K- symmetrization ($\mathcal{H}^x$):

$$|p^S, q^S, p^I, q^I; L, M, K, j^K\rangle_K = [2(1+\delta_{K,0})]^{-1/2} (j^K)^{1/2} |p^S, q^S, p^I, q^I\rangle$$
$$\otimes \left(|L, M, K\rangle + j^K (-1)^{L+K} |L, M, -K\rangle \right)$$

Note $\quad C_2(y)|L, M, K\rangle = (-1)^{L+K} |L, M, -K\rangle \quad$ (Zare, ref 269)

($C_2(y)$ is a rotation by π about the y axis)

$$C_2(y)|p^S, q^S, p^I, q^I; L, M, K, j^K\rangle_K = [2(1+\delta_{K,0})]^{-1/2} (j^K)^{1/2} |p^S, q^S, p^I, q^I\rangle$$
$$\otimes \left((-1)^{L+K} |L, M, -K\rangle + j^K (-1)^{L+K} (-1)^{L-K} |L, M, K\rangle \right)$$
$$= [2(1+\delta_{K,0})]^{-1/2} (j^K)^{1/2} |p^S, q^S, p^I, q^I\rangle$$
$$\otimes \left(j^K |L, M, K\rangle + (-1)^{L+K} (j^K)^2 |L, M, -K\rangle \right)$$
$$= j^K |p^S, q^S, p^I, q^I; L, M, K, j^K\rangle \quad \checkmark$$

j^K is the parity of the K-symmetrized basis set

MUMF:

$$\langle \sigma_1 | \mathcal{H}^x | \sigma_2 \rangle = N_L(L_1, L_2)(-1)^{M_1+K_1} \sum_{\mu, l} \langle 1 | [A_\mu^{(l, \Delta p)}]^x | 2 \rangle$$
$$\times\, d^l_{\Delta p, M_1 - M_2}(\gamma)\, F_{M,D}^{(l, K_1 - K_2)*} \begin{pmatrix} L_1 & l & L_2 \\ M_1 & M_2 - M_1 & -M_2 \end{pmatrix} \begin{pmatrix} L_1 & l & L_2 \\ K_1 & K_2 - K_1 & -K_2 \end{pmatrix}$$

$$\langle \sigma_1 | \mathcal{H}^x | \sigma_2 \rangle_K = N_L(L_1, L_2)(-1)^{M_1+K_1} \sum_{\mu,l} \langle 1 | [A_\mu^{(l,\Delta p)}]^x | 2 \rangle$$

$$\times d^l_{\Delta p, M_1-M_2}(\Psi) \begin{pmatrix} L_1 & l & L_2 \\ M_1 & M_2-M_1 & -M_2 \end{pmatrix} [2(1+\delta_{K_1,0})\, 2(1+\delta_{K_2,0})]^{-1/2} [(j^{K_1})^{1/2}]^* [j^{K_2}]^{1/2}$$

$$\times \Big\{ F_{\mu,D}^{(l,K_1-K_2)*} \begin{pmatrix} L_1 & l & L_2 \\ K_1 & K_2-K_1 & -K_2 \end{pmatrix} + j^{K_2}(-1)^{L_2+K_2} F_{\mu,D}^{(l,K_1+K_2)*} \begin{pmatrix} L_1 & l & L_2 \\ K_1 & -K_2-K_1 & K_2 \end{pmatrix}$$

$$+ j^{K_1}(-1)^{L_1+K_1} F_{\mu,D}^{(l,-K_1-K_2)*} \begin{pmatrix} L_1 & l & L_2 \\ -K_1 & K_2+K_1 & -K_2 \end{pmatrix}$$

$$+ j^{K_1} j^{K_2} (-1)^{L_1+K_1} (-1)^{L_2+K_2} F_{\mu,D}^{(l,-K_1+K_2)*} \begin{pmatrix} L_1 & l & L_2 \\ -K_1 & K_1-K_2 & K_2 \end{pmatrix} \Big\}$$

