

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:

$a, b, c, d, \dots = \text{particles},$

$i, j, k, l, \dots = \text{holes},$

$p, q, r, s, \dots = \text{either}.$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\left. + (n_t - n_u) (1 - P_{pq}) (1 - P_{rs}) A_{tpur} B_{uqts} \right\} \quad (14)$$

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

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

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

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

$$\frac{1}{2} \sum_{ijab} \eta_{ijab} \Gamma_{abij}, \quad (17)$$

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

The one-body component simplifies to

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

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

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

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

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

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

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

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

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

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

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

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

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

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

And the two-body component is

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

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

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

$$\left. + (n_t - n_u) (1 - P_{ij}) (1 - P_{kl}) A_{tpur} B_{uqts} \right\}, \quad (35)$$

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

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

$$\left. + (n_t - n_u) (1 - P_{ij}) (1 - P_{kl}) A_{tpur} B_{uqts} \right\}, \quad (38)$$

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

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

$$(41)$$