Fourth-order perturbative extension of the single-double excitation coupled-cluster method,
Part II: Angular reduction

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Abstract

We tabulate angularly reduced fourth-order many-body corrections to matrix elements for univalent atoms, derived in [A. Derevianko and E.D. Emmons, Phys. Rev. A 65, 052115 (2002)]. In particular we focus on practically important diagrams complementary to those included in the coupled-cluster method truncated at single and double excitations. Derivation and angular reduction of a large number of diagrams have been carried out with the help of symbolic algebra software.

1 Generalities

This e-print serves as an electronic supplement to Ref. [DE02]. In that paper we derived fourth-order many-body corrections to matrix elements for univalent atoms. Based on the derived diagrams we proposed next-generation many-body method for calculating atomic properties such as parity-violating amplitudes. Here I carry out the next necessary step required in a practical implementation of this method — angular reduction of the relevant diagrams.

In Ref. [DE02] the fourth-order diagrams were classified using coupled-cluster-inspired separation into contributions from \( n \)-particle excitations from the lowest-order wavefunction. It was found that the complete set of fourth-order diagrams involves only connected single, double, and disconnected quadruple excitations. Approximately half of the fourth-order diagrams is not accounted for by the popular coupled-cluster method truncated at single and double excitations (CCSD). To devise a practical scheme capable of improving accuracies of the existing many-body methods, we proposed to combine direct order-by-order many-body perturbation theory (MBPT) with the truncated CCSD method. As shown in Fig. 1, the CCSD method recovers all many-body diagrams up to the third order of MBPT for matrix elements, but misses contributions starting from the fourth order. Such a fusion of (truncated) all-order methods with order-by-order MBPT promises improved accuracy in calculating parity-violating effects for several practically interesting atoms such as Cs, Fr, and with some modifications to Tl. It is worth noting...
fourth-order diagrams we also devised a partial summation scheme to all orders of MBPT \[DE02\]. The discussion of that approach is beyond the scope of the present e-print.

We considered a matrix element $M_{wv}$ of non-scalar operator $Z$ between two states of valence electron $w$ and $v$. The set of MBPT diagrams complementary to CCSD is entirely due to omitted triple excitations from the reference Hartree-Fock determinant. We separated these additional contributions into three major classes by noting that triples enter the fourth order matrix element $M_{wv}^{(4)}$ via

1. an indirect effect of triples on single and double excitations in the third-order wavefunction — we denote this class as $Z_{0 \times 3}$,
2. direct contribution of triples to matrix elements — class $Z_{1 \times 2}$,
3. correction to normalization — $Z_{\text{norm}}$.

Further these classes are broken into subclasses based on the nature of triples, so that

$$
\left( M_{wv}^{(4)} \right)_{\text{non-CCSD}} = Z_{1 \times 2}(T_v) + Z_{1 \times 2}(T_c) + \\
Z_{0 \times 3}(S_v[T_v]) + Z_{0 \times 3}(D_v[T_v]) + Z_{0 \times 3}(S_c[T_c]) + Z_{0 \times 3}(D_v[T_c]) + \\
Z_{\text{norm}}(T_v) .
$$
Here we distinguished between valence \( (T_v) \) and core \( (T_c) \) triples and introduced a similar notation for singles \( (S) \) and doubles \( (D) \). Notation like \( S_v[T_c] \) stands for an effect of second-order core triples \( (T_c) \) on third-order valence singles \( S_v \). The reader is referred to Ref. \[DE02\] for further details and discussion. Representative diagrams are shown in Fig. 2 and algebraic expressions are tabulated in the Appendix of Ref. \[DE02\].

\[ \begin{align*}
Z_{1x3} (T_c), 44 & \quad Z_{1x2} (T_c), 20 & \quad Z_{0x3} (S_v[T_c]), 8 \\
Z_{0x3} (D_v[T_c]), 36 & \quad Z_{0x3} (D_v[T_c]), 12 & \quad Z_{0x3} (S_v[T_c]), 8 \\
\end{align*} \]

**Figure 2:** Sample fourth-order diagrams involving triple excitations. The one-particle matrix element is denoted by a wavy horizontal line. The number of contributions for each class of diagrams is also shown; direct, all possible exchange, and the conjugated graphs of a given diagram.

### 1.1 Sample contribution and notation

Here is a sample fourth-order term derived in Ref. \[DE02\]

\[ Z_{0x3}(S_v[T_c]) = - \sum_{abcmnr} \frac{z_{bvw} \tilde{g}_{acnr} \tilde{g}_{rmw} \tilde{g}_{ab}}{\left( \varepsilon_w - \varepsilon_b \right) \left( \varepsilon_{mw} - \varepsilon_{ab} \right) \left( \varepsilon_{nrw} - \varepsilon_{abc} \right)} + 7 \text{ additional terms} + \text{h.c.s.} \]

In energy denominators, abbreviation \( \varepsilon_{xy...z} \) stands for \( \varepsilon_x + \varepsilon_y + \cdots + \varepsilon_z \), with \( \varepsilon_z \) being single-particle Dirac-Hartree-Fock (DHF) energies. Coulomb interaction in the basis of DHF orbitals \( u_i(\mathbf{r}) \)

\[ g_{ijkl} = \int u_i^\dagger (\mathbf{r}) \, u_j^\dagger (\mathbf{r}') \, \frac{1}{|\mathbf{r} - \mathbf{r}'|} \, u_k (\mathbf{r}) \, u_l (\mathbf{r}') \, d^3r \, d^3r'. \]

The quantities \( \tilde{g}_{ijkl} \) are antisymmetric combinations \( \tilde{g}_{ijkl} = g_{ijkl} - g_{jikl} \). The summation is over single-particle DHF states, following convention: core orbitals are enumerated by letters \( a, b, c, d \), complementary excited states are labelled by \( m, n, r, s \), denoted by \( v \) and \( w \). Finally matrix elements of operator \( \hat{Z} \) in the DHF basis are denoted \( z_{ij} \) and the h.c.s. contribution is to be calculated by taking the hermitian conjugate of all preceding terms and swapping labels \( v \) and \( w \).
1.2 Angular reduction

Having introduced building blocks of a many-body contribution to matrix elements, now we proceed to angular reduction, which means carrying out a summation over magnetic quantum numbers in a closed form.

One-particle DHF orbital may be conventionally represented as

\[ u(r) = \frac{1}{r} \left( i P_m(r) \Omega_{\kappa m}(\hat{r}) \right), \]

where \( P \) and \( Q \) are large and small radial components, \( \kappa = (l - j)(2j + 1) \), and \( \Omega_{\kappa m} \) is the spherical spinor. Then in Eq. (2) an orbital \( i \) encapsulates summation over principal quantum number \( n_i \), angular momentum \( j_i \) (or \( \kappa_i \)), and magnetic quantum numbers \( m_i \).

The Wigner-Eckart (WE) theorem [Edm85] allows to “peel off” \( m \)-dependence of various matrix elements. WE theorem states that if an operator \( Z^K_{Q} \) is the \( Q \)th component of an irreducible tensor operator of rank \( K \), then the matrix element \( \langle n_1 j_1 m_1 | Z^K_{Q} | n_2 j_2 m_2 \rangle \) may be expressed as

\[ \langle n_1 j_1 m_1 | Z^K_{Q} | n_2 j_2 m_2 \rangle = (-1)^{j_1 - m_1} \left( \begin{array}{ccc} j_1 & K & j_2 \\ -m_1 & Q & m_2 \end{array} \right) \langle n_1 j_1 || Z^K || n_2 j_2 \rangle, \]

where \( \langle n_j || Z^K || n'_j' \rangle \) is a reduced matrix element. Using the WE theorem and expansion of \( 1/|r - r'| \) into Legendre polynomials, the Coulomb matrix element (3) is traditionally represented as

\[ g_{abcd} = \sum_{LM} (-1)^{L-M} (-1)^{j_a - m_a} \left( \begin{array}{ccc} j_a & L & j_c \\ -m_a & M & m_c \end{array} \right) (-1)^{j_b - m_b} \left( \begin{array}{ccc} j_b & L & j_d \\ -m_b & M & m_d \end{array} \right) X_L(abcd), \]

where Coulomb integral

\[ X_L(abcd) = (-1)^{L} \langle \kappa_a || C(L) || \kappa_b \rangle \langle \kappa_c || C(L) || \kappa_d \rangle R_L(abcd) \]

is defined in terms of reduced matrix element of normalized spherical harmonics \( C(L) \) [VMK88] and a Slater integral expressed in terms of radial components of single-particle orbitals

\[ R_L(abcd) = \int_{r_2}^{r_1} dr_1 \int_{r_2}^{r_1} dr_2 \left[ P_a(r_1)P_c(r_1) + Q_a(r_1)Q_c(r_1) \right] \int_{r_2}^{r_1} dr_2 \frac{r_2}{r_2+1} \left[ P_b(r_2)P_d(r_2) + Q_b(r_2)Q_d(r_2) \right] \]

with \( r_2 = \min(r_1, r_2) \) and \( r_1 = \max(r_1, r_2) \). The anti-symmetrized combinations \( \tilde{g}_{abcd} = g_{abcd} - g_{abdc} \) are reduced similar to \( X_L(abcd) \) is replaced with

\[ Z_L(abcd) = X_L(abcd) + [L] \sum_{L'} \left\{ b a d c k k' \right\} X_{L'}(bacd) \].
Here $[L] = 2L + 1$. It is worth emphasizing that both $Z_L(\text{abcd})$ and $X_L(\text{abcd})$ do not depend on magnetic quantum numbers.