Note $\begin{pmatrix} L_1 & l & L_2 \\ -\alpha & -\beta & -\gamma \end{pmatrix} = (-1)^{L_1+l+L_2} \begin{pmatrix} L_1 & l & L_2 \\ \alpha & \beta & \gamma \end{pmatrix}$

$$\{\ \} = \Big[F_{\mu,D}^{(l,K_1-K_2)*} + j^{K_1} j^{K_2} (-1)^{L_1+K_1} (-1)^{L_2+K_2} (-1)^{L_1+l+L_2} F_{\mu,D}^{(l,-K_1+K_2)*} \Big] \times$$

$$\times \begin{pmatrix} L_1 & l & L_2 \\ K_1 & K_2-K_1 & -K_2 \end{pmatrix}$$

$$+ \Big[j^{K_2}(-1)^{L_2+K_2} F_{\mu,D}^{(l,K_1+K_2)*} + j^{K_1}(-1)^{L_1+K_1}(-1)^{L_1+l+L_2} F_{\mu}^{(l,-K_1-K_2)*} \Big] \times$$

$$\times \begin{pmatrix} L_1 & l & L_2 \\ K_1 & -K_1-K_2 & K_2 \end{pmatrix}$$

$$\langle \sigma_1 | \mathcal{H}^x | \sigma_2 \rangle = N_L(L_1, L_2)\, N_K(K_1, K_2)(-1)^{M_1+K_1} \sum_{\mu,l} \langle 1 | [A_\mu^{(l,\Delta p)}]^x | 2 \rangle \times$$

$$\times d^l_{\Delta p, M_1-M_2}(\Psi) \begin{pmatrix} L_1 & l & L_2 \\ M_1 & M_2-M_1 & -M_2 \end{pmatrix} \frac{1}{2} [(j^{K_1})^{1/2}]^* [j^{K_2}]^{1/2}$$

$$\times \{\ \}$$

$R_{\mu,\ell}(L_1 K_1 j_1^K ; L_2 K_2 j_2^K)$

$$= \frac{1}{2}\left[(j_1^K)^{1/2}\right]^* \left[j_2^K\right]^{1/2} \times \Big\{ \begin{pmatrix} L_1 & \ell & L_2 \\ K_1 & K_2-K_1 & -K_2 \end{pmatrix}$$

$$\times \left[F_{\mu,D}^{(\ell,K_1-K_2)*} + j_1^K j_2^K (-1)^{K_1+K_2} F_{\mu,D}^{(\ell,-K_1+K_2)*} \right]$$

$$+ \begin{pmatrix} L_1 & \ell & L_2 \\ K_1 & -K_1-K_2 & K_2 \end{pmatrix} \left[j_2^K (-1)^{L_2+K_2} F_{\mu,D}^{(\ell,K_1+K_2)*} + j_1^K (-1)^{L_2+K_1} F_{\mu,D}^{(\ell,-K_1-K_2)*} \right]$$

Given a tensor $T^{(k,q)}$ there is a relationship between the q and $-q$ components

$$T^{(k,q)*} = (-1)^q T^{(k,-q)}$$

Thus:

$$R_{\mu,\ell}(L_1 K_1 j_1^K ; L_2 K_2 j_2^K) = \frac{1}{2}\left[(j_1^K)^{1/2}\right]^* \left[j_2^K\right]^{1/2} \times$$

$$\times \Big\{ \begin{pmatrix} L_1 & \ell & L_2 \\ K_1 & K_2-K_1 & -K_2 \end{pmatrix} \left[F_{\mu,D}^{(\ell,K_1-K_2)*} + j_1^K j_2^K (-1)^{K_1+K_2} (-1)^{K_1-K_2} F_{\mu,D}^{(\ell,K_1-K_2)} \right]$$

