

Calculation of derivative properties in XMS-CASPT2

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Calculation of matrix elements for many electron operators



- We need a generic approach for evaluating terms of the form

$$\sum_{\substack{ijkl \\ wxyz}} \sum_J T_{ijkl}^{\dagger} g_{wxyz} q_{uv} \langle I | a_i a_j a_k^{\dagger} a_l^{\dagger} a_w^{\dagger} a_x^{\dagger} a_y a_z a_u^{\dagger} a_v | J \rangle c_J$$

- These terms can be decomposed into a sum of expressions of the following form:

$$\sum_{ijklmn}^{act} \sum_J \langle I | a_i^{\dagger} a_j^{\dagger} a_k^{\dagger} a_l a_m a_n | J \rangle c_J A_{ijklmn}$$

- Jae used code from SMITH3 to develop an efficient method of doing this in a non-relativistic framework.
- However, for cases involving spin-flipping interactions, we need to develop a method which takes advantage of spin symmetry.

Outline of method



Step 1 : Get operator information.

- Split input tensors up into blocks.
- Generate all possible contractions of these blocks.
- Identify which blocks/contracted blocks are equivalent.

Step 2 : Manipulate indexes.

- Rearrange indexes to normal order, applying range constraints.
- Put indexes into alternating order and group common indexes.

Step 3 : Generate computational procedure.

- Merge all contributions from different brackets.
- Generate a task list to obtain contracted A-tensors.

Step 4 : Execute computational procedure.

- Contract A-tensors with gamma matrices.

Step 5 : Loop over spin sectors and states.

- Repeat for all necessary spin sectors.

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Step 5 : Loop over spin sectors and states.

- Repeat for all necessary spin sectors.

Generation of A-tensors



- Each A-tensor is defined by the original operators, T_{ijkl}^\dagger , g_{wxyz} , q_{uv} , and a set, X , of contraction indices and factors:

$$A_{abcd} = \sum_t^{x_t \in X} s_t \sum_{e_t f_t g_t h_t m_t n_t} \delta_{e_t f_t} \delta_{g_t h_t} \delta_{m_t n_t} T_{ijkl}^\dagger g_{wxyz} q_{uv}$$

$$X = \{(\{(a_1, b_1), (c_1, d_1), (e_1, f_1)\}, s_1), (\{(a_2, b_2), (c_2, d_2), (e_2, f_2)\}, s_2), \dots\}$$

$$\{e_t, f_t, g_t, h_t, m_t, n_t\} \subset \{i, j, k, l, w, x, y, z, u, v\}$$

Contraction of γ_{ijklmn}^I and A_{ijklmn}



- Contraction of A-tensor with reduced density matrix (or similar) term:

$$\sum_{ijklmn}^{act} \sum_J \langle I | a_i^\dagger a_j a_k^\dagger a_l a_m^\dagger a_n | J \rangle c_J A_{ijklmn}$$

- The middle term is often too large to be stored in memory.
- Two possible methods may be used to calculate this term “on-the-fly” will be discussed at the end.

Contraction of γ_{ijklmn}^I and A_{ijklmn}



- Final step is to contract the A-tensor with the reduced density matrix or similar terms :

$$\sum_{ijklmn}^{act} \sum_J \langle I | a_i^\dagger a_j a_k^\dagger a_l a_m^\dagger a_n | J \rangle c_J A_{ijklmn}$$

- Aim to avoid storing the six index reduced density matrix derivative term in memory.

$$\sum_{ijkl} H_{ijkl}^\dagger \sum_K \langle I | ijk^\dagger | K \rangle \sum_{nop} \sum_J T_{lnop} \langle K | n^\dagger op | J \rangle c_J^N$$

