

## 1 Equations

### 1.1 Diagram components of $\bar{H}$

These are the equations for the components of  $\bar{H}$ .

$$\text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3} \quad (1.1.1)$$

$$\begin{aligned}
& \text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} \\
& + \text{Diagram 5} + \text{Diagram 6}
\end{aligned}
\tag{1.1.2}$$

$$\begin{aligned}
& \text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} \\
& + \text{Diagram 5} + \text{Diagram 6}
\end{aligned}
\tag{1.1.3}$$

[illegible]

$$\begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \end{array} \text{---} \text{wavy line} \text{---} \begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \end{array} = \begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \end{array} \text{---} \text{dashed line} \text{---} \begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \end{array} \quad (1.1.5)$$

$$\begin{array}{c} \diagdown \\ | \\ \text{---} w \text{---} \\ | \\ \diagup \end{array} = \begin{array}{c} \diagdown \\ | \\ \text{---} \\ | \\ \diagup \end{array} + \begin{array}{c} \diagdown \\ | \\ \text{---} \\ | \\ \diagup \end{array} \quad (1.1.6)$$

$$\begin{array}{c} \diagdown \\ \text{---} \\ \diagup \end{array} \begin{array}{c} \diagup \\ \text{---} \\ \diagdown \end{array} = \begin{array}{c} \diagdown \\ \text{---} \\ \diagup \end{array} \begin{array}{c} \text{---} \\ \diagup \end{array} \begin{array}{c} \diagdown \\ \text{---} \\ \diagup \end{array} + \begin{array}{c} \diagdown \\ \text{---} \\ \diagup \end{array} \begin{array}{c} \diagup \\ \text{---} \\ \diagdown \end{array} \begin{array}{c} \diagup \\ \text{---} \\ \diagdown \end{array} \begin{array}{c} \diagdown \\ \text{---} \\ \diagup \end{array} \begin{array}{c} \diagup \\ \text{---} \\ \diagdown \end{array} \quad (1.1.7)$$

$$\begin{aligned}
& \text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + \text{Diagram 5} \\
& \text{Diagram 1: } \text{Two vertices connected by a wavy line.} \\
& \text{Diagram 2: } \text{Two vertices connected by a dashed line.} \\
& \text{Diagram 3: } \text{Two vertices connected by a dashed line, with a loop on the right.} \\
& \text{Diagram 4: } \text{Two vertices connected by a dashed line, with a loop on the left.} \\
& \text{Diagram 5: } \text{Two vertices connected by a dashed line, with a loop on both sides.}
\end{aligned}
\tag{1.1.8}$$

$$\begin{aligned}
& \text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} \\
& \text{Diagram 5}
\end{aligned}
\tag{1.1.9}$$

$$\begin{aligned}
 & \text{Diagram 1} = \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + \text{Diagram 5} + \text{Diagram 6} \\
 & \text{Diagram 7} + \text{Diagram 8} \quad (1.1.10)
 \end{aligned}$$

Diagram (1.1.11) shows the expansion of a vertex correction. The left-hand side is a vertex with two incoming fermion lines and one outgoing fermion line, connected by a wavy line. The right-hand side is a sum of diagrams representing the expansion of this vertex. The first row shows three diagrams with a dashed line and a fermion loop. The second row shows three diagrams with a dashed line and a fermion loop, and a diagram with a dashed line and a fermion loop. The third row shows three diagrams with a dashed line and a fermion loop. The fourth row shows two diagrams with a dashed line and a fermion loop. The fifth row shows one diagram with a dashed line and a fermion loop. The label (1.1.11) is at the bottom right.

Diagram (1.1.12) shows the expansion of a vertex correction. The left-hand side is a vertex with two incoming fermion lines and one outgoing fermion line, connected by a wavy line. The right-hand side is a sum of diagrams representing the expansion of this vertex. The first row shows three diagrams with a dashed line and a fermion loop. The second row shows three diagrams with a dashed line and a fermion loop. The third row shows three diagrams with a dashed line and a fermion loop. The fourth row shows two diagrams with a dashed line and a fermion loop. The fifth row shows one diagram with a dashed line and a fermion loop. The label (1.1.12) is at the bottom right.

