This document is meant to help me organize my thoughts. I kept losing track of indices and factors while doing this by hand. I want expressions that can be easily and efficiently implemented.

Index convention:

$$a, b, c, d, ... = \text{particles},$$
$$i, j, k, l, ... = \text{holes},$$
$$p, q, r, s, ... = \text{either}.$$

One- and two- body operators have the following form:

$$A^{(1)} = \sum_{pq} A_{pq} : a_p^\dagger a_q :, \tag{1}$$

$$A^{(2)} = \frac{1}{4} \sum_{pqrs} A_{pqrs} : a_p^\dagger a_q^\dagger a_s a_r :, \tag{2}$$

where the colons indicate normal ordering. I want to write a function that returns the zero-, one-, and two-body components of the commutator

$$[A^{(1)} + A^{(2)}, B^{(1)} + B^{(2)}]. \tag{3}$$

I will name these components $C^{(0)}$, $C^{(1)}$, and $C^{(2)}$, respectively. Note: the three-body component will be omitted. Since this commutator is equivalent to the following sum of commutators

$$[A^{(1)}, B^{(1)}] + [A^{(1)}, B^{(2)}] + [A^{(2)}, B^{(1)}] + [A^{(2)}, B^{(2)}], \tag{4}$$

we can use the fundamental commutator expressions to evaluate each term. For reference, I will write the relevant expressions here:

$$[A^{(1)}, B^{(1)}]^{(0)} = \sum_{pq} (n_p - n_q) A_{pq} B_{qp}, \tag{5}$$

$$[A^{(1)}, B^{(1)}]^{(1)} = \sum_{pq} \sum_{r} : a_p^\dagger a_q : (A_{pr} B_{rq} - B_{pr} A_{rq}), \tag{6}$$

$$[A^{(1)}, B^{(2)}]^{(1)} = \sum_{pq} \sum_{rs} : a_p^\dagger a_q : (n_r - n_s) A_{rs} B_{sprq}, \tag{7}$$

$$[A^{(1)}, B^{(2)}]^{(2)} = \frac{1}{4} \sum_{pqrs} \sum_{t} : a_p^\dagger a_q^\dagger a_s a_r : \{(1 - P_{pq}) A_{pt} B_{tqrs} - (1 - P_{rs}) A_{tr} B_{pqts}\}, \tag{8}$$

$$[A^{(2)}, B^{(1)}]^{(1)} = -[B^{(1)}, A^{(2)}]^{(1)} = \sum_{pq} \sum_{rs} : a_p^\dagger a_q : (n_s - n_r) B_{rs} A_{sprq}, \tag{9}$$

$$[A^{(2)}, B^{(1)}]^{(2)} = -[B^{(1)}, A^{(2)}]^{(2)} = \frac{1}{4} \sum_{pqrs} \sum_{t} : a_p^\dagger a_q^\dagger a_s a_r : \{(1 - P_{rs}) B_{tr} A_{pqts} - (1 - P_{pq}) B_{pt} A_{tqrs}\}, \tag{10}$$

$$[A^{(2)}, B^{(2)}]^{(0)} = \frac{1}{4} \sum_{pqrs} n_p n_q \bar{n}_r \bar{n}_s (A_{pqrs} B_{rspq} - B_{pqrs} A_{rspq}), \tag{11}$$

$$[A^{(2)}, B^{(2)}]^{(1)} = \frac{1}{2} \sum_{pq} \sum_{rst} : a_p^\dagger a_q : (\bar{n}_r \bar{n}_s n_t + n_r n_s \bar{n}_t)(A_{tprs} B_{rstq} - B_{tprs} A_{rstq}), \tag{12}$$

$$[A^{(2)}, B^{(2)}]^{(2)} = \frac{1}{4} \sum_{pqrs} \sum_{tu} : a_p^\dagger a_q^\dagger a_s a_r : \Big\{ \frac{1}{2} (1 - n_t - n_u)(A_{pqtu} B_{turs} - B_{pqtu} A_{turs}) \tag{13}$$

$$+ (n_t - n_u)(1 - P_{pq})(1 - P_{rs}) A_{tpur} B_{uqts} \Big\} \tag{14}$$

Now, we can simplify this a bit because many of the terms in the summations vanish. Using the index notation mentioned above, the zero-body component is

$$C^{(0)} = \sum_{pq}(n_p - n_q)A_{pq}B_{qp} + \frac{1}{4}\sum_{pqrs} n_p n_q \bar{n}_r \bar{n}_s (A_{pqrs}B_{rspq} - B_{pqrs}A_{rspq}), \tag{15}$$

$$= \sum_{ia}(A_{ia}B_{ai} - A_{ai}B_{ia}) + \frac{1}{4}\sum_{ijab}(A_{ijab}B_{abij} - B_{ijab}A_{abij}) \tag{16}$$

Note: when $A^{(2)} = \eta^{(2)}$ and $B^{(2)} = \Gamma = H^{(2)}$, the second term in (16) can be simplified further to

$$\frac{1}{2}\sum_{ijab}\eta_{ijab}\Gamma_{abij}, \tag{17}$$

because $\eta_{ijab} = -\eta_{abij}$ and $\Gamma_{ijab} = \Gamma_{abij}$.

