^{-l+1+n} \sqrt{2l+3} \begin{pmatrix} l & 1 & l+1 \\ -m & q & n \end{pmatrix} e_q Y_{l,-m}(\hat{\mathbf{k}}) \right] Y_{l+1,n}(\hat{\mathbf{r}}) \\ &= -\sum_n \sqrt{\frac{2l+1}{2l+3}} \mathbf{Y}_{l+1,l,n}(\hat{\mathbf{k}}) Y_{l+1,n}^*(\hat{\mathbf{r}}) \end{aligned} \quad (85)$$

$$\begin{aligned}
\sum_m Y_{lm}^*(\hat{\mathbf{k}}) Y_{l-1m}(\hat{\mathbf{r}}) &= \sum_{m,n,q} Y_{lm}^*(\hat{\mathbf{k}}) \left[(-)^{-l-m} \sqrt{2l+1} \begin{pmatrix} l-1 & 1 & l \\ n & q & -m \end{pmatrix} \mathbf{e}_q Y_{l-1,n}(\hat{\mathbf{r}}) \right] \\
&= \sum_n (-)^{n+1} \sqrt{\frac{2l+1}{2l-1}} \left[\sum_{m,q} (-)^{-l+1+n} \sqrt{2l-1} \begin{pmatrix} l & 1 & l-1 \\ -m & q & n \end{pmatrix} \mathbf{e}_q Y_{l,-m}(\hat{\mathbf{k}}) \right] Y_{l-1,n}(\hat{\mathbf{r}}) \\
&= - \sum_n \sqrt{\frac{2l+1}{2l-1}} Y_{l-1,l,n}(\hat{\mathbf{k}}) Y_{l-1,n}^*(\hat{\mathbf{r}})
\end{aligned} \tag{86}$$

we get

$$\begin{aligned}
\nabla e^{+i\mathbf{k}\mathbf{r}} &= -4\pi k \sum_{lm} i^l \left[\sqrt{\frac{l+1}{2l+3}} Y_{l+1,l,m}(\hat{\mathbf{k}}) Y_{l+1,m}^*(\hat{\mathbf{r}}) j_{l+1}(kr) + \sqrt{\frac{l}{2l-1}} Y_{l-1,l,m}(\hat{\mathbf{k}}) Y_{l-1,m}^*(\hat{\mathbf{r}}) j_{l-1}(kr) \right] \\
&\quad (l \rightarrow l-1 \text{ and } l \rightarrow l+1 \text{ for the 1st and 2nd terms, respectively.}) \\
&= 4\pi k \sum_{lm} i^{l+1} \left[\sqrt{\frac{l}{2l+1}} Y_{l,l-1,m}(\hat{\mathbf{k}}) - \sqrt{\frac{l+1}{2l+1}} Y_{l,l+1,m}(\hat{\mathbf{k}}) \right] Y_{l,m}^*(\hat{\mathbf{r}}) j_l(kr)
\end{aligned} \tag{87}$$

Using the formula,

$$\hat{\mathbf{k}} Y_{lm}(\hat{\mathbf{k}}) = \sqrt{\frac{l}{2l+1}} Y_{l,l-1,m}(\hat{\mathbf{k}}) - \sqrt{\frac{l+1}{2l+1}} Y_{l,l+1,m}(\hat{\mathbf{k}}) \tag{88}$$

finally we can obtain

$$\nabla e^{+i\mathbf{k}\mathbf{r}} = ik \hat{\mathbf{k}} 4\pi \sum_{lm} i^l Y_{lm}(\hat{\mathbf{k}}) Y_{l,m}^*(\hat{\mathbf{r}}) j_l(kr) = i\mathbf{k} e^{+i\mathbf{k}\mathbf{r}} \tag{89}$$

If we choose $\hat{\mathbf{k}} = \mathbf{e}_z$, i.e. $\theta_k = \varphi_k = 0$, then we have

$$Y_{lm}(\hat{\mathbf{k}}) = Y_{lm}(\mathbf{e}_z) = \sqrt{\frac{2l+1}{4\pi}} \delta_{m0}. \tag{90}$$