Contraction of γ_{ijklmn}^I and A_{ijklmn}



- Another alternative is to use two three index terms

$$\begin{aligned} & \sum_J \sum_{\substack{ijkl \\ lno p}} H_{ijkl}^\dagger T_{lno p} \langle I | ijk^\dagger l^\dagger n^\dagger o | J \rangle c_J^N \\ &= \sum_{ijkl} H_{ijkl}^\dagger \sum_K \langle I | ijk^\dagger | K \rangle \sum_{lno p} \sum_J T_{lno p} \langle K | l^\dagger n^\dagger o | J \rangle c_J^N \end{aligned}$$

- Often there are only a few contributions to the A-tensor, which
- One possible method is to decompose it into a four index and two index term:

Generation of A-tensors



- Each A-tensor is defined by the original operators, T_{ijkl}^\dagger , g_{wxyz} , q_{uv} , and a set, X , of contraction indices and factors:

$$A_{abcd} = \sum_x^{x \in X} \sum_{efghmn} \delta_{ef} \delta_{gh} \delta_{mn} T_{ijkl}^\dagger g_{wxyz} q_{uv}$$

$$X = \{(\{(a_1, b_1), (c_1, d_1), (e_1, f_1)\}, s_1), (\{(a_2, b_2), (c_2, d_2), (e_2, f_2)\}, s_2), \dots\}$$

- Each contribution, A^x , to the A-tensor is obtained by performing a recursive sequence of operations:

$$A_{abcd}^x = B(A_{abcdefgh}^x, (g, h)) =$$

$$= B(B(A_{abcdefgh}^x, (g, h)), (e, f)) = B(B(B(A_{abcdefgh}^x, (g, h)), (e, f)), (c, d))$$

Contraction tree



5el

$$T_{ijkl}^{\dagger} g_{wxyz} q_{uv}$$

4el

$$A_{ijkwxyuv}$$

$$A_{ijlwxyzuv}$$

3el

$$A_{jkxyuv}$$

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$$A_{lzuv}$$

$$A_{ilwv}$$

Building contraction tree



- The contraction tree is quite large; at each vertex connects to N_{el}^2 paths.
- This leads to $(N_{el}!)^2$ distinct paths (14400 for a five electron operator).
- Which paths we need are determined by how we reorder the expression in question:

$$\sum_{\substack{ijkl \\ wxyz}} \sum_J T_{ijkl}^\dagger g_{wxyz} q_{uv} \langle I | a_i a_j a_k^\dagger a_l^\dagger a_w^\dagger a_x^\dagger a_y a_z a_u^\dagger a_v | J \rangle c_J$$

- Obtaining all A-tensors efficiently is not the only consideration; we must also consider the evaluation of final contraction:

$$\sum_{ijklmn}^{act} \sum_J \langle I | a_i^\dagger a_j a_k^\dagger a_l a_m^\dagger a_n | J \rangle c_J A_{ijklmn}$$

Generation of contraction task list



- Each A-tensor is defined by the original operators, T_{ijkl}^\dagger , g_{wxyz} , q_{uv} , and a set, X , of contraction indices and factors:

$$A_{abcd} = \sum_x^{x \in X} \sum_{efghmn} \delta_{ef} \delta_{gh} \delta_{mn} T_{ijkl}^\dagger g_{wxyz} q_{uv}$$

$$X = \{(\{(a_1, b_1), (c_1, d_1), (e_1, f_1)\}, s_1), (\{(a_2, b_2), (c_2, d_2), (e_2, f_2)\}, s_2), \dots\}$$

- Each path from top to bottom corresponds to a member of X .
- Order of contractions is not important.
- Reorder the individual members of X to get the most efficient tree.

