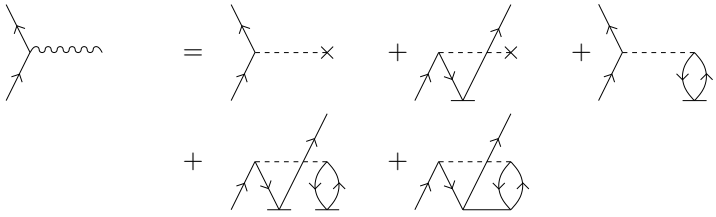
1 Equations

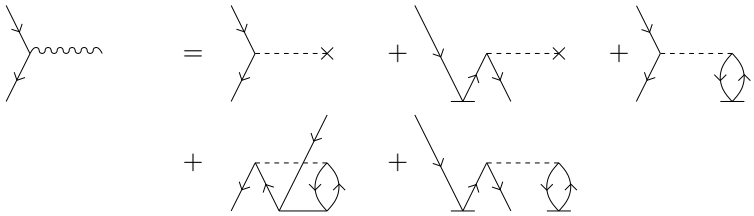
1.1 Diagram components of $\bar{H}$

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

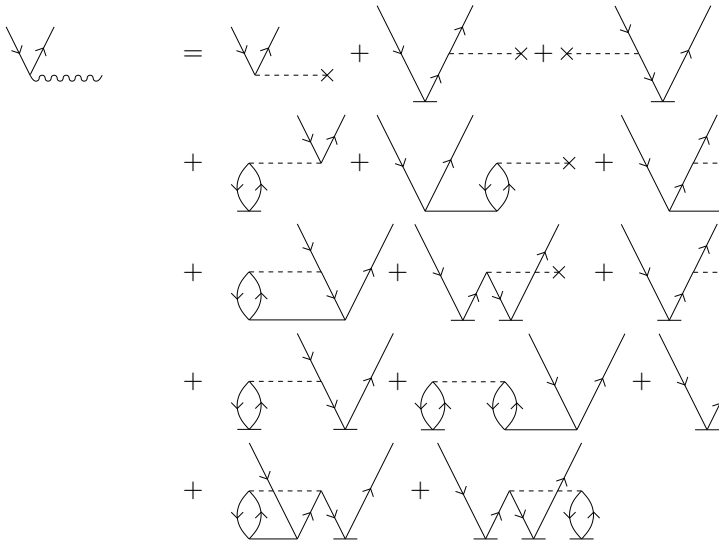
(1.1.1)



(1.1.2)

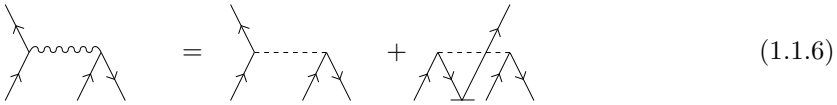


(1.1.3)

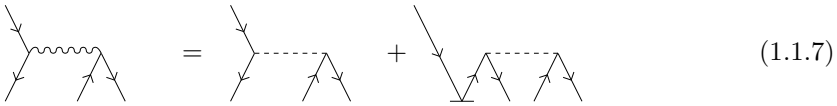


(1.1.4)

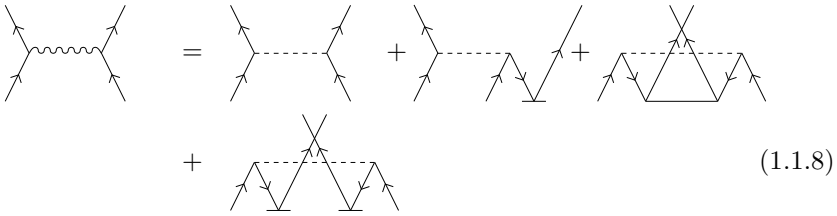
(1.1.5)



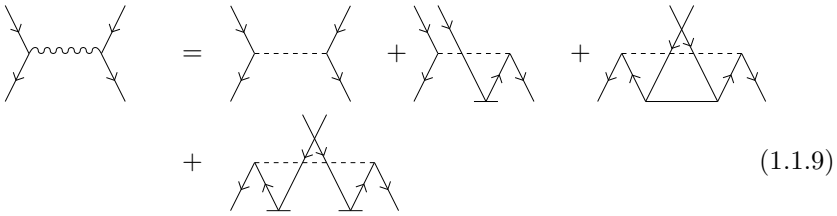
(1.1.6)



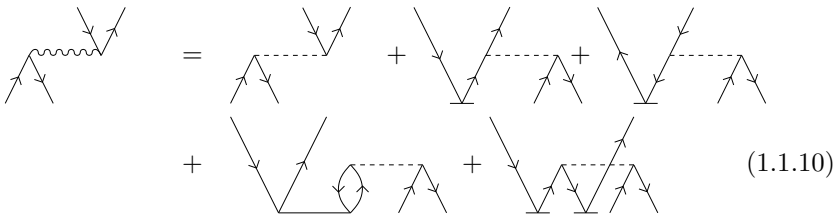
(1.1.7)