Angular reduction, i.e. summation over magnetic quantum numbers of atomic single-particle orbitals in many-body diagrams, leads to many-body correction to reduced matrix elements, $\bar{M}_{wv}$, as prescribed by the WE theorem:

$$\mathcal{M}_{wv} = (-1)^{j_w - m_w} \left( \begin{array}{cc} j_w & K_j \\ -m_w & Q \\ j_v & m_v \end{array} \right) \bar{M}_{wv},$$

where $K$ and $Q$ are the rank and component of the underlying one-particle operator $Z$. In symbolic calculations it is more convenient to invert this relation and compute

$$\bar{M}_{wv} = \sum_{m_w, m_v, Q} (-1)^{j_w - m_w} \left( \begin{array}{cc} j_w & K_j \\ -m_w & Q \\ j_v & m_v \end{array} \right) \mathcal{M}_{wv}.$$

To derive many-body diagrams and carry out angular reduction we developed a symbolic tool based on Mathematica [Wol99] and a publicly available angular reduction routine [Tak92]. This package allows to work with MBPT expressions in an interactive regime. For example, all the LA TEX formulae tabulated in the Section 2 have been generated automatically. Without the help of symbolic tools, the sheer number of diagrams in the fourth order of MBPT would have made the traditional “pencil-and-paper” approach unmanageable and error-prone. The correctness of the developed code has been verified by repeating results of angular reduction for the third-order corrections to matrix elements, tabulated by Johnson, Liu, and Sapirstein [JLS96].

The results of the angular reduction is given in Section 2. In addition to the Coulomb matrix elements $X_L(\text{abcd})$ and $X_L(\text{abcd})$, we used the following notation. Reduced matrix elements of a non-scalar one-particle operator $Z$ are denoted as $\langle i || z || j \rangle$, $K$ is the rank of the operator, $(-1)^{a+\ldots} = (-1)^{j_a+\ldots}$, $\delta_{\kappa}(a, b) = \delta_{\kappa_a, \kappa_b}$, and $[a] = 2j_a + 1$.

As to the angular reduction of h.c.s. terms, it is given simply by adding a phase factor and swapping labels $w$ and $v$ in the reduced matrix element:

$$\text{h.c.s. (} M_{wv} \text{)} = (-1)^{w-v} \bar{M}_{wv}(w \leftrightarrow v),$$

provided reduced matrix element of one-particle operator satisfies

$$\langle a||z||b \rangle = (-1)^{a-b} \langle b||z||a \rangle.$$

The relation (8) allows us to carry out angular reduction and code only half of the diagrams, which is of a great utility considering a couple of hundreds of diagrams in the fourth order MBPT. The requirement (9) is not restrictive, it holds for all practically important matrix elements: non-retarded electric and magnetic multipoles, hyperfine, and parity-violating matrix elements.

To reiterate, in this e-print we have tabulated angularly reduced fourth-order corrections to matrix elements for univalent atoms. Due to overwhelmingly large number of diagrams we focused on the diagrams complementary to those included in the coupled cluster method truncated at single and double excitations. The derivation of the diagrams and angular reduction has been carried out with the help of symbolic algebra software. In the future we plan to extend the suite to automatically generate Fortran code for these contributions and to perform numerical evaluations.

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2 Formulae

2.1 $Z_{1\times 2}(T_c)$

\[
Z_{1\times 2}(T_c) =
\]

\[
- \sum_{abcmnr} \sum_{L_1L_2} (-1)^{L_2-r-v-w} \left\{ \begin{array}{ccc} a & b & c \\ K & v & w \end{array} \right\} \left\{ \begin{array}{ccc} L_1 & L_2 & n \\ a & m & n \end{array} \right\} Z_{L_1}(cbv) Z_{L_1}(rcm) Z_{L_2}(mwa) \langle a || z || n \rangle \\
(\varepsilon_{mw} - \varepsilon_{ab}) (\varepsilon_{rv} - \varepsilon_{bc}) (\varepsilon_{nrw} - \varepsilon_{abc}) [L_1]
\]

\[
- \left( \frac{1}{[K]} \right) \sum_{abcmnr} \sum_{L_1} (-1)^{L_1-r-v-w} \left\{ \begin{array}{ccc} w & b & c \\ L_1 & m & n \end{array} \right\} Z_{K}(mna) Z_{L_1}(cbv) Z_{L_1}(rcm) \langle a || z || n \rangle \\
(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{rv} - \varepsilon_{bc}) (\varepsilon_{nrw} - \varepsilon_{abc}) [L_1]
\]

\[
- \sum_{abcmnr} \sum_{L_1L_3} (-1)^{b+K+L_1-r-v-w} \left\{ \begin{array}{ccc} K & c & b \\ e & L_1 & L_3 \end{array} \right\} \left\{ \begin{array}{ccc} L_3 & K & L_1 \\ a & m & r \end{array} \right\} Z_{L_3}(bcv) Z_{L_1}(mna) Z_{L_3}(rcm) \langle a || z || r \rangle \\
(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{rv} - \varepsilon_{bc}) (\varepsilon_{nrw} - \varepsilon_{abc}) [L_1]
\]
\[
\frac{1}{[w]} \sum_{abcdmn} \sum_{L_1L_3} \delta_e(a, w) \delta_e(b, m) (-1)^{c+L_3-n+r+w} X_{L_1(nrnm)} Z_{L_1(cnrb)} Z_{L_3(mwab)} \langle a || z || v \rangle + \\
- \left( \frac{1}{[w]} \right) \sum_{abcdmn} \sum_{L_1L_2} \delta_e(a, w) (-1)^{b+c+L_2+m-n-r+w} X_{L_1(bcnr)} Z_{L_1(mnab)} Z_{L_2(rwcm)} \langle a || z || v \rangle + \\
\frac{1}{[K]} \sum_{abcdmn} \sum_{L_1L_2} \delta_e(a, v) (-1)^{b-c+d+K-m-n-v} X_{L_1(anrd)} Z_{K(mnba)} Z_{L_1(dcnv)} \langle b || z || m \rangle + \\
\frac{1}{[K]} \sum_{abcdmn} \sum_{L_1L_2L_3} \delta_e(a, m) \delta_e(b, w) (-1)^{a-c+d-n} X_{L_1(ancd)} Z_0(mwab) Z_{L_1(edmnn)} \langle b || z || v \rangle + \\
\sum_{abcdmn} \sum_{L_1L_2L_3} \delta_e(b, w) \left( \frac{K \ v \ w}{a \ c \ m} \right) \left( \frac{L_2 \ L_1}{d \ L_3} \right) \left( \frac{L_3 \ L_1}{a \ c \ m} \right) X_{L_1(awcd)} X_{L_1(mnab)} Z_{L_1(dmnn)} \langle b || z || v \rangle + \\
\frac{1}{[w]} \sum_{abcdmn} \sum_{L_1} \delta_e(a, m) \delta_e(b, w) (-1)^{d+L_1-n-v-w} X_{L_1(ancd)} Z_{L_1(wnab)} Z_{L_1(dmnn)} \langle c || z || m \rangle + \\
\sum_{abcdmn} \sum_{L_1} \delta_e(a, m) \delta_e(b, w) (-1)^{d+L_1-n-v-w} X_{L_1(ancd)} Z_{L_1(dmnn)} \langle c || z || m \rangle + \\
\frac{1}{[K]} \sum_{abcdmn} \sum_{L_2} (-1)^{a+b+c+d+L_2-m-n} X_{L_1(mnab)} Z_{K(nrncm)} Z_{L_1(abrv)} \langle c || z || n \rangle + \\
\frac{1}{[K]} \sum_{abcdmn} \sum_{L_2} (-1)^{c-n-v-w} X_{L_1(mnab)} Z_{K(nrncm)} Z_{L_1(abrv)} \langle c || z || n \rangle + \\
7
\]
\[ -\sum_{\text{abcmnr, } L_1 L_2 L_3} (-1)^{-c+K+L_3-v} \left\{ \begin{array}{ccc} L_3 & L_2 & L_1 \\ a & m & r \end{array} \right\} \left\{ \begin{array}{ccc} L_3 & v & n \\ b & L_1 & L_2 \end{array} \right\} \left\{ \begin{array}{ccc} v & L_3 & n \\ c & K & w \end{array} \right\} X_{L_1}(mnab) Z_{L_2(bavr)} Z_{L_3(rwmc)} \right] \\
\left[ \epsilon_{mn} - \epsilon_{ab} \right] \left[ \epsilon_{rv} - \epsilon_{ab} \right] \left[ \epsilon_{nrw} - \epsilon_{abc} \right] \]