Initial reordering



$$T_{ijkl}^{\dagger} g_{wxyz} q_{uv} \langle I | a_i a_j a_k^{\dagger} a_l^{\dagger} a_w^{\dagger} a_x^{\dagger} a_y a_z a_u^{\dagger} a_v | J \rangle c_J$$

- Initial ordering is ill-suited to efficient computation. Reorder to normal order :

$$= T_{ijkl}^{\dagger} g_{wxyz} q_{uv} \langle I | a_k^{\dagger} a_l^{\dagger} a_w^{\dagger} a_x^{\dagger} a_u^{\dagger} a_i a_j a_y a_z a_v | J \rangle s_0$$

$$+ \sum_{\{\mu, \nu\}} T_{abcd} g_{efgh} q_{ij} \langle I | a_q^{\dagger} a_r^{\dagger} a_u^{\dagger} a_v^{\dagger} a_w a_x a_y a_z | J \rangle \delta_{\mu\nu} s_{\mu\nu}$$

$$+ \sum_{\{\mu, \nu\}} \sum_{\{\tau, \epsilon\}} T_{abcd} g_{efgh} q_{ij} \langle I | a_q^{\dagger} a_r^{\dagger} a_u^{\dagger} a_x a_y a_z | J \rangle \delta_{\mu\nu} \delta_{\tau\epsilon} s_{\mu\nu\tau\epsilon}$$

$$+ \sum_{\{\mu, \nu\}} \sum_{\{\tau, \epsilon\}} \sum_{\{\eta, \theta\}} T_{abcd} g_{efgh} q_{ij} \langle I | a_q^{\dagger} a_r^{\dagger} a_u^{\dagger} a_x a_y a_z | J \rangle \delta_{\mu\nu} \delta_{\tau\epsilon} \delta_{\eta\theta} s_{\mu\nu\tau\epsilon\eta\theta}$$

- Now all indexes in the BraKet must be active; this constraint greatly reduces the computational cost as typically $N_{act} \ll N_{virt}$ and $N_{act} \ll N_{core}$.

Six electron contribution



- The order of the indexes on the bra-ket and contractions still have the same indexes as the operators, T, g and q, but the ordering is changed:

$$\sum_{\{\mu, \nu\}} \sum_{\{\tau, \epsilon\}} T_{abcd} g_{efgh} q_{ij} \langle I | a_q^\dagger a_r^\dagger a_u^\dagger a_x a_y a_z | J \rangle \delta_{\mu\nu} \delta_{\tau\epsilon} S_{\mu\nu\tau\epsilon}$$

$$\{a, b, c, d, e, f, g, h, i, j\} = P\{\mu, \nu, \tau, \eta, u, v, w, x, y, z\}$$

- The ordering, sign and any constraints on the indexes are determined by the entire sequence of permutation operations necessary to get to that point.
- In terms of computational cost, which sequence of permutations is used is (almost) as important as the final index order.
- New terms due to reordering are always of equal or lower rank; apply reordering recursively from largest term to smallest.

Optimal ordering sequence



- By passing *through* certain orders, it is possible to eliminate terms and simplify the final expression.

Normal order

- Indexes in bra-ket must be active.

$$\langle I | a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n | J \rangle$$

Spin maximizing/minimizing order

- Reorder so as to maximally decrease or increase spin.
- May result in contractions (depending on the spin-sector).

$$\langle I | \alpha_i^\dagger \beta_j \beta_k^\dagger \alpha_l \beta_m^\dagger \alpha_n | J \rangle$$

$$\alpha_i^\dagger = a_{i,\alpha}^\dagger$$

$$\beta_i^\dagger = a_{i,\beta}^\dagger$$

Spin constraints



Chose order so as to push the wavefunction out of the active space.

Spin sector	$\{ J\rangle\}$	$\{ K\rangle\}$	$\{ L\rangle\}$	$\{ I\rangle\}$
$[7\alpha 0\beta]$				
$[6\alpha 1\beta]$				
$[5\alpha 2\beta]$				
$[4\alpha 3\beta]$				
$[3\alpha 4\beta]$				
$[2\alpha 5\beta]$				
$[1\alpha 6\beta]$				
$[0\alpha 7\beta]$				

$$\sum_{KL} \langle I | \beta_k^\dagger \alpha_l | K \rangle \langle K | \alpha_i^\dagger \beta_j | L \rangle \langle L | \beta_m^\dagger \alpha_n | J \rangle =$$

$$= \begin{cases} 0 & \text{if } i \neq n \text{ and } i \neq k \\ \pm 1 & \text{otherwise} \end{cases}$$