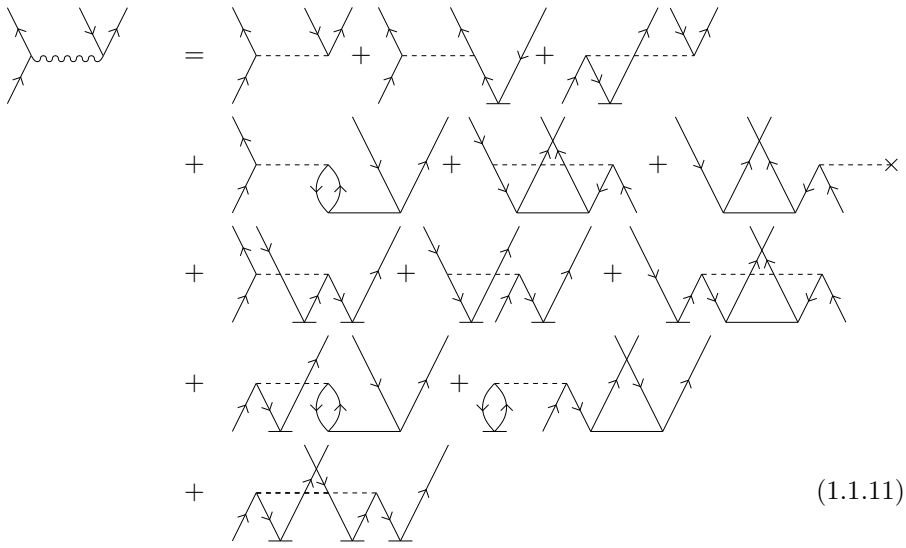
(1.1.8)



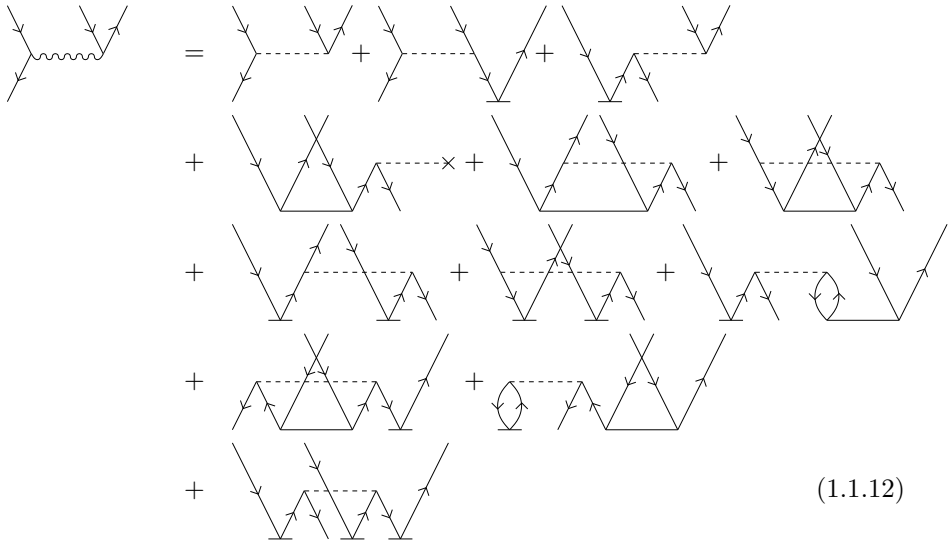
(1.1.9)



