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:

$$a, b, c, d, \dots =$$
particles,  
 $i, j, k, l, \dots =$ holes,  
 $p, q, r, s, \dots =$ 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

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

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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$+\frac{1}{2}\sum_{pq}\sum_{rst}:a_{p}^{\dagger}a_{q}:(n_{r}n_{s}+n_{t}(1-n_{r}-n_{s}))(A_{tprs}B_{rstq}-B_{tprs}A_{rstq}),$$
(23)

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

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

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

$$+\frac{1}{2}\sum_{pq}\sum_{rsi}:a_{p}^{\dagger}a_{q}:(1-n_{r}-n_{s})(A_{iprs}B_{rsiq}-B_{iprs}A_{rsiq}),$$
(27)

$$= \sum_{pq} : a_p^{\dagger} a_q : \left\{ \sum_r (A_{pr} B_{rq} - B_{pr} A_{rq}) \right\}$$
 (28)

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

$$\tag{29}$$

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

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

And the two-body component is

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

$$+\frac{1}{4}\sum_{pars}\sum_{t}:a_{p}^{\dagger}a_{q}^{\dagger}a_{s}a_{r}:\{(1-P_{rs})B_{tr}A_{pqts}-(1-P_{pq})B_{pt}A_{tqrs}\}$$
(33)

$$+\frac{1}{4}\sum_{pqrs}\sum_{tu}:a_{p}^{\dagger}a_{q}^{\dagger}a_{s}a_{r}:\left\{\frac{1}{2}(A_{pqtu}B_{turs}-B_{pqtu}A_{turs})(1-n_{t}-n_{u})\right\}$$
(34)

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

$$= \frac{1}{4} \sum_{pqrs} \sum_{t} : a_{p}^{\dagger} a_{q}^{\dagger} a_{s} a_{r} : \{ (1 - P_{pq})(A_{pt} B_{tqrs} - B_{pt} A_{tqrs}) - (1 - P_{rs})(A_{tr} B_{pqts} - B_{tr} A_{pqts}) \}$$
(36)

$$+\frac{1}{4}\sum_{pqrs}\sum_{tu}:a_{p}^{\dagger}a_{q}^{\dagger}a_{s}a_{r}:\left\{\frac{1}{2}(A_{pqtu}B_{turs}-B_{pqtu}A_{turs})(1-n_{t}-n_{u})\right\}$$
(37)

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

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

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

(41)