With this condition, Eqs.(85) and (86) become

$$\begin{aligned}
\sum_m Y_{lm}^*(\hat{\mathbf{k}}) Y_{l+1m}(\hat{\mathbf{r}}) &= \sum_{q=0,\pm 1} \sqrt{\frac{2l+1}{4\pi}} \left[(-)^{-l} \sqrt{2l+1} \begin{pmatrix} l+1 & 1 & l \\ -q & q & 0 \end{pmatrix} \mathbf{e}_q Y_{l+1,-q}(\hat{\mathbf{r}}) \right] \\
&= -\sqrt{\frac{2l+1}{4\pi(2l+3)}} \left[\sqrt{l+1} \mathbf{e}_0 Y_{l+1,0}(\hat{\mathbf{r}}) + \sqrt{\frac{l+2}{2}} (\mathbf{e}_{+1}^* Y_{l+1,1}(\hat{\mathbf{r}}) + \mathbf{e}_{+1} Y_{l+1,1}^*(\hat{\mathbf{r}})) \right]
\end{aligned} \tag{91}$$

$$\begin{aligned}
\sum_m Y_{lm}^*(\hat{\mathbf{k}}) Y_{l-1m}(\hat{\mathbf{r}}) &= \sum_{q=0,\pm 1} \sqrt{\frac{2l+1}{4\pi}} \left[(-)^{-l} \sqrt{2l+1} \begin{pmatrix} l-1 & 1 & l \\ -q & q & 0 \end{pmatrix} \mathbf{e}_q Y_{l-1,-q}(\hat{\mathbf{r}}) \right] \\
&= \sqrt{\frac{2l+1}{4\pi(2l-1)}} \left[\sqrt{l} \mathbf{e}_0 Y_{l-1,0}(\hat{\mathbf{r}}) - \sqrt{\frac{l-1}{2}} (\mathbf{e}_{+1} Y_{l-1,1}^*(\hat{\mathbf{r}}) + \mathbf{e}_{+1}^* Y_{l-1,1}(\hat{\mathbf{r}})) \right]
\end{aligned} \tag{92}$$

Therefore we can obtain

$$e^{+i\mathbf{k}\mathbf{r}} = 4\pi \sum_l i^l \sqrt{\frac{2l+1}{4\pi}} Y_{l0}(\hat{\mathbf{r}}) j_l(kr) \tag{93}$$

$$\begin{aligned}
\nabla e^{+i\mathbf{k}\mathbf{r}} &= 4\pi k \sum_l i^l \left[-\sqrt{\frac{l+1}{4\pi(2l+3)}} \left\{ \sqrt{l+1} \mathbf{e}_0 Y_{l+1,0}(\hat{\mathbf{r}}) + \sqrt{\frac{l+2}{2}} (\mathbf{e}_{+1}^* Y_{l+1,1}(\hat{\mathbf{r}}) + \mathbf{e}_{+1} Y_{l+1,1}^*(\hat{\mathbf{r}})) \right\} j_{l+1}(kr) \right. \\
&\quad \left. + \sqrt{\frac{l}{4\pi(2l-1)}} \left\{ \sqrt{l} \mathbf{e}_0 Y_{l-1,0}(\hat{\mathbf{r}}) - \sqrt{\frac{l-1}{2}} (\mathbf{e}_{+1} Y_{l-1,1}^*(\hat{\mathbf{r}}) + \mathbf{e}_{+1}^* Y_{l-1,1}(\hat{\mathbf{r}})) \right\} j_{l-1}(kr) \right]
\end{aligned} \tag{94}$$

$$\begin{aligned}
&= 4\pi k \sum_l \frac{i^{l+1}}{\sqrt{4\pi(2l+1)}} \left[\left\{ l e_0 Y_{l,0}(\hat{\mathbf{r}}) + \sqrt{\frac{l(l+1)}{2}} (e_{+1}^* Y_{l,1}(\hat{\mathbf{r}}) + e_{+1} Y_{l,1}^*(\hat{\mathbf{r}})) \right\} \right. \\
&\quad \left. + \left\{ (l+1) e_0 Y_{l,0}(\hat{\mathbf{r}}) - \sqrt{\frac{l(l+1)}{2}} (e_{+1} Y_{l,1}^*(\hat{\mathbf{r}}) + e_{+1}^* Y_{l,1}(\hat{\mathbf{r}})) \right\} \right] j_l(kr) \tag{95}
\end{aligned}$$

$$= i k e_0 \left[4\pi \sum_l i^l \sqrt{\frac{2l+1}{4\pi}} Y_{l,0}(\hat{\mathbf{r}}) j_l(kr) \right] = i \mathbf{k} e^{+i \mathbf{k} \mathbf{r}} \tag{96}$$