4

## 1.2 Algebraic components of $\bar{H}$

$$I_{ia} = f_{ia} + \langle ik||ac\rangle t_k^c \quad (1.2.1)$$

$$I_b^a = f_{ab} - f_{kb}t_k^a + \langle ak||bc\rangle t_k^c - \langle kl||bc\rangle t_k^a t_l^c - \frac{1}{2}\langle kl||bc\rangle t_{kl}^{ac} \quad (1.2.2)$$

$$I_i^j = f_{ij} + f_{ic}t_j^c + \langle ik||jc\rangle t_k^c + \langle ik||cd\rangle t_j^c t_k^d + \frac{1}{2}\langle ik||cd\rangle t_{jk}^{cd} \quad (1.2.3)$$

$$\begin{aligned} I^{ai} &= f_{ai} + f_{ac}t_i^c - f_{ki}t_k^a + \langle ka||ci\rangle t_k^c + f_{kc}t_{ik}^{ac} + \frac{1}{2}\langle ak||cd\rangle t_{ik}^{cd} \\ &\quad - \frac{1}{2}\langle kl||ci\rangle t_{kl}^{ca} - f_{kc}t_i^c t_k^a + \langle ak||cd\rangle t_i^c t_k^d - \langle kl||ci\rangle t_k^c t_l^a + \langle kl||cd\rangle t_k^c t_{li}^{da} \\ &\quad - \frac{1}{2}\langle kl||cd\rangle t_i^c t_{kl}^{ad} - \frac{1}{2}\langle kl||cd\rangle t_l^a t_{ki}^{cd} - \langle kl||cd\rangle t_i^c t_k^a t_c^d \end{aligned} \quad (1.2.4)$$

$$I_{ijab} = \langle ij||ab\rangle \quad (1.2.5)$$

$$I_{ibc}^a = \langle ai||bc\rangle - \langle mi||bc\rangle t_m^a \quad (1.2.6)$$

$$I_{ika}^j = \langle ik||ja\rangle + \langle ik||ea\rangle t_j^e \quad (1.2.7)$$

$$\begin{aligned} I_{cd}^{ab} &= \langle ab||cd\rangle - P(ab)\langle am||cd\rangle t_m^b + \frac{1}{2}\langle mn||cd\rangle t_{mn}^{ab} \\ &\quad + P(ab)\langle mn||cd\rangle t_m^a t_n^b \end{aligned} \quad (1.2.8)$$

$$\begin{aligned} I_{ij}^{kl} &= \langle ij||kl\rangle + P(kl)\langle ij||ke\rangle t_l^e + \frac{1}{2}\langle ij||ef\rangle t_{kl}^{ef} \\ &\quad + P(kl)\langle ij||ef\rangle t_k^e t_l^f \end{aligned} \quad (1.2.9)$$

$$\begin{aligned} I_{ib}^{aj} &= \langle ia||bj\rangle + \langle ai||eb\rangle t_j^e - \langle mi||jb\rangle t_m^a \langle mi||eb\rangle t_{jm}^{ae} \\ &\quad - \langle mi||eb\rangle t_j^e t_m^a \end{aligned} \quad (1.2.10)$$

$$\begin{aligned} I_c^{abi} &= \langle ab||ci\rangle + \langle ab||ce\rangle t_i^e - P(ab)\langle mb||ci\rangle t_m^a + P(ab)\langle am||ce\rangle t_{mi}^{eb} + \frac{1}{2}\langle mn||ic\rangle t_{mn}^{ab} \\ &\quad - f_{mc}t_{im}^{ab} - P(ab)\langle am||ce\rangle t_i^e t_m^b + P(ab)\langle mn||ic\rangle t_m^a t_n^b + P(ab)\langle mn||ec\rangle t_i^e t_{mn}^{ab} \\ &\quad - P(ab)\langle mn||ce\rangle t_m^a t_{ni}^{eb} - \langle mn||ec\rangle t_m^e t_{ni}^{ab} + P(ab)\langle mn||ce\rangle t_m^a t_i^e t_n^b \end{aligned} \quad (1.2.11)$$

$$\begin{aligned} I_i^{ajk} &= \langle ia||jk\rangle - \langle im||jk\rangle t_m^a + P(jk)\langle ia||ek\rangle t_j^e + f_{ic}t_{jk}^{ac} + \frac{1}{2}\langle ai||ef\rangle t_{jk}^{ef} - \langle mi||je\rangle t_{mk}^{ae} \\ &\quad + P(jk)\langle ai||ef\rangle t_j^e t_k^f - P(jk)\langle mi||je\rangle t_m^a t_k^e + P(jk)\langle im||ef\rangle t_j^e t_{mk}^{fa} \\ &\quad - \frac{1}{2}\langle im||ef\rangle t_{jk}^{ef} t_m^a + \langle mi||ef\rangle t_m^e t_{jk}^{fa} - P(jk)\langle im||ef\rangle t_j^e t_k^f t_m^a \end{aligned} \quad (1.2.12)$$