$$+ \begin{pmatrix} L_1 & \ell & L_2 \\ K_1 & -K_1-K_2 & K_2 \end{pmatrix} \left[j_2^K (-1)^{L_2+K_2} F_{\mu,D}^{(\ell,K_1+K_2)*} + j_1^K (-1)^{L_2+K_1} (-1)^{K_1+K_2} F_{\mu,D}^{(\ell,K_1+K_2)} \right] \Big\}$$

$$= \frac{1}{2}\left[(j_1^K)^{1/2}\right]^* \left[j_2^K\right]^{1/2} \times$$

$$\times \Big\{ \begin{pmatrix} L_1 & \ell & L_2 \\ K_1 & K_2-K_1 & -K_2 \end{pmatrix} \left[F_{\mu,D}^{(\ell,K_1-K_2)*} + j_1^K j_2^K F_{\mu,D}^{(\ell,K_1-K_2)} \right]$$

$$+ \begin{pmatrix} L_1 & \ell & L_2 \\ K_1 & -K_1-K_2 & K_2 \end{pmatrix} \left[j_2^K (-1)^{L_2+K_2} F_{\mu,D}^{(\ell,K_1+K_2)*} + j_1^K (-1)^{L_2+K_2} F_{\mu,D}^{(\ell,K_1+K_2)} \right] \Big\}$$

$$R_{\mu,l}\,(L_1 K_1 j_1^K;\ L_2 K_2 j_2^K) = \tfrac{1}{2}\left[(j_1^K)^{1/2}\right]^* (j_2^K)^{1/2} \times$$

$$\times \left\{ \begin{pmatrix} L_1 & l & L_2 \\ K_1 & K_2-K_1 & -K_2 \end{pmatrix} \left[F_{\mu,D}^{(l,K_2-K_1)} + j_1^K j_2^K F_{\mu,D}^{(l,K_2-K_1)} \right] \right.$$

$$\left. + \begin{pmatrix} L_1 & l & L_2 \\ K_1 & -K_1-K_2 & K_1 \end{pmatrix} j_2^K (-1)^{L_2+K_2} \left[F_{\mu,D}^{(l,K_1+K_2)*} + j_1^K j_2^K F_{\mu,D}^{(l,K_1+K_2)} \right] \right\}$$

$$G_{\mu,l}\,(j_1^K, j_2^K; K) \equiv \tfrac{1}{2}\left[(j_1^K)^{1/2}\right]^* (j_2^K)^{1/2} \left[F_{\mu,D}^{(l,K)*} + j_1^K j_2^K F_{\mu,D}^{(l,K)} \right]$$

$$= \delta_{j_1^K, j_2^K}\, \mathrm{Re}\left\{ F_{\mu,D}^{(l,K)} \right\} + (1-\delta_{j_1^K, j_2^K})\, j_1^K\, \mathrm{Im}\left\{ F_{\mu,D}^{(l,K)} \right\} \checkmark$$

if $j_1^K = -1$, $j_2^K = 1$ $\mathrm{Im}\{F_{\mu,D}^{(l,K)}\}$ changes sign compared to $j_1^K = 1$, $j_2^K = -1$

$$\langle \sigma_1 | \mathcal{H}^X | \sigma_2 \rangle = N_L(L_1, L_2)\, N_K(K_1, K_2)\, (-1)^{M_1+K_1} \times$$

$$\times \sum_{\mu,l} \langle p_1^S q_1^S; p_1^I q_1^I | \left[A^{(l,\Delta p)}\right]^X | p_2^S, q_2^S; p_2^I, q_2^I \rangle\, d^{\,l}_{\Delta p, M_1-M_2}(\psi) \begin{pmatrix} L_1 & l & L_2 \\ M_1 & M_2-M_1 & -M_2 \end{pmatrix} \times$$

$$\times R_{\mu,l}\,(L_1 K_1 j_1^K;\ L_2 K_2 j_2^K) \checkmark$$

K- symmetrization (Γ_K):