Operator	Density
Y_{LM}	$\rightarrow \rho$
$Y_{LM}\nabla_\mu$	$\rightarrow \mathbf{j}$
$Y_{LM}\sigma_\mu$	$\rightarrow \mathbf{s}$
$Y_{LM}\sigma_\mu\nabla_\nu$	$\rightarrow J_{\mu\nu}$

TABLE I:

IV. REDUCED MATRIX ELEMENT(WIGNER-ECKART'S THEOREM)

The definition of the reduced matrix element is given by

$$\langle j'm'|T_{LM}|jm\rangle = (-)^{j'-m'} \begin{pmatrix} j' & L & j \\ -m' & M & m \end{pmatrix} \langle j'||T_L||j\rangle \quad (97)$$

where T_{LM} is the so-called “*polarization operator*”, and this relation between the matrix element and the reduced one is called as “*Wick's theorem*”. There are some correspondences between the linear response quantities of the various density(density matrices) and the (polarization) operators. We show the correspondences on the Table.I.

A. Reduced matrix element of the Spin-independent operator

$$\begin{aligned} \langle l'j'm'|Y_{LM}|ljm\rangle &= \sum_{\sigma} \int d\hat{\mathbf{r}} \mathcal{Y}_{l'j'm'}^*(\hat{\mathbf{r}}\sigma) Y_{LM}(\hat{\mathbf{r}}) \mathcal{Y}_{ljm}(\hat{\mathbf{r}}\sigma) \\ &= \sum_{m'_l, m_l, m_s} \langle l'm'_l : \frac{1}{2}m_s | j'm'\rangle \langle lm_l : \frac{1}{2}m_s | jm\rangle \langle l'm'_l | Y_{LM} | lm_l\rangle \\ &= \sum_{m'_l, m_l, m_s} (-)^{l+l'+m-m'+l'-m'_l} \begin{pmatrix} l' & \frac{1}{2} & j' \\ m'_l & m_s & -m' \end{pmatrix} \begin{pmatrix} l & \frac{1}{2} & j \\ m_l & m_s & -m \end{pmatrix} \\ &\quad \times \begin{pmatrix} l' & L & l \\ -m'_l & M & m_l \end{pmatrix} \langle l' || Y_L || l \rangle \\ &= (-)^{j'-m'} \begin{pmatrix} j' & L & j \\ -m' & M & m \end{pmatrix} \langle l'j' || Y_L || lj \rangle \end{aligned} \quad (98)$$

where

$$\langle l' || Y_L || l \rangle = (-)^{l'} \frac{\widehat{L}\widehat{l}\widehat{l}}{\sqrt{4\pi}} \begin{pmatrix} L & l' & l \\ 0 & 0 & 0 \end{pmatrix} \quad (99)$$

$$\langle l'j' || Y_L || lj \rangle = \left[(-)^{j+l'+L+1/2} \widehat{j}\widehat{j} \left\{ \begin{matrix} j & j' & L \\ l' & l & \frac{1}{2} \end{matrix} \right\} \langle l' || Y_L || l \rangle \right] \quad (100)$$

Using Eq.(99), Eq.(100) and Eq.(10), one can get

$$\langle l'j' || Y_L || lj \rangle = (-)^{j'+L-1/2} \frac{\widehat{j}\widehat{j}}{\sqrt{4\pi}} \left\{ \frac{1 + (-)^{L+l+l'}}{2} \right\} \langle j1/2; j' - 1/2 | L0 \rangle \quad (101)$$

1. Example of the application: $\langle l' j' || \mathbf{Y}_{L\lambda} \cdot \nabla || l j \rangle$

Using Eq.(80) and Eq.(73), one can get

$$\langle l' m'_l | \mathbf{Y}_{L\lambda M} \cdot \vec{\nabla} | l m_l \rangle = \int d\hat{\mathbf{r}} Y_{l' m'_l}^*(\hat{\mathbf{r}}) \mathbf{Y}_{L\lambda M} \cdot \vec{\nabla} Y_{l m_l}(\hat{\mathbf{r}}) \quad (102)$$

$$= \sum_{l''=l\pm 1} \frac{(-)^{\frac{1}{2}(l''-l+1)}}{\hat{l}} \sqrt{\frac{l''+l+1}{2}} \int d\hat{\mathbf{r}} Y_{l' m'_l}^*(\hat{\mathbf{r}}) \mathbf{Y}_{L\lambda M}(\hat{\mathbf{r}}) \cdot \mathbf{Y}_{l'' m_l}(\hat{\mathbf{r}}) \\ \times \left[\frac{\vec{\partial}}{\partial r} - (-)^{\frac{1}{2}(l+1-l'')} \left(\frac{3l+1-l''}{2} \right) \frac{1}{r} \right] \quad (103)$$