\[ -\left( \frac{1}{[K][v]} \right) \sum_{\text{abcmnr, } L_1} \sum_{\delta_{\kappa}(m, v)} (-1)^{-a+b+c+K-n-r-v} X_{L_1}(mnab) Z_{K(rwcm)} Z_{L_1(banv)} \langle c|z||v \rangle + \]

\[ -\left( \frac{1}{[w]} \right) \sum_{\text{abcmnr, } L_1 L_2 L_3} \sum_{\delta_{\kappa}(c, w)} \left\{ \begin{array}{ccc} L_2 & L_3 & L_1 \\ a & m & r \end{array} \right\} \left\{ \begin{array}{ccc} L_2 & n & w \\ b & L_1 & L_3 \end{array} \right\} X_{L_1(mwab)} X_{L_2(nrcm)} Z_{L_3(banr)} \langle c|z||v \rangle \]

\[ \left[ \epsilon_{mw} - \epsilon_{ab} \right] \left[ \epsilon_{nr} - \epsilon_{ab} \right] \left[ \epsilon_{nrw} - \epsilon_{abc} \right] \]

\[ \frac{1}{[w]} \sum_{\text{abcdmn, } L_1 L_2} \sum_{\delta_{\kappa}(a, d)} \delta_{\kappa}(c, w) (-1)^{b+L_2+m-n-w} X_{L_1(mnab)} Z_{L_1(bdmm)} Z_{L_2(awcd)} \langle c|z||v \rangle + \]

\[ \left[ \epsilon_{mn} - \epsilon_{ab} \right] \left[ \epsilon_{mn} - \epsilon_{bd} \right] \left[ \epsilon_{mnw} - \epsilon_{bcd} \right] \left[ a \right] [L_1] \]

\[ \frac{1}{[w]} \sum_{\text{abcdmn, } L_1 L_2} \sum_{\delta_{\kappa}(c, w)} (-1)^{-a+b+d+L_1-m-n-w} Z_{L_1(ancd)} Z_{L_1(mwba)} Z_{L_2(bdmm)} \langle c|z||v \rangle + \]

\[ \left[ \epsilon_{mn} - \epsilon_{bd} \right] \left[ \epsilon_{mn} - \epsilon_{ab} \right] \left[ \epsilon_{mnw} - \epsilon_{bcd} \right] [L_1]^2 \]

\[ -\left( \frac{1}{[w]} \right) \sum_{\text{abcmnr, } L_1 L_3} \sum_{\delta_{\kappa}(c, w)} \delta_{\kappa}(m, r) (-1)^{-a+b+L_3-n+w} X_{L_1(mnab)} Z_{L_2(banr)} Z_{L_3(rwmc)} \langle c|z||v \rangle + \]

\[ \left[ \epsilon_{mn} - \epsilon_{ab} \right] \left[ \epsilon_{nr} - \epsilon_{ab} \right] \left[ \epsilon_{nrw} - \epsilon_{abc} \right] [L_1][c] \]

\[ \text{h.c.s.} \]
2.2 \(Z_{1x2}(T^h_v)\)

\[
Z_{1x2}(T^h_v) = \\
\sum_{abcmnr L_1 L_2 L_3} (-1)^{-a+K+L_3+v} \left\{ \frac{L_1}{b} \frac{L_2}{m} \frac{L_3}{n} \right\} \left\{ \frac{L_1}{c} \frac{L_2}{r} \frac{L_3}{c} \right\} X_{L_1}(nmwv) Z_{L_2}(bcrm) Z_{L_3}(rm) (a||z||c) + \\
(\frac{1}{[K]}) \sum_{abcmnr L_1} \frac{\delta_s(c,m) (-1)^{a+b+K-n+r} X_{L_1}(nrwm) Z_K(mwv) Z_{L_1}(bcrm) (a||z||c)}{(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{nr} - \varepsilon_{bc}) (\varepsilon_{nrw} - \varepsilon_{abc}) [L_1]} + \\
(\frac{1}{[K]}) \sum_{abcmnr L_1 L_2} \frac{(-1)^{b+K+L_1-r+v+w} \left\{ \frac{L_1}{a} \frac{L_2}{c} \frac{K}{n} \right\} \left\{ \frac{m}{w} \frac{L_1}{v} \frac{K}{L_2} \right\} Z_{L_1}(bcrm) Z_{L_1}(rwmv) Z_K(mnab) (a||z||c)}{(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{nr} - \varepsilon_{bc}) (\varepsilon_{nrw} - \varepsilon_{abc}) [L_1]} + \\
(\frac{1}{[K]^2}) \sum_{abcmnr L_1 L_2} \sum_{L_1} \frac{(-1)^{a-b-c+L_1+m-n-r} \left\{ \frac{r}{a} \frac{m}{c} \frac{K}{L_1} \right\} Z_K(rwmv) Z_{L_1}(bcrm) Z_{L_1}(mnab) (a||z||c)}{(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{nr} - \varepsilon_{bc}) (\varepsilon_{nrw} - \varepsilon_{abc}) [L_1]} + \\
(\frac{1}{[K]^2}) \sum_{abcmnr L_1 L_2} \sum_{L_1} \frac{(-1)^{a-n-v-w} \left\{ \frac{L_1}{b} \frac{L_2}{m} \frac{K}{r} \right\} \left\{ \frac{w}{v} \frac{L_1}{K} \frac{K}{L_2} \frac{s}{L_2} \right\} X_{L_1}(rwmv) Z_K(mnab) Z_{L_2}(burs) (a||z||n)}{(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{rs} - \varepsilon_{bu}) (\varepsilon_{nr} - \varepsilon_{abc}) [L_1]} + \\
(\frac{1}{[K]^2}) \sum_{abcmnr L_1 L_2} \sum_{L_1} \frac{(-1)^{b+K+L_1-s+v+w} \left\{ \frac{L_1}{a} \frac{K}{m} \frac{L_2}{r} \right\} \left\{ \frac{n}{w} \frac{L_1}{L_2} \frac{K}{v} \right\} Z_{L_1}(burs) Z_{L_1}(rwmv) Z_K(mnab) (a||z||r)}{(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{ns} - \varepsilon_{bu}) (\varepsilon_{nr} - \varepsilon_{abc}) [L_1]} + \\
(\frac{1}{[K]^2}) \sum_{abcmnr L_1 L_2} \sum_{L_2} \frac{(-1)^{b+L_3-n+v+w} \left\{ \frac{L_3}{a} \frac{K}{m} \frac{L_1}{r} \right\} \left\{ \frac{s}{v} \frac{L_3}{L_1} \frac{K}{w} \right\} Z_{L_1}(burs) Z_{L_1}(mnab) Z_{L_3}(rwmv) (a||z||r)}{(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{ns} - \varepsilon_{bu}) (\varepsilon_{nr} - \varepsilon_{abc}) [L_1]} + \\
(\frac{(-1)^{1K}}{[K]}) \sum_{abcmnr L_1 L_2} \sum_{L_1} \frac{\left\{ \frac{L_1}{a} \frac{L_2}{m} \frac{K}{r} \right\} \left\{ \frac{L_2}{b} \frac{L_1}{c} \frac{K}{n} \right\} X_{L_1}(nrwm) Z_K(mwv) Z_{L_2}(acr) (b||z||c)}{(\varepsilon_{mw} - \varepsilon_{ab}) (\varepsilon_{nr} - \varepsilon_{ac}) (\varepsilon_{nrw} - \varepsilon_{abc}) [L_1]} + \\
9
\[
\frac{1}{\sqrt{|v|}} \sum_{abmnrs} \sum_{L_1} \delta_c(a, m) \delta_c(n, v) (-1)^{a+b-r+s} X_{L_1}(rsbm) Z_0(mnav) Z_{L_1}(bars) \langle w||z||n \rangle + \\
\frac{1}{|v|} \sum_{abmnrs} \sum_{L_1, L_2} \delta_c(r, v) (-1)^{a+b+L_2+m-n-s+v} Z_{L_1}(abns) Z_{L_1}(nmav) Z_{L_2}(srbm) \langle w||z||r \rangle + \\
\frac{1}{|v|} \sum_{abmnrs} \sum_{L_1, L_3} \delta_c(m, s) \delta_c(r, v) (-1)^{-a+b+L_3-n+v} X_{L_1}(mnab) Z_{L_1}(bans) Z_{L_3}(rmsv) \langle w||z||r \rangle + \\
\text{h.c.s.}
\]
2.3 \( Z_{1\times 2}(T_v^p) \)