$\langle L_1 M_1 K_1 | \Gamma_K | L_2 M_2 K_2 \rangle$

$$= \delta_{M_1 M_2} \sum_L X^L_{K_1-K_2} N_L(L_1, L_2)(-1)^{K_1+M_1} \begin{pmatrix} L_1 & L & L_2 \\ M_1 & 0 & -M_1 \end{pmatrix} \begin{pmatrix} L_1 & L & L_2 \\ K_1 & K_2-K_1 & -K_2 \end{pmatrix}$$

$\langle L_1 M_1 K_1 | \Gamma_K | L_2 M_2 K_2 \rangle_K$

$$= \delta_{M_1 M_2} N_L(L_1 L_2) N_K(K_1 K_2)(-1)^{M_1+K_1} \sum_L \begin{pmatrix} L_1 & L & L_2 \\ M_1 & 0 & -M_1 \end{pmatrix} \frac{(j_1^K)^{1/2} (j_2^K)^{1/2}}{2} \times$$

$$\Big\{ X^L_{K_1-K_2} \begin{pmatrix} L_1 & L & L_2 \\ K_1 & K_2-K_1 & -K_2 \end{pmatrix} + j_2^K (-1)^{L_2+K_2} X^L_{K_1+K_2} \begin{pmatrix} L_1 & L & L_2 \\ K_1 & -K_1-K_2 & K_2 \end{pmatrix}$$

$$+ j_1^K (-1)^{L_1+K_1} X^L_{-K_1-K_2} \begin{pmatrix} L_1 & L & L_2 \\ -K_1 & K_2+K_1 & -K_2 \end{pmatrix} + j_1^K j_2^K (-1)^{L_1+L_2+K_1+K_2} X^L_{-K_1+K_2} \begin{pmatrix} L_1 & L & L_2 \\ -K_1 & -K_2+K_1 & K_2 \end{pmatrix} \Big\}$$

$$\frac{()()}{2}\{\ \} = \frac{(j_1^K)^{1/2*} (j_2^K)^{1/2}}{2} \Big\{ \Big[X^L_{K_1-K_2} + j_1^K j_2^K (-1)^{L_1+L_2+K_1+K_2} (-1)^{L_1+L+L_2} X^L_{-K_1+K_2} \Big] \times$$

$$\times \begin{pmatrix} L_1 & L & L_2 \\ K_1 & K_2-K_1 & -K_2 \end{pmatrix}$$

$$+ j_2^K (-1)^{L_2+K_2} \Big[X^L_{K_1+K_2} + j_1^K j_2^K (-1)^{L_1+L_2+K_1+K_2} (-1)^{L_1+L+L_2} X^L_{-K_1-K_2} \Big] \times$$

$$\times \begin{pmatrix} L_1 & L & L_2 \\ K_1 & -K_2-K_1 & K_2 \end{pmatrix} \Big\}$$

Note $X^L_K = X^L_{-K}$, K, L even

$$\frac{()^*()}{2}\{\ \} = \frac{(j_1^K)^{1/2*} (j_2^K)^{1/2}}{2} \Big\{ X^L_{K_1-K_2} (1 + j_1^K j_2^K) \begin{pmatrix} L_1 & L & L_2 \\ K_1 & K_2-K_1 & -K_2 \end{pmatrix}$$

$$+ X^L_{K_1+K_2} (1 + j_1^K j_2^K) \begin{pmatrix} L_1 & L & L_2 \\ K_1 & -K_2-K_1 & K_2 \end{pmatrix} \Big\}$$

(vanishes unless $j_1^K = j_2^K$)

So

$$\langle L_1 M_1 K_1 | T_k | L_2 M_2 K_2 \rangle_K$$

$$= \delta_{M_1 M_2} \delta_{j_1^k j_2^k} N_L(L_1, L_2) N_K(K_1, K_2) (-1)^{M_1+K_1} \sum_L \begin{pmatrix} L_1 & L & L_2 \\ M_1 & 0 & -M_1 \end{pmatrix} \times$$

$$\times \left\{ X^L_{K_1-K_2} \begin{pmatrix} L_1 & L & L_2 \\ K_1 & K_2-K_1 & -K_2 \end{pmatrix} + j_2^K (-1)^{L_2+K_2} X^L_{K_1+K_2} \begin{pmatrix} L_1 & L & L_2 \\ K_1 & -K_1-K_2 & K_2 \end{pmatrix} \right\}$$