$$= (-)^{l'-m'_l} \begin{pmatrix} l' & L & l \\ -m'_l & M & m_l \end{pmatrix} \\ \times \sum_{l''=l\pm 1} (-)^{L+\lambda+l'+\frac{1}{2}(l''-l+1)} \widehat{L\lambda l''} \widehat{l'} \sqrt{\frac{l''+l+1}{8\pi}} \begin{pmatrix} \lambda & l'' & l' \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} L & l & l' \\ l'' & \lambda & 1 \end{matrix} \right\} \\ \times \left[\frac{\vec{\partial}}{\partial r} - (-)^{\frac{1}{2}(l+1-l'')} \left(\frac{3l+1-l''}{2} \right) \frac{1}{r} \right] \quad (104)$$

$$= (-)^{l'-m'_l} \begin{pmatrix} l' & L & l \\ -m'_l & M & m_l \end{pmatrix} \langle l' || \mathbf{Y}_{L\lambda} \cdot \vec{\nabla} || l \rangle \quad (105)$$

where

$$\langle l' || \mathbf{Y}_{L\lambda} \cdot \vec{\nabla} || l \rangle = \sum_{l''=l\pm 1} (-)^{L+\lambda+l'+\frac{1}{2}(l''-l+1)} \widehat{L\lambda l''} \widehat{l'} \sqrt{\frac{l''+l+1}{8\pi}} \begin{pmatrix} \lambda & l'' & l' \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} L & l & l' \\ l'' & \lambda & 1 \end{matrix} \right\} \\ \times \left[\frac{\vec{\partial}}{\partial r} - (-)^{\frac{1}{2}(l+1-l'')} \left(\frac{3l+1-l''}{2} \right) \frac{1}{r} \right] \quad (106)$$

$$= (-)^{\lambda+l'+1} \frac{\widehat{L\lambda l''}}{\sqrt{4\pi}} \left[\begin{pmatrix} \lambda & 1 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} \frac{\vec{\partial}}{\partial r} \right. \\ \left. + \frac{1+(-)^{\lambda+l'+1}}{2} \sqrt{2l(l+1)} \begin{pmatrix} \lambda & 1 & L \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} l' & l & L \\ 0 & 1 & -1 \end{pmatrix} \frac{1}{r} \right] \quad (107)$$

$$= \langle l' || Y_L || l \rangle (-)^L \widehat{\lambda} \begin{pmatrix} \lambda & 1 & L \\ 0 & 0 & 0 \end{pmatrix} \\ \times \left[\frac{\vec{\partial}}{\partial r} + \left\{ \frac{\lambda(\lambda+1)-2-L(L+1)}{4L(L+1)} \right\} \frac{l'(l'+1)-l(l+1)-L(L+1)}{r} \right] \quad (108)$$

$$\langle l' m'_l | \vec{\nabla} \cdot \mathbf{Y}_{L\lambda M} | l m_l \rangle = \int d\hat{\mathbf{r}} Y_{l' m'_l}^*(\hat{\mathbf{r}}) \vec{\nabla} \cdot \mathbf{Y}_{L\lambda M}(\hat{\mathbf{r}}) Y_{l m_l}(\hat{\mathbf{r}}) \quad (109)$$

$$= \sum_{l''=l'\pm 1} \left[\frac{\overleftarrow{\partial}}{\partial r} - (-)^{\frac{1}{2}(l'+1-l'')} \left(\frac{3l'+1-l''}{2} \right) \frac{1}{r} \right] \frac{(-)^{\frac{1}{2}(l''-l'+1)}}{\hat{l'}} \sqrt{\frac{l''+l'+1}{2}} \\ \times \int d\hat{\mathbf{r}} Y_{l'' m'_l}^*(\hat{\mathbf{r}}) \cdot \mathbf{Y}_{L\lambda M}(\hat{\mathbf{r}}) Y_{l m_l}(\hat{\mathbf{r}}) \quad (110)$$