\[
Z_{1\times 2}(T_v^p) = \sum_{abcdmn} \sum_{L_1 L_2 L_3} (-1)^{b+K+L_2-v} \left\{ \begin{array}{ccc}
L_1 & n & v \\
d & L_2 & L_3 \\
a & c & m
\end{array} \right\} \left\{ \begin{array}{ccc}
L_3 & L_1 & L_2 \\
v & b & K \\
d & w & n
\end{array} \right\} \frac{X_{L_1}(mnav) Z_{L_2}(awcb) Z_{L_3}(cdmn)}{(\varepsilon_{mn} - \varepsilon_{av}) (\varepsilon_{mn} - \varepsilon_{cd}) (\varepsilon_{mnw} - \varepsilon_{bcv})} \\
-\left( \frac{1}{|K|} \right) \sum_{abcdmn} \sum_{L_1 L_3} \left\{ \begin{array}{ccc}
L_3 & L_1 & K \\
a & c & m
\end{array} \right\} \left\{ \begin{array}{ccc}
L_3 & L_1 & K \\
b & d & n
\end{array} \right\} \frac{X_{L_1}(mnab) Z_K(awc) Z_{L_3}(cdmn) \langle b\|z\|d \rangle}{(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{mn} - \varepsilon_{cd}) (\varepsilon_{mnw} - \varepsilon_{bcv})} + \\
-\frac{1}{|K|} \sum_{abcdmn} \sum_{L_1} (-1)^{-a-b-c-d+L_1+m-n} \left\{ \begin{array}{ccc}
d & L_2 & v \\
a & L_1 & m
\end{array} \right\} \left\{ \begin{array}{ccc}
v & w & K \\
b & d & L_2
\end{array} \right\} \frac{Z_{L_1}(cdmn) Z_{L_1}(nace) Z_{L_2}(mwan) \langle b\|z\|d \rangle}{(\varepsilon_{mn} - \varepsilon_{cd}) (\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{mnw} - \varepsilon_{bcv})} \\
-\frac{1}{|K|} \sum_{abcdmn} \sum_{L_1} (-1)^{a-b+c+K+L_1+L_2-m-n} \left\{ \begin{array}{ccc}
d & L_2 & v \\
a & L_1 & m
\end{array} \right\} \left\{ \begin{array}{ccc}
v & w & K \\
b & d & L_2
\end{array} \right\} \frac{Z_{L_1}(mnab) Z_K(awc) Z_{L_3}(cdmn) \langle b\|z\|d \rangle}{(\varepsilon_{mn} - \varepsilon_{cd}) (\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{mnw} - \varepsilon_{bcv})} \\
-\frac{1}{|K|} \sum_{abcdmn} \sum_{L_1} (-1)^{c+L_3-r+v+w} \left\{ \begin{array}{ccc}
K & L_3 & L_1 \\
a & b & m
\end{array} \right\} \left\{ \begin{array}{ccc}
n & v & L_3 \\
L_1 & w & L_2
\end{array} \right\} \frac{Z_{L_1}(arbc) Z_{L_1}(cwrn) Z_{L_3}(mnab) \langle b\|z\|m \rangle}{(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{mn} - \varepsilon_{cw}) (\varepsilon_{mnw} - \varepsilon_{bcw})} \\
-\frac{1}{|K|} \sum_{abcdmn} \sum_{L_1 L_3} (-1)^{b-r-v+w} \left\{ \begin{array}{ccc}
K & L_3 & L_1 \\
a & c & m
\end{array} \right\} \left\{ \begin{array}{ccc}
w & n & L_3 \\
L_1 & K & v
\end{array} \right\} \frac{X_{L_1}(mnav) Z_K(arcb) Z_{L_3}(cwmn) \langle b\|z\|r \rangle}{(\varepsilon_{mn} - \varepsilon_{av}) (\varepsilon_{mn} - \varepsilon_{cw}) (\varepsilon_{mnw} - \varepsilon_{bcw})} \\
\sum_{abcdmn} \sum_{L_1 L_2 L_3} (-1)^{K+L_2-r+w} \left\{ \begin{array}{ccc}
L_2 & w & b \\
K & r & v
\end{array} \right\} \left\{ \begin{array}{ccc}
L_3 & L_1 & L_2 \\
K & c & m
\end{array} \right\} \left\{ \begin{array}{ccc}
L_3 & w & n \\
L_1 & b & L_2
\end{array} \right\} \frac{X_{L_1}(mnab) Z_{L_2}(arcv) Z_{L_3}(cwmn)}{(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{mn} - \varepsilon_{cw}) (\varepsilon_{mnw} - \varepsilon_{bcw})} \right. \]
\[
\left(\frac{1}{[K]}\right) \sum_{abcdmn L_1} \delta_{\epsilon}(a, d) \left(-1\right)^{b+c+K+m-n} X_{L_1}(mnab) Z_K(awcv) Z_{L_1}(bdmn) (c||z||d) + \\
- \sum_{abcdmn L_1 L_3} \left(-1\right)^{b+K+L_1-m+v-w} K_{a} L_1 L_3 \{ L_1 K \ a c d \ c \ m \ n \} Z_{L_1}(bdmn) Z_{L_1}(mwba) Z_{L_1}(nacv) (c||z||d) \\
- \sum_{abcdmn L_1 L_2} \left(-1\right)^{b+K+L_2-n+v+w} K_{a} L_2 L_1 \{ L_1 K \ a c m \ n \} Z_{L_1}(arcv) Z_{L_2}(bcnr) Z_{L_2}(mnab) (c||z||m) \\
- \left(\frac{1}{[K]}\right) \sum_{abcdmn L_1} \delta_{\epsilon}(a, w) \left(-1\right)^{b+c+K+m-n-r+w} X_{L_1}(mnab) Z_K(arvc) Z_{L_1}(bwnm) (c||z||r) \\
- \sum_{abcdmn L_1 L_3} \left(-1\right)^{a+b-c+L_2+m-n-r} K_{a} L_2 L_1 \{ L_2 L_3 L_1 \ a \ b \ c \ n \} Z_{L_2}(awbc) Z_{L_2}(cbnr) Z_{L_2}(mnab) (r||z||m) \\
- \sum_{abcdmn L_1 L_2 L_3} \left(-1\right)^{c+K+L_1-n+v-w} K_{a} L_1 \{ L_1 \ a \ b \ n \} \{ L_3 L_2 L_1 \ r \ w \ m \ n \} Z_{L_1}(cbmr) Z_{L_1}(nacv) Z_{L_1}(mwba) (r||z||m) \\
+ \sum_{abcdmn L_1 L_2} \left(-1\right)^{c+K+L_1-n+v-w} K_{a} L_1 \{ L_1 \ a \ b \ n \} \{ L_2 L_3 L_1 \ r \ w \ m \ n \} Z_{L_1}(cbmr) Z_{L_1}(nacv) Z_{L_1}(mwba) (r||z||m) \\
+ \left(\frac{1}{[K]}\right) \sum_{abcdmn L_1} \delta_{\epsilon}(a, r) \left(-1\right)^{-b+c+K+m-n} X_{L_1}(anbc) Z_K(mwav) Z_{L_1}(cbmr) (r||z||m) \\
+ \sum_{abcdmn L_1 L_2} \left(-1\right)^{a+b-c+K+L_1+L_2-m-n+r} K_{a} L_2 \{ L_2 L_1 \ a \ b \ c \ n \} \{ L_1 L_2 L_1 \ r \ w \ m \ n \} Z_{L_1}(anbc) Z_{L_1}(bcrm) Z_{L_1}(mwba) (r||z||n) \\
+ \left(\frac{1}{[K]}\right) \sum_{abcdmn L_1 L_2} \left\{ K_{a} L_2 \{ L_2 L_1 \ a \ b \ m \} \{ L_1 \ r \ w \ m \ n \} X_{L_1}(anbc) Z_K(mwav) Z_{L_1}(bcrm) (r||z||n) \\
+ \left(-\frac{1}{[w]}\right) \sum_{abcdmn L_1 L_2} \delta_{\epsilon}(m, v) \left(-1\right)^{-a+b+c+L_2-n-r-v} Z_{L_1}(bcrm) Z_{L_1}(mnab) Z_{L_2}(racv) (w||z||m) \\
+ \sum_{abcdmn L_1 L_2} \left(-\frac{1}{[w]}\right) \sum_{abcdmn L_1 L_2} \left\{ K_{a} L_2 \{ L_2 L_1 \ a \ b \ m \} \{ L_1 \ r \ w \ m \ n \} X_{L_1}(anbc) Z_K(mwav) Z_{L_1}(bcrm) (r||z||n) \\
+ \left(-\frac{1}{[w]}\right) \sum_{abcdmn L_1 L_2} \delta_{\epsilon}(m, v) \left(-1\right)^{-a+b+c+L_2-n-r-v} Z_{L_1}(bcrm) Z_{L_1}(mnab) Z_{L_2}(racv) (w||z||m) \\
+ \sum_{abcdmn L_1 L_2} \left(-\frac{1}{[w]}\right) \sum_{abcdmn L_1 L_2} \left\{ K_{a} L_2 \{ L_2 L_1 \ a \ b \ m \} \{ L_1 \ r \ w \ m \ n \} X_{L_1}(anbc) Z_K(mwav) Z_{L_1}(bcrm) (r||z||n) \\
+ \left(-\frac{1}{[w]}\right) \sum_{abcdmn L_1 L_2} \delta_{\epsilon}(m, v) \left(-1\right)^{-a+b+c+L_2-n-r-v} Z_{L_1}(bcrm) Z_{L_1}(mnab) Z_{L_2}(racv) (w||z||m) \\
+ 13
\]
\[- \left( \frac{1}{[v]} \right) \sum_{abcmnr} \sum_{L_1 L_3} \delta_\kappa(a, n) \delta_\kappa(m, v) (-1)^{-b+c+L_3-r+v} X_{L_1}^{ab} Z_{L_1}^{bc} Z_{L_3}^{mn} \langle w \| z \| m \rangle +
\]