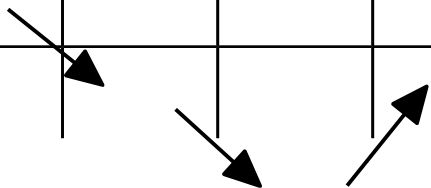
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$[2\alpha 5\beta]$				
$[1\alpha 6\beta]$				
$[0\alpha 7\beta]$				

$$\sum_{KL} \langle I | \alpha_i^\dagger \beta_j | K \rangle \langle K | \beta_k^\dagger \alpha_l | L \rangle \langle L | \beta_m^\dagger \alpha_n | J \rangle = 0$$



Optimal ordering



- By passing *through* certain orders, it is possible to eliminate terms and simplify the final expression.

Grouped operator index order

- May decompose expression into product of two sub expressions

$$\sum_K \sum_{\substack{ijkl \\ wxyz \\ uv}} T_{ijkl}^\dagger g_{wxyz} q_{uv} \langle I | a_k^\dagger a_l^\dagger a_w^\dagger a_x^\dagger a_u^\dagger a_i a_j a_y a_z a_v | J \rangle c_J$$

$$\rightarrow \sum_J \sum_{\substack{ijkl \\ wxyz}} T_{ijkl}^\dagger g_{wxyz} \langle I | a_k^\dagger a_l^\dagger a_w^\dagger a_x^\dagger a_i a_j a_y a_z | K \rangle \sum_{uv} \sum_J q_{uv} \langle K | a_u^\dagger a_v | J \rangle c_J$$

$$\rightarrow \sum_J \sum_{\substack{ijkl \\ wxyz}} T_{ijkl}^\dagger g_{wxyz} \langle I | a_k^\dagger a_l^\dagger a_w^\dagger a_x^\dagger a_i a_j a_y a_z | K \rangle \tilde{c}_K$$

Optimal ordering



- By passing *through* certain orders, it is possible to eliminate terms and simplify the final expression.
- Final order should be determined from symmetry constraints, and the need to minimize the number of vertices high in the contraction tree.

Application of block symmetry



Example : CASPT2 perturbation coefficients $T_{(ij),(kl)}$.

	$c \rightarrow a$	$c \rightarrow v$	$a \rightarrow a$	$a \rightarrow v$
$c \rightarrow a$				
$c \rightarrow v$				
$a \rightarrow a$				
$a \rightarrow v$				

Possible transitions

closed \rightarrow active

closed \rightarrow virtual

active \rightarrow active

active \rightarrow virtual

Application of symmetry



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Contraction of tensor blocks



Contract over all possible pairs of indexes, e.g.,

$$\hat{H}\hat{T} \rightarrow \sum_{wxyz} \sum_{ijkl} H_{wxyz} a_w^\dagger a_x^\dagger a_y a_z T_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

$$A_{abcdef}^{HT,st} = \sum_{wxyz} \sum_{ijkl} H_{wxyz} T_{ijkl} \delta_{st}$$

$$s := w, x, i, \text{ or } j$$

$$t := y, z, k \text{ or } l$$

Use the block range constraints to rule out possible contractions, e.g.

$$A_{abcdef}^{HT,st} = \begin{cases} A_{abcdef}^{HT,st} & \text{if } rng(s) = rng(t) \\ 0 & \text{otherwise} \end{cases}$$

Contraction list is different for every range block.

Contraction tree



5el

$$T_{ijkl}^{\dagger} g_{wxyz} q_{uv}$$

4el

$$A_{ijkwxyuv}$$

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$$A_{lzuv}$$

$$A_{lzuv}$$

$$A_{ilwv}$$

$$\delta_{lz}$$

$$\delta_{ky}$$

$$\delta_{iw}$$

$$\delta_{kv}$$

$$\delta_{iw}$$

$$\delta_{jx}$$

$$\delta_{jx}$$

$$\delta_{ky}$$

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Block specific contraction trees



- Which paths contribute is depends on the block(s) under consideration.