$$= \sum_{l''=l'\pm 1} \left[\frac{\overleftarrow{\partial}}{\partial r} - (-)^{\frac{1}{2}(l'+1-l'')} \left(\frac{3l'+1-l''}{2} \right) \frac{1}{r} \right] \frac{(-)^{\frac{1}{2}(l''-l'+1)}}{\hat{l'}} \sqrt{\frac{l''+l'+1}{2}} \\ \times (-)^{l'+l''+1+m'_l+m_l} \int d\hat{\mathbf{r}} Y_{l-m_l}^*(\hat{\mathbf{r}}) \mathbf{Y}_{L\lambda M}(\hat{\mathbf{r}}) \cdot \mathbf{Y}_{l'' m'_l}(\hat{\mathbf{r}}) \quad (111)$$

$$\begin{aligned}
&= (-)^{l'-m'_l} \begin{pmatrix} l' & L & l \\ -m'_l & M & m_l \end{pmatrix} \\
&\quad \times \sum_{l''=l'\pm 1} \left[\frac{\overleftarrow{\partial}}{\partial r} - (-)^{\frac{1}{2}(l'+1-l'')} \left(\frac{3l'+1-l''}{2} \right) \frac{1}{r} \right] \sqrt{\frac{l''+l'+1}{2}} \\
&\quad \times (-)^{\lambda+l+l'+l''+1+\frac{1}{2}(l''-l'+1)} \frac{\widehat{L}\widehat{\lambda}\widehat{l''}\widehat{l}}{\sqrt{4\pi}} \begin{pmatrix} \lambda & l'' & l \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} L & l' & l \\ l'' & \lambda & 1 \end{matrix} \right\} \quad (112)
\end{aligned}$$

$$= (-)^{l'-m'_l} \begin{pmatrix} l' & L & l \\ -m'_l & M & m_l \end{pmatrix} \langle l' || \overleftarrow{\nabla} \cdot \mathbf{Y}_{L\lambda} || l \rangle \quad (113)$$

where

$$\begin{aligned}
\langle l' || \overleftarrow{\nabla} \cdot \mathbf{Y}_{L\lambda} || l \rangle &= \sum_{l''=l'\pm 1} \left[\frac{\overleftarrow{\partial}}{\partial r} - (-)^{\frac{1}{2}(l'+1-l'')} \left(\frac{3l'+1-l''}{2} \right) \frac{1}{r} \right] \sqrt{\frac{l''+l'+1}{2}} \\
&\quad \times (-)^{\lambda+l+l'+l''+1+\frac{1}{2}(l''-l'+1)} \frac{\widehat{L}\widehat{\lambda}\widehat{l''}\widehat{l}}{\sqrt{4\pi}} \begin{pmatrix} \lambda & l'' & l \\ 0 & 0 & 0 \end{pmatrix} \left\{ \begin{matrix} L & l' & l \\ l'' & \lambda & 1 \end{matrix} \right\} \quad (114)
\end{aligned}$$

$$\begin{aligned}
&= (-)^{L+\lambda+l+1} \frac{\widehat{L}\widehat{\lambda}\widehat{l''}}{\sqrt{4\pi}} \left[\begin{pmatrix} \lambda & 1 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} \frac{\overleftarrow{\partial}}{\partial r} \right. \\
&\quad \left. + \frac{1+(-)^{\lambda+l+l'+1}}{2} \sqrt{2l'(l'+1)} \begin{pmatrix} \lambda & 1 & L \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} l' & l & L \\ -1 & 0 & 1 \end{pmatrix} \frac{1}{r} \right] \quad (115)
\end{aligned}$$

$$\begin{aligned}
&= \langle l' || Y_L || l \rangle (-)^L \widehat{\lambda} \begin{pmatrix} \lambda & 1 & L \\ 0 & 0 & 0 \end{pmatrix} \\
&\quad \times \left[\frac{\overleftarrow{\partial}}{\partial r} + \left\{ \frac{\lambda(\lambda+1) - 2 - L(L+1)}{4L(L+1)} \right\} \frac{l(l+1) - l'(l'+1) - L(L+1)}{r} \right] \quad (116)
\end{aligned}$$

2.

$$\begin{aligned}
&\langle l' j' m' | \sigma_\mu Y_{LM} | l j m \rangle \\
&= \sum_{JM_J} (-)^{j'-m'} \begin{pmatrix} j' & J & j \\ -m' & M_J & m \end{pmatrix} \widehat{J}\widehat{j}\widehat{j'} \sqrt{6} \langle l' || Y_L || l \rangle \left\{ \begin{matrix} 1 & \frac{1}{2} & \frac{1}{2} \\ L & l & l' \\ J & j & j' \end{matrix} \right\} \widehat{J}(-)^{-L+1-M_J} \begin{pmatrix} L & 1 & J \\ M & \mu & -M_J \end{pmatrix} \quad (117)
\end{aligned}$$