\[- \left( \frac{1}{[v]} \right) \sum_{abcmnr} \sum_{L_1 L_2 L_3} \delta_\kappa(r, v) \left\{ \frac{L_2}{c} \frac{n}{L_1} \frac{v}{L_3} \right\} \left\{ \frac{L_3}{a} \frac{L_2}{b} \frac{L_1}{m} \right\} X_{L_1}^{ab} X_{L_2}^{mn} Z_{L_3}^{bc} \langle w \| z \| r \rangle +
\]

\[- \frac{1}{\sqrt[14]{[v]}} \sum_{abcmnr} \sum_{L_1} \delta_\kappa(a, c) \delta_\kappa(r, v) (-1)^{a+b+m-n} X_{L_1}^{mnab} Z_0^{ac} Z_{L_1}^{bc} \langle w \| z \| r \rangle +
\]

\[\text{h.c.s.}\]
2.4 \( Z_{0 \times 3} (S_v[T_v]) \)

\[ Z_{0 \times 3} (S_v[T_v]) = \]

\[
\frac{1}{v} \sum_{abmnr} \sum_{L_1 L_2 L_3} \delta_{n,v} \left\{ \begin{array}{ccc} L_2 & L_3 & L_1 \\ a & m & r \end{array} \right\} \left\{ \begin{array}{ccc} L_2 & s & v \\ b & L_1 & L_3 \end{array} \right\} X_{L_1(mnab)} X_{L_2(rsmv)} Z_{L_3(abrs)} \langle w||z||n \rangle \times \]

\[
\left( \varepsilon_n - \varepsilon_v \right) \left( \varepsilon_{mn} - \varepsilon_{ab} \right) \left( \varepsilon_{nrs} - \varepsilon_{abe} \right) +
\]

\[
- \left( \frac{1}{[v]} \right) \sum_{abcmnr} \sum_{L_1 L_2} \delta_{n,v} (-1)^{-a+b+c+L_2-m-r-v} Z_{L_1(bcmr)} Z_{L_1(mnba)} Z_{L_2(racv)} \langle w||z||n \rangle \\
\left( \varepsilon_n - \varepsilon_v \right) \left( \varepsilon_{mn} - \varepsilon_{ab} \right) \left( \varepsilon_{nrs} - \varepsilon_{bcv} \right) \left[ L_2 \right]^2 +
\]

\[
\frac{1}{\sqrt{v}} \sum_{abmnr} \sum_{L_1} \delta_{n,v} (1+a+b-r+s) X_{L_1(rsmv)} Z_{0(mnab)} Z_{L_1(bars)} \langle w||z||n \rangle \\
\left( \varepsilon_n - \varepsilon_v \right) \left( \varepsilon_{mn} - \varepsilon_{av} \right) \left( \varepsilon_{nrs} - \varepsilon_{abo} \right) \sqrt{a} \left[ L_1 \right] +
\]

\[
- \frac{1}{\sqrt{v}} \sum_{abcmnr} \sum_{L_1} \delta_{n,v} (1-a-b+c-r) X_{L_1(tva)} Z_{0(mnab)} Z_{L_1(bcmv)} \langle w||z||n \rangle \\
\left( \varepsilon_n - \varepsilon_v \right) \left( \varepsilon_{mn} - \varepsilon_{av} \right) \left( \varepsilon_{nrs} - \varepsilon_{bcv} \right) \sqrt{a} \left[ L_1 \right] +
\]

\[
- \frac{1}{\sqrt{v}} \sum_{abcmnr} \sum_{L_1} \delta_{n,v} (1-a+c-r-s) X_{L_1(rsmv)} Z_{0(mnba)} Z_{L_1(bcrs)} \langle w||z||n \rangle \\
\left( \varepsilon_n - \varepsilon_v \right) \left( \varepsilon_{mn} - \varepsilon_{av} \right) \left( \varepsilon_{nrs} - \varepsilon_{bcv} \right) \sqrt{a} \left[ L_1 \right] +
\]

\[
- \frac{1}{\sqrt{v}} \sum_{abcmnr} \sum_{L_1} \delta_{n,v} (-1)^{a+b+L_2-m-n-r+v} Z_{L_1(abnr)} Z_{L_1(mnba)} Z_{L_2(rsmv)} \langle w||z||s \rangle \\
\left( \varepsilon_n - \varepsilon_v \right) \left( \varepsilon_{mn} - \varepsilon_{ab} \right) \left( \varepsilon_{nrs} - \varepsilon_{abe} \right) \left[ L_2 \right]^2 +
\]

\[
\frac{1}{\sqrt{v}} \sum_{abmnr} \sum_{L_1} \delta_{n,v} (-1)^a+b-m-n X_{L_1(mnab)} Z_{0(rsmv)} Z_{L_1(banr)} \langle w||z||s \rangle \\
\left( \varepsilon_n - \varepsilon_v \right) \left( \varepsilon_{mn} - \varepsilon_{ab} \right) \left( \varepsilon_{nrs} - \varepsilon_{abe} \right) \left[ L_1 \right] \sqrt{m} +
\]

h.c.s.
\[ Z_{0 \times 3} (S_c | T_c) = \]

\[
\sum_{abcdmn} \sum_{L_1 L_2 L_3} \frac{1}{[w]} \delta_a(b, w) \left\{ \begin{array}{ccc} L_2 & n & w \\ d & L_1 & L_3 \end{array} \right\} \left\{ \begin{array}{ccc} L_3 & L_2 & L_1 \\ a & c & m \end{array} \right\} X_{L_1}(awcd) X_{L_2}(mnab) Z_{L_3}(cdmn) \langle b||z||v \rangle +
\]

\[
\frac{1}{\sqrt{[w]}} \sum_{abcdmn} \sum_{L_1} \delta_a(a, m) \delta_c(b, w) (-1)^{a+c-n+r} X_{L_1}(ncrm) Z_0(mwab) Z_{L_1}(canr) \langle b||z||v \rangle +
\]

\[
\frac{1}{\sqrt{[w]}} \sum_{abcdmn} \sum_{L_1} \delta_a(a, m) \delta_c(b, w) (-1)^{a-c+d-n} X_{L_1}(acnr) Z_0(mwab) Z_{L_1}(cdmn) \langle b||z||v \rangle +
\]

\[
\left( \frac{1}{[w]} \right) \sum_{abcdmn} \sum_{L_1 L_2} \delta_a(a, m) \delta_c(c, w) (-1)^{a+c+L_2+m-n+r+w} X_{L_1}(acnr) Z_0(mnab) Z_{L_1}(rwcm) \langle b||z||v \rangle +
\]

\[
\left( \frac{1}{[w]} \right) \sum_{abcdmn} \sum_{L_1 L_2 L_3} \delta_a(a, c) \delta_c(c, m, r) (-1)^{a+b+L_3-n+w} X_{L_1}(mnab) Z_0(awcd) Z_{L_1}(bcnm) \langle d||z||v \rangle +
\]

\[
\sum_{abcdmn} \sum_{L_1} \delta_a(a, c) \delta_c(d, w) (-1)^{a+b+L_2-m-n-w} X_{L_1}(bcnm) Z_0(bcmn) Z_{L_1} (nacd) \langle d||z||v \rangle +
\]

\[ \text{h.c.s.} \]
2.6 \( Z_{0 \times 3}(D_v[T_c]) \)