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$$A_{lzuv}$$

$$A_{lzuv}$$

$$A_{ilwv}$$

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$$\delta_{ky}$$

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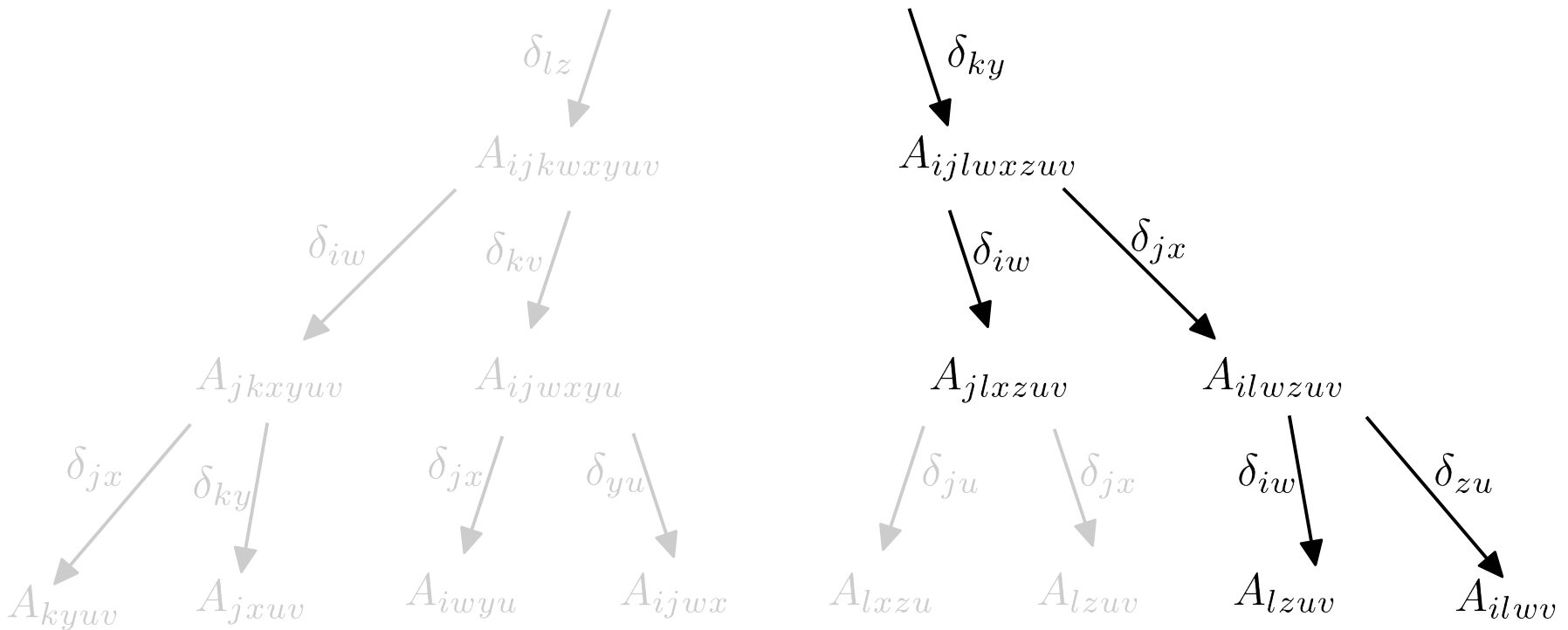
$$A_{ijwx}$$