On the other hand,

$$\sigma_\mu Y_{LM} = \sum_{JM_J} \widehat{J}(-)^{-L+1-M_J} \begin{pmatrix} L & 1 & J \\ M & \mu & -M_J \end{pmatrix} \mathbf{Y}_{JLM_J} \cdot \boldsymbol{\sigma} \quad (118)$$

Therefore we can obtain

$$\langle l'j'm' | \mathbf{Y}_{JLM_J} \cdot \boldsymbol{\sigma} | ljm \rangle = (-)^{j'-m'} \begin{pmatrix} j' & J & j \\ -m' & M_J & m \end{pmatrix} \langle l'j' || \mathbf{Y}_{JL} \cdot \boldsymbol{\sigma} || lj \rangle \quad (119)$$

where

$$\langle l'j' || \mathbf{Y}_{JL} \cdot \boldsymbol{\sigma} || lj \rangle = \widehat{J} \widehat{j} \widehat{j}' \sqrt{6} \begin{Bmatrix} 1 & \frac{1}{2} & \frac{1}{2} \\ L & l & l' \\ J & j & j' \end{Bmatrix} \langle l' || Y_L || l \rangle \quad (120)$$

and also

$$\begin{aligned} & \langle l'j'm' | \sigma_\mu Y_{LM} | ljm \rangle \\ &= \sum_{JM_J} (-)^{j'-m'} \begin{pmatrix} j' & J & j \\ -m' & M_J & m \end{pmatrix} \widehat{J}(-)^{-L+1-M_J} \begin{pmatrix} L & 1 & J \\ M & \mu & -M_J \end{pmatrix} \langle l'j' || \mathbf{Y}_{JL} \cdot \boldsymbol{\sigma} || lj \rangle \end{aligned} \quad (121)$$

B.

$$\langle l'm'_l | \overleftarrow{\nabla} \cdot Y_{LM} \overrightarrow{\nabla} | lm_l \rangle = \int d\hat{\mathbf{r}} Y_{l'm'_l}^*(\hat{\mathbf{r}}) \overleftarrow{\nabla} \cdot Y_{LM}(\hat{\mathbf{r}}) \overrightarrow{\nabla} Y_{lm_l}(\hat{\mathbf{r}}) \quad (122)$$

$$\begin{aligned} &= \sum_{\eta'=l' \pm 1} \sum_{\eta=l \pm 1} \frac{(-)^{\frac{1}{2}(\eta'+\eta-l'-l+2)}}{2\widehat{l}'\widehat{l}} \sqrt{(\eta'+l'+1)(\eta+l+1)} \int d\hat{\mathbf{r}} \mathbf{Y}_{l'\eta'm'_l}^*(\hat{\mathbf{r}}) \cdot Y_{LM}(\hat{\mathbf{r}}) \mathbf{Y}_{l\eta m_l}(\hat{\mathbf{r}}) \\ &\times \left[\frac{\overleftarrow{\partial}}{\partial r} - (-)^{\frac{1}{2}(l'+1-\eta')} \left(\frac{3l'+1-\eta'}{2} \right) \frac{1}{r} \right] \left[\frac{\overrightarrow{\partial}}{\partial r} - (-)^{\frac{1}{2}(l+1-\eta)} \left(\frac{3l+1-\eta}{2} \right) \frac{1}{r} \right] \end{aligned} \quad (123)$$

$$\begin{aligned} & \int d\hat{\mathbf{r}} \mathbf{Y}_{l'\eta'm'_l}^*(\hat{\mathbf{r}}) \cdot Y_{LM}(\hat{\mathbf{r}}) \mathbf{Y}_{l\eta m_l}(\hat{\mathbf{r}}) \\ &= \sum_{IJM_J} (-)^{J+I} \frac{\widehat{l}\widehat{L}\widehat{\eta}\widehat{I}\widehat{J}}{\sqrt{4\pi}} \begin{pmatrix} \eta & L & I \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} 1 & I & J \\ L & l & \eta \end{Bmatrix} \begin{pmatrix} L & J & l \\ M & M_J & m_l \end{pmatrix} \int d\hat{\mathbf{r}} \mathbf{Y}_{l'\eta'm'_l}^*(\hat{\mathbf{r}}) \cdot \mathbf{Y}_{JIM_J}^*(\hat{\mathbf{r}}) \\ &= (-)^{-m'_l} \frac{\widehat{l}\widehat{L}\widehat{\eta}\widehat{\eta}'\widehat{l}'}{\sqrt{4\pi}} \begin{pmatrix} \eta & L & \eta' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} 1 & \eta' & l' \\ L & l & \eta \end{Bmatrix} \begin{pmatrix} L & l' & l \\ M & -m'_l & m_l \end{pmatrix} \end{aligned} \quad (124)$$