\[
Z_{0 \times 3}(D_v[T_c]) = \\
\frac{1}{|K|} \sum_{abcdmn} \sum_{L_1} \delta_k(a, v) \left( -1 \right)^{b+c+d+K-m-n-v} X_{L_1}(an) Z_K(mnab) Z_{L_1}(dcm) \langle b || z || m \rangle + \\
\frac{1}{|K|} \sum_{abcdmn} \sum_{L_1 L_2} (-1)^{b-n-v-w} \left\{ \begin{array}{ccc} K & v & w \\ d & L_1 & L_2 \end{array} \right\} X_{L_1}(aw) Z_K(mnab) Z_{L_2}(edm) \langle b || z || n \rangle + \\
\sum_{abcdmn} \sum_{L_1 L_2 L_3} (-1)^{a+b+c+L_1-m-n-r} \left\{ \begin{array}{ccc} w & L_1 & m \\ a & K & v \end{array} \right\} Z_K(mnab) Z_{L_1}(carv) Z_{L_1}(rcm) \langle b || z || n \rangle + \\
\sum_{abcdmn} \sum_{L_1 L_2} (-1)^{a+b+c+K+L_1+L_2-m-n+r} \left\{ \begin{array}{ccc} r & L_2 & v \\ a & L_1 & m \end{array} \right\} \left\{ \begin{array}{ccc} v & L_2 & r \\ b & K & w \end{array} \right\} Z_{L_1}(an) Z_{L_1}(nrcm) Z_{L_1}(cw) \langle b || z || r \rangle + \\
- \sum_{abcdmn} \sum_{L_1 L_3} (-1)^{a+K+L_1-n-v-w} \left\{ \begin{array}{ccc} K & w & v \\ c & L_2 & L_3 \end{array} \right\} Z_{L_1}(acm) Z_{L_1}(mnab) Z_{L_1}(wrcm) \langle b || z || r \rangle + \\
- \sum_{abcdmn} \sum_{L_1 L_2 L_3} (-1)^{c+K+L_3-v} \left\{ \begin{array}{ccc} L_3 & L_2 & L_1 \\ a & m & r \end{array} \right\} \left\{ \begin{array}{ccc} v & L_3 & n \\ b & L_1 & L_2 \end{array} \right\} X_{L_1}(mnab) Z_{L_2}(ba) Z_{L_3}(wcm) \langle b || z || r \rangle + \\
- \left( \frac{1}{|K|} \right) \sum_{abcdmn} \sum_{L_1 L_2} (-1)^{c-r-v-w} \left\{ \begin{array}{ccc} K & L_2 & L_1 \\ a & m & n \end{array} \right\} \left\{ \begin{array}{ccc} K & v & w \\ b & L_1 & L_2 \end{array} \right\} X_{L_1}(mnab) Z_{L_2}(nrm) Z_{L_2}(an) \langle c || z || r \rangle + \\
17
\]

\( K \)
\[ -\left(\frac{1}{K^2}\right) \sum_{abc} \sum_{L_1} \delta_\varepsilon(m, v) (-1)^{-a+b+c+K-n-r-v} X_{L_1}(mnab) Z_K(rwcm) Z_{L_1}(banv) \langle c||z||r \rangle + \]

\[ \sum_{abc} \sum_{L_1} \left\{ \begin{array}{ccc} K & L_1 & L_1 \\ a & d & m \\ b & v & w \end{array} \right\} \left\{ \begin{array}{ccc} K & L_1 & L_1 \\ v & w & L_1 \end{array} \right\} Z_{L_1}(cbmv) Z_{L_1}(nacd) Z_{L_2}(mwbv) \langle d||z||m \rangle \]

\[ -\sum_{abc} \sum_{L_1 L_2} (-1)^{-a+b-c-d+K+L_1+L_2-m+n} \left\{ \begin{array}{ccc} v & L_1 & n \\ d & K & w \end{array} \right\} \left\{ \begin{array}{ccc} v & n & L_1 \\ a & c & L_2 \end{array} \right\} Z_{L_1}(awcd) Z_{L_2}(bcmv) Z_{L_2}(mnba) \langle d||z||n \rangle \frac{(\varepsilon_{mn} - \varepsilon_{ab})(\varepsilon_{nw} - \varepsilon_{dv})(\varepsilon_{mnw} - \varepsilon_{bcd})}{[L_1]} \]

\[ -\frac{1}{K} \sum_{abc} \sum_{L_2} (-1)^{-a+b-c+d+L_2-m-n} \left\{ \begin{array}{ccc} v & w & K \\ a & c & L_2 \end{array} \right\} Z_K(ancd) Z_{L_2}(bcmv) Z_{L_2}(mwbv) \langle d||z||n \rangle \frac{(\varepsilon_{mw} - \varepsilon_{ab})(\varepsilon_{nw} - \varepsilon_{dv})(\varepsilon_{mnw} - \varepsilon_{bcd})}{[L_2]} \]
\[2.7 \quad Z_{0 \times 3}(D_v[T_r^m]) = \] 

\[-\left(\frac{1}{|K|}\right) \sum_{abcmnr} \sum_{L_1} (-1)^{a+b+c+L_1-m-n-r} \left\{ \begin{array}{ccc} w & L_1 & m \\ a & K & v \end{array} \right\} Z_K(mnab) Z_{L_1}(cwrm) Z_{L_1}(race) \langle b||z||n \rangle \left(\varepsilon_{mn} - \varepsilon_{ab}\right) \left(\varepsilon_{nw} - \varepsilon_{be}\right) \left(\varepsilon_{mrn} - \varepsilon_{bcv}\right) [L_1] + \] 

\[\frac{1}{|K|} \sum_{abcmnr} \sum_{L_1 L_3} \left\{ \begin{array}{ccc} L_3 & L_1 & K \\ a & c & m \end{array} \right\} \left\{ \begin{array}{ccc} L_3 & r & n \\ b & L_1 & K \end{array} \right\} X_{L_1}(mnab) Z_K(awcv) Z_{L_1}(crmn) \langle b||z||r \rangle \left(\varepsilon_{mn} - \varepsilon_{ab}\right) \left(\varepsilon_{rw} - \varepsilon_{be}\right) \left(\varepsilon_{mrn} - \varepsilon_{bcv}\right) [L_1] + \] 

\[\sum_{abcmnr} \sum_{L_1 L_2 L_3} (-1)^{K+L_2-r+w} \left\{ \begin{array}{ccc} L_2 & w & b \\ K & r & v \end{array} \right\} \left\{ \begin{array}{ccc} L_3 & L_1 & L_2 \\ a & c & m \end{array} \right\} \left\{ \begin{array}{ccc} L_3 & w & n \\ b & L_1 & L_2 \end{array} \right\} X_{L_1}(mnab) Z_{L_2}(arcv) Z_{L_3}(cwmn) \left(\varepsilon_{mn} - \varepsilon_{ab}\right) \left(\varepsilon_{rw} - \varepsilon_{be}\right) \left(\varepsilon_{mrn} - \varepsilon_{bcv}\right) [L_1] \] 

\[+ \sum_{abcmnr} \sum_{L_1 L_2} (-1)^{-a-b+c+K+L_1+L_2-m-n+r} \left\{ \begin{array}{ccc} r & L_2 & v \\ a & L_1 & m \end{array} \right\} \left\{ \begin{array}{ccc} v & L_2 & r \\ b & K & w \end{array} \right\} Z_{L_1}(crnm) Z_{L_1}(nace) Z_{L_1}(mwab) \langle b||z||r \rangle \left(\varepsilon_{mn} - \varepsilon_{ab}\right) \left(\varepsilon_{rw} - \varepsilon_{be}\right) \left(\varepsilon_{mrn} - \varepsilon_{bcv}\right) [L_1] \] 

\[+ \sum_{abcmnr} \sum_{L_1 L_2} (-1)^{b+K+L_2-m+v+w} \left\{ \begin{array}{ccc} K & L_2 & L_1 \\ a & c & n \end{array} \right\} \left\{ \begin{array}{ccc} r & w & L_2 \\ K & L_1 & v \end{array} \right\} Z_{L_1}(arcv) Z_{L_2}(bwmr) Z_{L_2}(mnba) \langle c||z||n \rangle \left(\varepsilon_{mn} - \varepsilon_{ab}\right) \left(\varepsilon_{nw} - \varepsilon_{ev}\right) \left(\varepsilon_{mrn} - \varepsilon_{bec}\right) [L_1] \] 

\[+ \sum_{abcmnr} \sum_{L_1 L_2} (-1)^{-a+b-c+K+L_1+L_2-m+n-r} \left\{ \begin{array}{ccc} v & L_2 & n \\ c & K & w \end{array} \right\} \left\{ \begin{array}{ccc} w & L_2 & c \\ a & L_1 & m \end{array} \right\} Z_{L_1}(bwrm) Z_{L_1}(rabc) Z_{L_2}(mnav) \langle c||z||n \rangle \left(\varepsilon_{mn} - \varepsilon_{ab}\right) \left(\varepsilon_{nw} - \varepsilon_{ev}\right) \left(\varepsilon_{mrn} - \varepsilon_{bec}\right) [L_1] \] 