$$A_{lxzu}$$

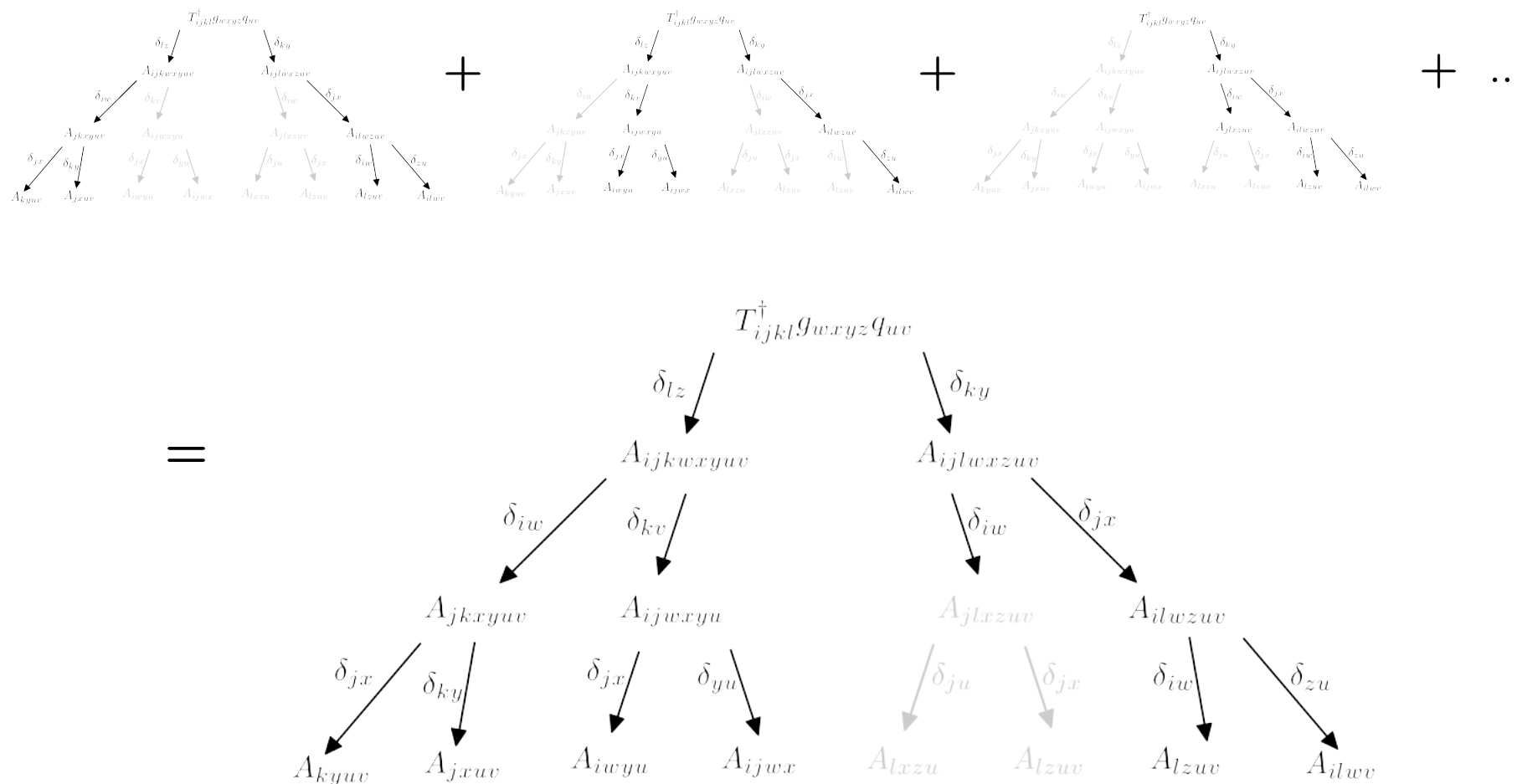
$$A_{lzuv}$$

$$A_{lzuv}$$

$$A_{ilwv}$$



Merge block specific contraction trees



Application of block symmetry



- The tree for each block is generated separately.
- Each vertex on the tree is an object which contains information about itself and it's position in the tree.
 - All requirements (vertexes higher up in the tree).
 - All dependents (vertexes lower in the tree).
- Due to the block symmetry several vertexes are equivalent, which can lead to redundancies.
- To avoid redundancies, block symmetry should be accounted for not just in the final contraction, but also in the construction of the tree.
- Currently, a very basic approach based on index substitution and standardized ordering is used.