$$\begin{aligned}
I^{abij} = & \langle ab||ij\rangle + P(ij)\langle ab||ej\rangle t_i^e - P(ab)\langle am||ij\rangle t_m^b + P(ab)f_{be}t_{ij}^{ae} - P(ij)f_{mi}t_{mj}^{ab} \\
& + \frac{1}{2}\langle ab||ef\rangle t_{ij}^{ef} + \frac{1}{2}\langle mn||ij\rangle t_{mn}^{ab} + P(ij)P(ab)\langle mb||ej\rangle t_{im}^{ae} \\
& + \frac{1}{2}P(ij)\langle ab||ef\rangle t_i^e t_j^f + \frac{1}{2}P(ab)\langle mn||ij\rangle t_m^a t_n^b - P(ij)P(ab)\langle mb||ej\rangle t_i^e t_m^a \\
& + \frac{1}{4}\langle mn||ef\rangle t_{ij}^{ef} t_{mn}^{ab} + \frac{1}{2}P(ij)P(ab)\langle mn||ef\rangle t_{im}^{ae} t_{nj}^{fb} - \frac{1}{2}P(ab)\langle mn||ef\rangle t_{ij}^{ae} t_{mn}^{bf} \\
& - \frac{1}{2}P(ij)\langle mn||ef\rangle t_{mi}^{ef} t_{nj}^{ab} - P(ij)f_{me}t_i^e t_{mj}^{ab} - P(ab)f_{mc}t_{ij}^{ae} t_m^b \\
& + P(ij)P(ab)\langle am||ef\rangle t_i^e t_{mj}^{fb} - \frac{1}{2}P(ab)\langle am||ef\rangle t_{ij}^{ef} t_m^b + P(ab)\langle bm||ef\rangle t_{ij}^{ae} t_m^f \\
& - P(ij)P(ab)\langle mn||ej\rangle t_{im}^{ae} t_n^b + \frac{1}{2}P(ij)\langle mn||ej\rangle t_i^e t_{mn}^{ab} - P(ij)\langle mn||ei\rangle t_m^e t_{nj}^{ab} \\
& - \frac{1}{2}P(ij)P(ab)\langle am||ef\rangle t_i^e t_j^f t_m^b + \frac{1}{2}P(ij)P(ab)\langle mn||ej\rangle t_i^e t_m^a t_n^b \\
& + \frac{1}{4}P(ij)\langle mn||ef\rangle t_i^e t_{mn}^{ab} t_j^f - P(ij)P(ab)\langle mn||ef\rangle t_i^e t_m^a t_{nj}^{fb} \\
& + \frac{1}{4}P(ab)\langle mn||ef\rangle t_m^a t_{ij}^{ef} t_n^b - P(ij)\langle mn||ef\rangle t_m^e t_i^f t_{mj}^{ab} - P(ab)\langle mn||ef\rangle t_{ij}^{ae} t_m^b t_n^f \\
& + \frac{1}{4}P(ij)P(ab)\langle mn||ef\rangle t_i^e t_m^a t_j^f t_n^b
\end{aligned} \tag{1.2.13}$$

## 2 Two particle attached EOM CCSD

### 2.1 Diagram equations

$$\begin{aligned}
 (\bar{H}R)^{ab} = & \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} \\
 & + \text{Diagram 4}
 \end{aligned}
 \tag{2.1.1}$$

The diagrams in (2.1.1) represent the following terms:

- Diagram 1: A horizontal line with an upward arrow on the left and a diagonal arrow on the right. A wavy line connects the right end of the horizontal line to the diagonal arrow.
- Diagram 2: A horizontal line with a diagonal arrow on the left and an upward arrow on the right. A wavy line connects the diagonal arrow to the right end of the horizontal line.
- Diagram 3: A horizontal line with an upward arrow on the left and a vertical arrow on the right. A wavy line connects the right end of the horizontal line to the vertical arrow.
- Diagram 4: A horizontal line with an upward arrow on the left and a diagonal arrow on the right. A wavy line connects the right end of the horizontal line to the diagonal arrow.

$$\begin{aligned}
 (\bar{H}R)_i^{abc} = & \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} \\
 & + \text{Diagram 4} + \text{Diagram 5}
 \end{aligned}
 \tag{2.1.2}$$

The diagrams in (2.1.2) represent the following terms:

- Diagram 1: A horizontal line with an upward arrow on the left and a diagonal arrow on the right. A wavy line connects the right end of the horizontal line to the diagonal arrow.
- Diagram 2: A horizontal line with a diagonal arrow on the left and an upward arrow on the right. A wavy line connects the diagonal arrow to the right end of the horizontal line.
- Diagram 3: A horizontal line with an upward arrow on the left and a vertical arrow on the right. A wavy line connects the right end of the horizontal line to the vertical arrow.
- Diagram 4: A horizontal line with an upward arrow on the left and a diagonal arrow on the right. A wavy line connects the right end of the horizontal line to the diagonal arrow.
- Diagram 5: A horizontal line with an upward arrow on the left and a diagonal arrow on the right. A wavy line connects the right end of the horizontal line to the diagonal arrow.

### 2.2 Algebraic equations

$$(\bar{H}R)^{ab} = P(ab)I_e^b r^{ae} + \frac{1}{2}I_{ef}^{ab} r^{ef} + I_{me} r_m^{abe} + \frac{1}{2}P(ab)I_{mef}^b r_m^{aef} \tag{2.2.1}$$

$$\begin{aligned}
 (\bar{H}R)_i^{abc} = & P(ab)P(ac)I_e^{bci} r^{ae} + P(ac)P(bc)I_e^c r_i^{abe} - P(ac)P(bc)I_m^i r_m^{abc} \\
 & + \frac{1}{2}P(ac)P(bc)I_{ef}^{ab} r_i^{efc} + P(ac)P(bc)I_{me}^{ci} r_m^{abe}
 \end{aligned}
 \tag{2.2.2}$$

$$\tag{2.2.3}$$

### 3 Two particle removed EOM CCSD

#### 3.1 Diagram equations

$$\begin{aligned}
 (\bar{H}R)^{ab} = & \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} \\
 & + \text{Diagram 4}
 \end{aligned}
 \tag{3.1.1}$$

The diagrams in (3.1.1) represent the two-particle removed EOM CCSD equation for the  $(\bar{H}R)^{ab}$  component. Diagram 1 shows a horizontal line with a vertical line entering from the left and a diagonal line exiting to the right, with a wavy line attached to the diagonal line. Diagram 2 shows a horizontal line with a vertical line entering from the left and a diagonal line entering from the right, with a wavy line attached to the diagonal line. Diagram 3 shows a horizontal line with a vertical line entering from the left and a vertical line exiting to the right, with a wavy line attached to the vertical line. Diagram 4 shows a horizontal line with a vertical line entering from the left and a diagonal line entering from the right, with a wavy line attached to the diagonal line.

$$\begin{aligned}
 (\bar{H}R)_i^{abc} = & \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} \\
 & + \text{Diagram 4} + \text{Diagram 5}
 \end{aligned}
 \tag{3.1.2}$$

The diagrams in (3.1.2) represent the two-particle removed EOM CCSD equation for the  $(\bar{H}R)_i^{abc}$  component. Diagram 1 shows a horizontal line with a vertical line entering from the left and a diagonal line exiting to the right, with a wavy line attached to the diagonal line. Diagram 2 shows a horizontal line with a vertical line entering from the left and a diagonal line entering from the right, with a wavy line attached to the diagonal line. Diagram 3 shows a horizontal line with a vertical line entering from the left and a vertical line exiting to the right, with a wavy line attached to the vertical line. Diagram 4 shows a horizontal line with a vertical line entering from the left and a diagonal line entering from the right, with a wavy line attached to the diagonal line. Diagram 5 shows a horizontal line with a vertical line entering from the left and a diagonal line entering from the right, with a wavy line attached to the diagonal line.

#### 3.2 Algebraic equations

$$\begin{aligned}
 (\bar{H}R)_{ij} = & -P(ij)I_m^j r_{im} + \frac{1}{2}I_{mn}^{ij} r_{mn} + I_{me} r_{ijm}^e \\
 & - \frac{1}{2}P(ij)I_{mne}^j r_{imn}^e
 \end{aligned}
 \tag{3.2.1}$$

$$\begin{aligned}
 (\bar{H}R)_{ijk}^e = & -P(ij)P(ik)I_m^{ajk} r_{im} + I_e^a r_{ijk}^e - P(ik)P(jk)I_m^k r_{ijm}^a \\
 & + \frac{1}{2}P(ik)P(jk)I_{mn}^{ij} r_{mnk}^a + P(ik)P(jk)I_{me}^{ak} r_{ijm}^e
 \end{aligned}
 \tag{3.2.2}$$

$$\tag{3.2.3}$$