\[+ \sum_{abcmnr} \sum_{L_1 L_2 L_3} (-1)^{-e+K+L_2+v} \left\{ \begin{array}{ccc} L_3 & L_1 & L_2 \\ a & b & m \end{array} \right\} \left\{ \begin{array}{ccc} r & n & L_3 \\ L_1 & L_2 & v \end{array} \right\} \left\{ \begin{array}{ccc} v & L_2 & r \\ c & K & w \end{array} \right\} X_{L_1}(mnab) Z_{L_2}(awbc) Z_{L_3}(brmn) \left(\varepsilon_{mn} - \varepsilon_{ab}\right) \left(\varepsilon_{nw} - \varepsilon_{ev}\right) \left(\varepsilon_{mrn} - \varepsilon_{bec}\right) [L_1] \] 

\[+ \left(\frac{1}{|K|}\right) \sum_{abcmnr} \sum_{L_1} \delta_s(a,r) (-1)^{b+c+K+m-n} X_{L_1}(mnab) Z_K(awcv) Z_{L_1}(brmn) \langle c||z||r \rangle \left(\varepsilon_{mn} - \varepsilon_{ab}\right) \left(\varepsilon_{rw} - \varepsilon_{be}\right) \left(\varepsilon_{mrn} - \varepsilon_{bcv}\right) [a] [L_1] + \]
\[
\begin{align*}
&- \left( \frac{1}{|K|} \right) \sum_{abemnr} \sum_{L_1 L_3} (-1)^{c-r-v-w} \left\{ \begin{array}{ccc} L_3 & L_1 & K \\ a & b & m \end{array} \right\} \left\{ \begin{array}{ccc} w & n & L_3 \\ L_1 & K & v \end{array} \right\} X_{L_1}(mnab) Z_K(abc) Z_{L_3}(bwnm) \langle c \| z \| r \rangle \\
&- \left( \frac{1}{|K| |w|} \right) \sum_{abemnr} \sum_{L_1} \delta_n(a, w) (-1)^{b+c+K-m+n-r+w} X_{L_1}(mnab) Z_K(abc) Z_{L_1}(bwnm) \langle c \| z \| r \rangle \\
&\sum_{abemnr} \sum_{L_1 L_3} (-1)^{b+K+L_1-m+v-w} \left\{ \begin{array}{ccc} K & L_1 & L_3 \\ a & v & w \end{array} \right\} \left\{ \begin{array}{ccc} L_1 & n & r \\ c & K & L_3 \end{array} \right\} Z_{L_1}(brmn) Z_{L_1}(mwna) Z_{L_1}(nacv) \langle c \| z \| r \rangle \\
&\sum_{abemnr} \sum_{L_1} (-1)^{-a+b-c+L_1+m+n} \left\{ \begin{array}{ccc} L_3 & L_1 & K \\ a & c & L_1 \end{array} \right\} Z_K(mnvw) Z_{L_1}(brmn) Z_{L_1}(nacv) \langle c \| z \| r \rangle \\
&- \sum_{abemnr} \sum_{L_1 L_3} (-1)^{c+K+L_1+n+v-w} \left\{ \begin{array}{ccc} K & L_3 & L_1 \\ a & v & w \end{array} \right\} \left\{ \begin{array}{ccc} K & L_3 & L_1 \\ b & d & m \end{array} \right\} Z_{L_1}(anvc) Z_{L_1}(bcda) Z_{L_1}(bmnv) \langle d \| z \| m \rangle \\
&\sum_{abemnr} \sum_{L_1} \frac{1}{|K|} \sum_{L_1} (-1)^{-a+b-c+L_1+m+n} X_{L_1}(anbc) Z_K(mnvw) Z_{L_1}(bcda) \langle d \| z \| m \rangle \\
&- \left( \frac{1}{|K|} \right) \sum_{abemnr} \sum_{L_2} (-1)^{-a+b-c-d+L_2-m+n} \left\{ \begin{array}{ccc} d & n & K \\ a & c & L_2 \end{array} \right\} Z_K(awcv) Z_{L_2}(bcmd) Z_{L_2}(mnba) \langle d \| z \| n \rangle \\
&\sum_{abemnr} \sum_{L_1 L_2} (-1)^{K+L_3+n+w} \left\{ \begin{array}{ccc} L_2 & L_3 & L_1 \\ a & b & m \end{array} \right\} \left\{ \begin{array}{ccc} L_3 & d & w \\ c & L_1 & L_2 \end{array} \right\} \left\{ \begin{array}{ccc} v & L_3 & n \\ d & K & w \end{array} \right\} X_{L_1}(awbc) Z_{L_2}(bcmd) Z_{L_3}(mnva) \\
&- \sum_{abemnr} \sum_{L_1 L_2} (-1)^{-a+b-c-d+K+L_1+L_2-m+n} \left\{ \begin{array}{ccc} d & w & L_1 \\ a & c & L_2 \end{array} \right\} \left\{ \begin{array}{ccc} v & L_1 & n \\ d & K & w \end{array} \right\} Z_{L_1}(ancv) Z_{L_2}(bcmd) Z_{L_2}(mwba) \langle d \| z \| n \rangle \\
&- \left( \frac{1}{|K|} \right) \sum_{abemnr} \sum_{L_1 L_2} \left\{ \begin{array}{ccc} K & L_1 & L_2 \\ c & d & n \end{array} \right\} \left\{ \begin{array}{ccc} L_2 & K & L_1 \\ a & b & m \end{array} \right\} X_{L_1}(anbc) Z_K(mnvw) Z_{L_2}(cdmb) \langle d \| z \| n \rangle \\
\end{align*}
\]
2.8 \( Z_{0\times3}(D_v[T^p_v]) \)

\[
Z_{0\times3}(D_v[T^p_v]) = \sum_{\text{abnmrs}} \sum_{L_1} \frac{\delta_c(m, w) (-1)^{a+b+K-n-r+s+w} X_{L_1}(rsbm) Z_K(mnva) Z_{L_1}(burs) \langle a||z||n \rangle}{(\varepsilon_{mn} - \varepsilon_{av}) (\varepsilon_{nw} - \varepsilon_{av}) (\varepsilon_{nrs} - \varepsilon_{abv}) [L_1]} + \\
\sum_{\text{abnmrs}} \sum_{L_2} \frac{\delta_c(m, s) (-1)^{a+b+K-n+r} X_{L_1}(nrbm) Z_K(mwav) Z_{L_1}(bsrn) \langle a||z||s \rangle}{(\varepsilon_{mw} - \varepsilon_{av}) (\varepsilon_{sw} - \varepsilon_{av}) (\varepsilon_{nrw} - \varepsilon_{abv}) [L_1][m]} + \\
\sum_{\text{abnmrs}} \sum_{L_1 L_2} \frac{(-1)^{b+K+L_1-r+v+w} \left\{ L_1 K L_2 \right\} \left\{ n w L_1 \right\} Z_{L_1}(bwm) Z_{L_1}(rsbm) Z_{L_2}(mnva) \langle a||z||s \rangle}{(\varepsilon_{mn} - \varepsilon_{av}) (\varepsilon_{sw} - \varepsilon_{av}) (\varepsilon_{nrs} - \varepsilon_{abv}) [L_1]} + \\
\sum_{\text{abnmrs}} \sum_{L_1 L_2} \frac{(-1)^{b+K+L_1-v+w} \left\{ L_1 a L_2 \right\} \left\{ w v K L_2 \right\} Z_{L_1}(bwm) Z_{L_1}(rvbm) Z_{L_2}(mnva) \langle a||z||s \rangle}{(\varepsilon_{mn} - \varepsilon_{av}) (\varepsilon_{sw} - \varepsilon_{av}) (\varepsilon_{nrs} - \varepsilon_{abv}) [L_1]} + \\
\sum_{\text{abnmrs}} \sum_{L_1 L_2} \frac{(-1)^{b-n-v-w} \left\{ L_1 L_2 K \right\} \left\{ w v K \right\} Z_{L_1}(rwmv) Z_K(mnab) Z_{L_2}(awrs) \langle b||z||n \rangle}{(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{nw} - \varepsilon_{be}) (\varepsilon_{brs} - \varepsilon_{abv})} + \\
- \sum_{\text{abnmrs}} \sum_{L_1 L_2 L_3} \frac{(-1)^{K+L_3-n+w} \left\{ L_1 L_2 L_3 \right\} \left\{ L_3 w r \right\} \left\{ L_1 L_2 L_3 \right\} \left\{ L_3 w b \right\} X_{L_1}(rsbm) Z_{L_2}(awsr) Z_{L_3}(mnab)}{(\varepsilon_{mn} - \varepsilon_{av}) (\varepsilon_{nw} - \varepsilon_{be}) (\varepsilon_{brs} - \varepsilon_{abv})} + \\
- \sum_{\text{abnmrs}} \sum_{L_1 L_2 L_3} \frac{(-1)^{-b+K+L_3-v} \left\{ L_1 L_2 L_3 \right\} \left\{ s v L_3 \right\} \left\{ v L_3 s \right\} \left\{ b L_1 K \right\} X_{L_1}(nrmv) Z_{L_2}(asrn) Z_{L_3}(mwab)}{(\varepsilon_{mn} - \varepsilon_{ab}) (\varepsilon_{sw} - \varepsilon_{be}) (\varepsilon_{nrw} - \varepsilon_{abv})} + \\
- \left( \frac{1}{[K]} \right) \sum_{\text{abnmrs}} \sum_{L_1 L_2} \frac{\left\{ L_1 L_2 K \right\} \left\{ L_2 s n \right\} X_{L_1}(nrbm) Z_K(mnva) Z_{L_2}(asrn) \langle b||z||s \rangle}{(\varepsilon_{mw} - \varepsilon_{av}) (\varepsilon_{sw} - \varepsilon_{av}) (\varepsilon_{nrw} - \varepsilon_{abv})} + \\
- \left( \frac{1}{[K]} \right) \sum_{\text{abnmrs}} \sum_{L_1} \frac{(-1)^{a+b+L_1+n-r-s} \left\{ K w v \right\} Z_K(rsmrb) Z_{L_1}(awnr) Z_{L_1}(mnva) \langle b||z||s \rangle}{(\varepsilon_{mn} - \varepsilon_{av}) (\varepsilon_{sw} - \varepsilon_{av}) (\varepsilon_{nrs} - \varepsilon_{abv}) [L_1]} + \\
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\[
\sum_{abmnrs} \sum_{L_1 L_3} (-1)^{a+b+K+L_1+L_3-m-n+r-s} \frac{K}{s} \left( \frac{L_3}{v} \right) \left( \frac{L_3}{w} \right) \left( \frac{r}{b} \right) \left( \frac{L_3}{m} \right) Z_{L_1}(awnr) Z_{L_1}(nmab) Z_{L_3}(rsmv) \langle b||z||s \rangle +
\]