where

$$\begin{aligned} & Y_{LM}(\hat{\mathbf{r}}) \mathbf{Y}_{l\eta m_l}(\hat{\mathbf{r}}) \\ &= \sum_{IJM_J} (-)^{J+I} \frac{\widehat{l}\widehat{L}\widehat{\eta}\widehat{I}\widehat{J}}{\sqrt{4\pi}} \begin{pmatrix} \eta & L & I \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} 1 & I & J \\ L & l & \eta \end{Bmatrix} \begin{pmatrix} L & J & l \\ M & M_J & m_l \end{pmatrix} \mathbf{Y}_{JIM_J}^*(\hat{\mathbf{r}}) \end{aligned} \quad (125)$$

and

$$\begin{aligned} & \int d\hat{\mathbf{r}} \mathbf{Y}_{l'\eta'm'_l}(\hat{\mathbf{r}}) \cdot \mathbf{Y}_{JIM_J}(\hat{\mathbf{r}}) \\ &= \sum_{J'M'_J} (-)^{l'+\eta} \frac{\widehat{l}'\widehat{J}\widehat{\eta}'\widehat{I}\widehat{J}'}{\sqrt{4\pi}} \begin{pmatrix} \eta' & I & J' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l' & J & J' \\ I & \eta' & 1 \end{Bmatrix} \begin{pmatrix} l' & J & J' \\ m'_l & M_J & M'_J \end{pmatrix} \int d\hat{\mathbf{r}} Y_{J'M'_J}^*(\hat{\mathbf{r}}) \\ &= (-)^{l'+\eta} \widehat{l}'\widehat{J}\widehat{\eta}'\widehat{I} \begin{pmatrix} \eta & I & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} l' & J & 0 \\ I & \eta' & 1 \end{Bmatrix} \begin{pmatrix} l' & J & 0 \\ m'_l & M_J & 0 \end{pmatrix} \\ &= (-)^{-m'_l} \widehat{l}'\widehat{\eta}' \begin{Bmatrix} l' & l' & 0 \\ \eta' & \eta' & 1 \end{Bmatrix} \delta_{l'J} \delta_{m'_l, -M_J} \delta_{\eta'I} = (-)^{l'+\eta'-m'_l} \delta_{l'J} \delta_{\eta'I} \delta_{m'_l, -M_J} \end{aligned} \quad (126)$$

1. In case of $L=0$.

$$\langle l' m'_l | \overleftarrow{\nabla} \cdot Y_{00} \overrightarrow{\nabla} | l m_l \rangle = \int d\hat{\mathbf{r}} Y_{l' m'_l}^*(\hat{\mathbf{r}}) \overleftarrow{\nabla} \cdot Y_{00}(\hat{\mathbf{r}}) \overrightarrow{\nabla} Y_{l m_l}(\hat{\mathbf{r}}) \quad (127)$$

$$= \sum_{\eta'=l'\pm 1} \sum_{\eta=l\pm 1} \frac{(-)^{\frac{1}{2}(\eta'+\eta-l'+l+2)}}{2\widehat{l}\widehat{l'}} \sqrt{(\eta'+l'+1)(\eta+l+1)} \int d\hat{\mathbf{r}} Y_{l' \eta' m'_l}^*(\hat{\mathbf{r}}) \cdot Y_{00}(\hat{\mathbf{r}}) Y_{l \eta m_l}(\hat{\mathbf{r}}) \\ \times \left[\frac{\overleftarrow{\partial}}{\partial r} - (-)^{\frac{1}{2}(l'+1-\eta')} \left(\frac{3l'+1-\eta'}{2} \right) \frac{1}{r} \right] \left[\frac{\overrightarrow{\partial}}{\partial r} - (-)^{\frac{1}{2}(l+1-\eta)} \left(\frac{3l+1-\eta}{2} \right) \frac{1}{r} \right] \quad (128)$$