The one-body component simplifies to

$$C^{(1)} = \sum_{pq}\sum_{r} : a_p^\dagger a_q : (A_{pr}B_{rq} - B_{pr}A_{rq}) \tag{18}$$

$$+ \sum_{pq}\sum_{rs} : a_p^\dagger a_q : (n_r - n_s)A_{rs}B_{sprq} + \sum_{pq}\sum_{rs} : a_p^\dagger a_q : (n_s - n_r)B_{rs}A_{sprq} \tag{19}$$

$$+ \frac{1}{2}\sum_{pq}\sum_{rst} : a_p^\dagger a_q : (\bar{n}_r\bar{n}_s n_t + n_r n_s \bar{n}_t)(A_{tprs}B_{rstq} - B_{tprs}A_{rstq}), \tag{20}$$

$$= \sum_{pq}\sum_{r} : a_p^\dagger a_q : (A_{pr}B_{rq} - B_{pr}A_{rq}) \tag{21}$$

$$+ \sum_{pq}\sum_{rs} : a_p^\dagger a_q : (n_r - n_s)(A_{rs}B_{sprq} - B_{rs}A_{sprq}) \tag{22}$$

$$+ \frac{1}{2}\sum_{pq}\sum_{rst} : a_p^\dagger a_q : (n_r n_s + n_t(1 - n_r - n_s))(A_{tprs}B_{rstq} - B_{tprs}A_{rstq}), \tag{23}$$

$$= \sum_{pq}\sum_{r} : a_p^\dagger a_q : (A_{pr}B_{rq} - B_{pr}A_{rq}) \tag{24}$$

$$+ \sum_{pq}\sum_{ia} : a_p^\dagger a_q : (A_{ia}B_{apiq} - B_{ia}A_{apiq} + B_{ai}A_{ipaq} - A_{ai}B_{ipaq}) \tag{25}$$

$$+ \frac{1}{2}\sum_{pq}\sum_{rst} : a_p^\dagger a_q : n_r n_s (A_{tprs}B_{rstq} - B_{tprs}A_{rstq}) \tag{26}$$

$$+ \frac{1}{2}\sum_{pq}\sum_{rsi} : a_p^\dagger a_q : (1 - n_r - n_s)(A_{iprs}B_{rsiq} - B_{iprs}A_{rsiq}), \tag{27}$$

$$= \sum_{pq} : a_p^\dagger a_q : \Bigg\{ \sum_{r}(A_{pr}B_{rq} - B_{pr}A_{rq}) \tag{28}$$

$$+ \sum_{ia}(A_{ia}B_{apiq} - B_{ia}A_{apiq} + B_{ai}A_{ipaq} - A_{ai}B_{ipaq}) \tag{29}$$

$$+ \frac{1}{2}\sum_{rst} n_r n_s (A_{tprs}B_{rstq} - B_{tprs}A_{rstq}) \tag{30}$$

$$+ \frac{1}{2}\sum_{rsi}(1 - n_r - n_s)(A_{iprs}B_{rsiq} - B_{iprs}A_{rsiq}) \Bigg\} \tag{31}$$

And the two-body component is

$$C^{(2)} = \frac{1}{4}\sum_{pqrs}\sum_{t} : a_p^\dagger a_q^\dagger a_s a_r : \{(1-P_{pq})A_{pt}B_{tqrs} - (1-P_{rs})A_{tr}B_{pqts}\} \tag{32}$$

$$+ \frac{1}{4}\sum_{pqrs}\sum_{t} : a_p^\dagger a_q^\dagger a_s a_r : \{(1-P_{rs})B_{tr}A_{pqts} - (1-P_{pq})B_{pt}A_{tqrs}\} \tag{33}$$

$$+ \frac{1}{4}\sum_{pqrs}\sum_{tu} : a_p^\dagger a_q^\dagger a_s a_r : \Big\{\frac{1}{2}(A_{pqtu}B_{turs} - B_{pqtu}A_{turs})(1-n_t-n_u) \tag{34}$$

$$+ (n_t-n_u)(1-P_{ij})(1-P_{kl})A_{tpur}B_{uqts}\Big\}, \tag{35}$$

$$= \frac{1}{4}\sum_{pqrs}\sum_{t} : a_p^\dagger a_q^\dagger a_s a_r : \{(1-P_{pq})(A_{pt}B_{tqrs} - B_{pt}A_{tqrs}) - (1-P_{rs})(A_{tr}B_{pqts} - B_{tr}A_{pqts})\} \tag{36}$$

$$+ \frac{1}{4}\sum_{pqrs}\sum_{tu} : a_p^\dagger a_q^\dagger a_s a_r : \Big\{\frac{1}{2}(A_{pqtu}B_{turs} - B_{pqtu}A_{turs})(1-n_t-n_u) \tag{37}$$

$$+ (n_t-n_u)(1-P_{ij})(1-P_{kl})A_{tpur}B_{uqts}\Big\}, \tag{38}$$

$$= \frac{1}{4}\sum_{pqrs} : a_p^\dagger a_q^\dagger a_s a_r : \Big\{\sum_{t}(1-P_{pq})(A_{pt}B_{tqrs} - B_{pt}A_{tqrs}) - (1-P_{rs})(A_{tr}B_{pqts} - B_{tr}A_{pqts}) \tag{39}$$

$$+ \sum_{tu}\big\{\frac{1}{2}(A_{pqtu}B_{turs} - B_{pqtu}A_{turs})(1-n_t-n_u) + (n_t-n_u)(1-P_{pq})(1-P_{rs})A_{tpur}B_{uqts}\big\}\Big\}, \tag{40}$$

$$\tag{41}$$