\[
\sum_{abmnrs} \sum_{L_1 L_3} (-1)^{a+b+L_1-n+w+L_1} \frac{L_1}{b} \left( \frac{K}{r} \right) \left( \frac{L_3}{s} \right) \left( \frac{L_3}{w} \right) \left( \frac{m}{a} \right) \left( \frac{L_3}{v} \right) Z_{L_1}(asnr) Z_{L_1}(nmav) Z_{L_3}(rwbm) \langle b||z||s \rangle +
\]

\[
- \left( \frac{1}{K_L} \right) \sum_{abmnrs} \sum_{L_1} (-1)^{a+b+L_1-m-n+r+s} \frac{K}{b} \frac{L_1}{m} \frac{K}{s} \left( \frac{L_3}{v} \right) \left( \frac{c}{a} \right) \left( \frac{K}{r} \right) Z_K(rwmuv) Z_{L_1}(asnr) Z_{L_1}(nmab) \langle b||z||s \rangle +
\]

\[
\sum_{abmnrs} \sum_{L_1 L_2} \frac{1}{K_L} \sum_{L_1 L_2} \frac{K}{b} \frac{L_1}{c} \frac{L_2}{n} \left( \frac{K}{a} \right) \left( \frac{L_2}{m} \right) \left( \frac{L_1}{r} \right) X_{L_1}(mnab) Z_K(rwmuv) Z_{L_2}(abcr) \langle c||z||n \rangle +
\]

\[
\sum_{abmnrs} \sum_{L_1} \frac{1}{K_L} \sum_{L_1} \left( \frac{K}{b} \right) \left( \frac{L_1}{c} \right) \left( \frac{K}{a} \right) \left( \frac{L_1}{m} \right) \left( \frac{K}{r} \right) Z_K(mwauv) Z_{L_1}(abcn) Z_{L_1}(nrbm) \langle c||z||r \rangle +
\]

\[
\sum_{abmnrs} \sum_{L_1 L_2 L_3} \left( -1 \right)^{a+b+L_1+L_3-n+w+L_1} \frac{K}{b} \frac{L_1}{c} \frac{L_2}{w} \left( \frac{L_3}{a} \right) \left( \frac{L_2}{m} \right) \left( \frac{L_3}{n} \right) \left( \frac{v}{c} \right) \left( \frac{L_3}{K} \right) \left( \frac{r}{w} \right) X_{L_1}(mwab) Z_{L_2}(bacn) Z_{L_3}(rwmn) +
\]

\[
\sum_{abmnrs} \sum_{L_1 L_3} \frac{1}{K_L} \sum_{L_1 L_3} \left( -1 \right)^{a+b+K+L_1-n+w+L_1} \frac{K}{b} \frac{L_1}{c} \frac{K}{r} \frac{L_1}{v} \left( \frac{m}{a} \right) \left( \frac{L_3}{w} \right) \left( \frac{L_3}{v} \right) Z_{L_1}(abmc) Z_{L_1}(nmav) Z_{L_3}(rwbnm) \langle c||z||r \rangle +
\]

\[
- \left( \frac{1}{K_L} \right) \sum_{abmnrs} \sum_{L_1} \delta_k(c,m) \left( -1 \right)^{a+b+K-n+r} \frac{K}{b} \frac{L_1}{c} \frac{K}{r} \frac{L_1}{v} \left( \frac{m}{a} \right) \left( \frac{L_3}{w} \right) \left( \frac{L_3}{v} \right) Z_{L_1}(mnab) Z_{K}(rwmuv) Z_{L_1}(abcm) \langle c||z||r \rangle +
\]

h.c.s.
2.9 Normalization correction

Finally, the angular reduction of normalization correction due to valence triple excitations is given by

\[
Z_{\text{norm}}(T_v) = -\frac{1}{2} \left( N_v^{(3)}(T_v) + N_w^{(3)}(T_v) \right) \langle w||z||v \rangle ,
\]

with

\[
\frac{1}{2} N_v^{(3)}(T_v) =
\]

\[
\frac{1}{|v|} \sum_{abmn} \sum_{L_1L_2L_3} \left\{ \begin{array}{ccc} L_2 & L_3 & L_1 \\ a & m & n \end{array} \right\} \left\{ \begin{array}{ccc} L_2 & r & v \\ b & L_1 & L_3 \end{array} \right\} X_{L_1}(mvab) X_{L_2}(mrvn) Z_{L_3}(abmn) \left( \varepsilon_{mv} - \varepsilon_ab \right) \left( \varepsilon_{mn} - \varepsilon_ab \right) \]

\[
- \left( \frac{1}{|v|} \right) \sum_{abmn} \sum_{L_1L_2L_3} \left\{ \begin{array}{ccc} L_2 & n & v \\ c & L_1 & L_3 \end{array} \right\} \left\{ \begin{array}{ccc} L_3 & L_2 & L_1 \\ a & b & m \end{array} \right\} X_{L_1}(avbc) X_{L_2}(mnab) Z_{L_3}(bcmn) \left( \varepsilon_{mn} - \varepsilon_av \right) \left( \varepsilon_{mn} - \varepsilon_bc \right) \]

\[
- \frac{1}{|v|} \sum_{abmn} \sum_{L_1} \delta_{\kappa(a,c)} (-1)^{a+b+m+n} X_{L_1}(mnab) Z_0(avec) Z_{L_1}(bcmn) \left( \varepsilon_{mn} - \varepsilon_{ab} \right) \left( \varepsilon_{mn} - \varepsilon_{bc} \right) \]

\[
+ \frac{1}{|v|} \sum_{abmn} \sum_{L_1L_2} (-1)^{a+b+c+L_1-m+n-v} X_{L_1}(anbc) Z_0(mncb) Z_{L_2}(bcnm) \left( \varepsilon_{mn} - \varepsilon_{bc} \right) \left( \varepsilon_{mv} - \varepsilon_{ab} \right) \left[ L_1 \right] \]

\[
- \frac{1}{|v|} \sum_{abmn} \sum_{L_1} \delta_{\kappa(a,m)} (-1)^{a+b-n+r} X_{L_1}(nrbm) Z_0(mvan) Z_{L_1}(banr) \left( \varepsilon_{m} - \varepsilon_{a} \right) \left( \varepsilon_{mn} - \varepsilon_{ab} \right) \]

\[
+ \frac{1}{|v|} \sum_{abmn} \sum_{L_1L_2} \delta_{\kappa(a,m)} (-1)^{a+b+e-n} X_{L_1}(anbc) Z_0(mncb) Z_{L_1}(bcmn) \left( \varepsilon_{mn} - \varepsilon_{ab} \right) \left( \varepsilon_{mn} - \varepsilon_{bc} \right) \]

\[
- \frac{1}{|v|} \sum_{abmn} \sum_{L_1} \delta_{\kappa(m,r)} (-1)^{a+b-m-n} X_{L_1}(mnab) Z_0(rvmb) Z_{L_1}(banr) \left( \varepsilon_{mn} - \varepsilon_{ab} \right) \left( \varepsilon_{nr} - \varepsilon_{ab} \right) \left[ L_1 \right] \left[ m \right] \]

\[
.\]