$$= \sum_{\eta=l\pm 1} \frac{(-)^{\eta-l}}{\widehat{l}^2 \sqrt{16\pi}} (\eta+l+1) \\ \times \left[\frac{\overleftarrow{\partial}}{\partial r} - (-)^{\frac{1}{2}(l+1-\eta)} \left(\frac{3l+1-\eta}{2} \right) \frac{1}{r} \right] \left[\frac{\overrightarrow{\partial}}{\partial r} - (-)^{\frac{1}{2}(l+1-\eta)} \left(\frac{3l+1-\eta}{2} \right) \frac{1}{r} \right] \quad (129)$$

$$\int d\hat{\mathbf{r}} Y_{l' \eta' m'_l}^*(\hat{\mathbf{r}}) \cdot Y_{00}(\hat{\mathbf{r}}) Y_{l \eta m_l}(\hat{\mathbf{r}}) = (-)^{-m'_l} \frac{\widehat{l} \widehat{\eta} \widehat{l'}}{\sqrt{4\pi}} \begin{pmatrix} \eta & 0 & \eta' \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} 1 & \eta' & l' \\ 0 & l & \eta \end{Bmatrix} \begin{pmatrix} 0 & l' & l \\ 0 & -m'_l & m_l \end{pmatrix} \quad (130)$$

$$= (-)^{-m'_l} \frac{1}{\sqrt{4\pi}} \delta_{\eta\eta'} \delta_{ll'} \delta_{m_l m'_l} \quad (131)$$

V. SPECIAL REDUCTION FORMULAS FOR 6J, 9J SYMBOL

There is a relation between 6j and 9j symbol,

$$\sum_X (-)^{2X} \widehat{X}^2 \begin{Bmatrix} a & b & X \\ c & d & p \end{Bmatrix} \begin{Bmatrix} c & d & X \\ e & f & q \end{Bmatrix} \begin{Bmatrix} e & f & X \\ b & a & r \end{Bmatrix} = \begin{Bmatrix} a & f & r \\ d & q & e \\ p & c & b \end{Bmatrix} \quad (132)$$

One can obtain a formula as following,

$$\sum_r \widehat{r}^2 \begin{Bmatrix} e & a & r \\ b & f & X \end{Bmatrix} \begin{Bmatrix} a & f & r \\ d & q & e \\ p & c & b \end{Bmatrix} = \sum_X (-)^{2X} \widehat{X}^2 \begin{Bmatrix} a & b & X \\ c & d & p \end{Bmatrix} \begin{Bmatrix} c & d & X \\ e & f & q \end{Bmatrix} \sum_r \widehat{r}^2 \begin{Bmatrix} e & a & r \\ b & f & X \end{Bmatrix} \begin{Bmatrix} e & a & r \\ b & f & X \end{Bmatrix} \quad (133)$$

$$= \sum_X (-)^{2X} \begin{Bmatrix} a & b & X \\ c & d & p \end{Bmatrix} \begin{Bmatrix} c & d & X \\ e & f & q \end{Bmatrix} \delta(e, f, X) \delta(a, b, X) \quad (134)$$

1. Special case

$$\sum_{j_f j_i} \widehat{j}_f \widehat{j}_i \langle l_f j_f || Y_L || l_i j_i \rangle \begin{Bmatrix} l_f & 1/2 & j_f \\ l_i & 1/2 & j_i \\ \lambda & S & L \end{Bmatrix} = \langle l_f || Y_L || l_i \rangle \sum_{j_f j_i} (-)^{j_i+l_f+L+1/2} \widehat{j}_f^2 \widehat{j}_i^2 \begin{Bmatrix} j_i & j_f & L \\ l_f & l_i & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} l_f & 1/2 & j_f \\ l_i & 1/2 & j_i \\ \lambda & S & L \end{Bmatrix} \quad (135)$$

$$= \langle l_f || Y_L || l_i \rangle \sum_{j_i} (-)^{j_i+l_f+L+1/2} \widehat{j}_i^2 \sum_{j_f} \widehat{j}_f^2 \begin{Bmatrix} \frac{1}{2} & l_f & j_f \\ L & j_i & l_i \end{Bmatrix} \begin{Bmatrix} l_f & 1/2 & j_f \\ l_i & 1/2 & j_i \\ \lambda & S & L \end{Bmatrix} \quad (136)$$