K-symmetrization (starting vector)

$$|v\rangle = \frac{1}{\sqrt{2}}\left(|v_1\rangle + |v_{-1}\rangle\right)$$

$$\langle p^S, q^S; p^I, q^I; LMK | v_m\rangle = \frac{1}{\sqrt{2I+1}}\,\delta_{p^I,0}\,\delta_{p^S,m}\,\delta_{M,0} \times$$

$$\times \sqrt{\frac{2L+1}{8\pi^2}} \int d\Omega \left(\mathcal{D}^L_{0K}\right)^* P^{1/2}(\Omega)$$

$$\langle p^S, q^S; p^I, q^I; LMKj^K | v_m\rangle = \frac{(j^K)^{1/2}}{\sqrt{2(1+\delta_{K,0})}}\,\frac{1}{\sqrt{2I+1}}\,\delta_{p^I,0}\,\delta_{p^S,m}\,\delta_{M,0}$$

$$\times \sqrt{\frac{2L+1}{8\pi^2}} \int \left[\mathcal{D}^{L\,*}_{MK} + j^K(-1)^{L+K}\mathcal{D}^{L\,*}_{M-K}\right] P^{1/2}(\Omega)$$

only even K, L have non-vanishing projection onto $P^{1/2}(\Omega)$ for uniaxial systems $j^K =$

$$[\ \ ] = \mathcal{D}^{L\,*}_{MK} + j^K \mathcal{D}^{L\,*}_{M-K}$$

Note $\left(\mathcal{D}^L_{MK}\right)^* = (-1)^{M_1+K_1}\mathcal{D}^L_{-M-K}$; however, we have the selection rule $M=0$ so $[\ ] = \mathcal{D}^{L\,*}_{0K} + j^K \mathcal{D}^{L\,*}_{0-K}$

$$= \mathcal{D}^{L\,*}_{0K} + j^K(-1)^K \mathcal{D}^L_{0K} = \mathcal{D}^{L\,*}_{0K} + j^K \mathcal{D}^L_{0K} \quad \text{since } K \text{ is even}$$

Note that $P(\beta,\gamma) = P(\beta,-\gamma)$ so for the starting vector to be non-vanishing we require the symmetric (even) combination of $\mathcal{D}^{L\,*}_{0K} + j^K \mathcal{D}^L_{0K} \Rightarrow j^K = 1$

So:

$$\langle p^S, q^S; p^I, q^I; L M K j^K | \sigma_m \rangle$$

$$= \sqrt{\frac{2}{1+\delta_{K,0}}} \frac{1}{\sqrt{2I+1}} \delta_{p^I,0}\, \delta_{p^S,m}\, \delta_{M,0}\, \delta_{j^K,1} \sqrt{\frac{2L+1}{8\pi^2}} \int d\Omega\, \mathrm{Re}\{D^L_{0K}\} \rho^{1/2}(\Omega)$$

K- symmetrization (Basis set normalization)

$$|p^S, q^S; p^I q^I; LMK; \kappa\rangle = \frac{(\gamma^\kappa)^{1/2}}{[2(1+\delta_{K,0})]^{1/2}} |p^S q^S; p^I, q^I\rangle$$

$$\otimes \left(|LMK\rangle + j^\kappa (-1)^{L+K} |LM-K\rangle\right)$$

$$\langle 1|1\rangle_\kappa = \frac{\left[|\gamma^\kappa|^2\right]^{1/2}}{[2(1+\delta_{K,0})]}\Big[\left(1 + (j^\kappa)^2\right) [1-\delta_{K,0}]$$

$$+ (1+1+1+1)\,\delta_{K,0}\Big] = 1 \checkmark$$