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Application of block symmetry



- Currently, a very basic approach based on index substitution is used.
- All indexes are named, and the program reorders them so they always occur in a certain order.

	closed	active	virtual
closed			
active			
virtual			

Closed-virtual block

Id names : $\{x_0, x_1\}$

Ranges : $\{clo, vir\}$

CA ops : $\{a^\dagger, a\}$

Virtual-closed block

Id names : $\{x_1, x_0\}$

Ranges : $\{clo, vir\}$

CA ops : $\{a^\dagger, a\}$

Contraction of γ_{ijklmn}^I and A_{ijklmn}



- Final step is to contract the A-tensor with the reduced density matrix or similar terms :

$$\sum_{ijklmn}^{act} \sum_J \langle I | a_i^\dagger a_j a_k^\dagger a_l a_m^\dagger a_n | J \rangle c_J A_{ijklmn}$$

- Aim to avoid storing the six index reduced density matrix derivative term in memory.
- One possible approach is to consider contributions to the A-tensor individually, enabling us to avoid evaluation of any density matrices with more than three indices :

$$\begin{aligned} & \sum_J \sum_{ijkl} H_{ijkl}^\dagger T_{lnop} \langle I | i j k^\dagger l^\dagger n^\dagger o | J \rangle c_J^N \\ &= \sum_{ijkl} H_{ijkl}^\dagger \sum_K^{lnop} \langle I | i j k^\dagger | K \rangle \sum_{lnop} \sum_J T_{lnop} \langle K | l^\dagger n^\dagger o | J \rangle c_J^N \end{aligned}$$

Contraction of γ_{ijklmn}^I and A_{ijklmn}



- May be evaluated by the following sequence:

$$\sum_{ijkp} H_{ijkp}^\dagger \sum_K \langle I | ijk^\dagger | K \rangle \sum_{lno} \sum_J T_{lnop} \langle K | l^\dagger n^\dagger o | J \rangle c_J^N$$

(1)	$\sum_{LJ}^{N_{det}} \langle K l^\dagger L \rangle \langle L n^\dagger o J \rangle c_J^N = \sigma_{lno}^K$	$N_{act}^3 N_{det}(J)$
(2)	$\sum_{nop}^{N_{act}} T_{lnop} \sigma_{lno}^K = \tilde{x}_p^K$	$N_{act}^3 N_{rng(p)} N_{det}(K)$
(3)	$\sum_l^{N_{rng(p)}} H_{ijkp}^\dagger \tilde{x}_p^K = \tilde{w}_{ijk}^K$	$N_{act}^3 N_{rng(p)} N_{det}(K)$
(4)	$\sum_{ijk}^{N_{act}} \sum_K^{N_{det}} \langle I ijk^\dagger K \rangle \tilde{w}_{ijk}^K = \tilde{c}^I$	$N_{act}^3 N_{rng(p)} N_{det}(K)$

Contraction of γ_{ijklmn}^I and A_{ijklmn}



$$\sum_{ijkp} H_{ijkp}^\dagger \sum_K \langle I | ijk^\dagger | K \rangle \sum_{lno} \sum_J T_{lnop} \langle K | l^\dagger n^\dagger o | J \rangle c_J^N$$

- Avoid storing the rdm derivatives and A-tensor at the cost of recalculating the third order rdm multiple times.
- Key advantage is that rdm derivatives (or similar) and large A-tensor terms are not stored.
- Only the ci-vector and relevant tensor blocks are required; reduces communication.
- No reordering of indexes of large tensors.
- Becomes very costly if there are multiple contractions between different tensors, due to the occurrence of N_{virt}^2 terms.