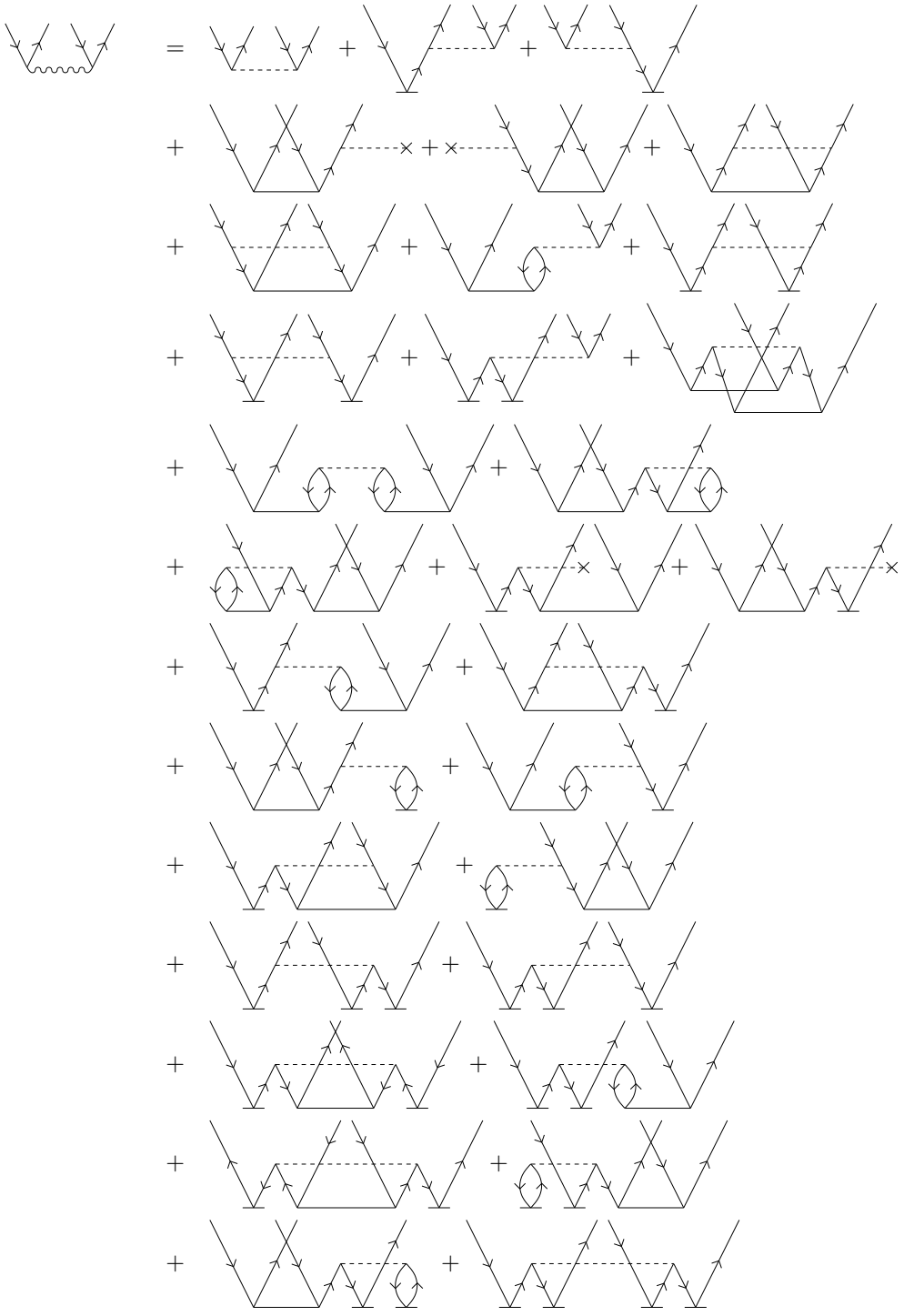
(1.1.10)



(1.1.11)



(1.1.12)



(1.1.13)

1.2 Algebraic components of $\bar{H}$

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

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

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

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

$$I_{ijab} = \langle ij||ab\rangle \tag{1.2.5}$$

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

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

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

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

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

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

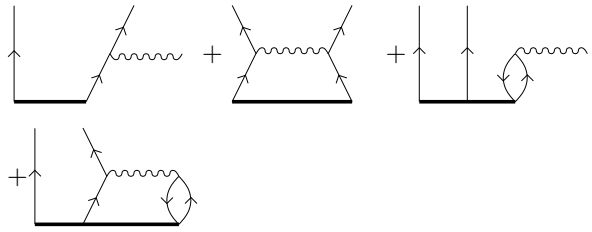
$$\begin{aligned} I_i^{ajk} = {} & \langle ia||jk\rangle - \langle im||jk\rangle t_m^a + P(jk)\langle ia||ek\rangle t_j^e + f_{ic}t_{jk}^{ac} + \frac{1}{2}\langle ai||ef\rangle t_{jk}^{ef} - \langle mi||je\rangle t_{mk}^{ae} \\ & +P(jk)\langle ai||ef\rangle t_j^e t_k^f - P(jk)\langle mi||je\rangle t_m^a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

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

2 Two particle attatched EOM CCSD

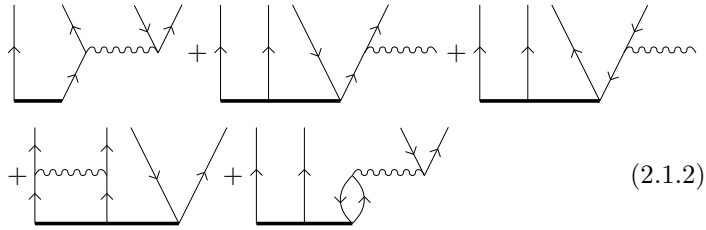
2.1 Diagram equations

$\left(\bar{H}R\right)^{ab}$ =



(2.1.1)

$\left(\bar{H}R\right)_{i}^{abc}$ =



(2.1.2)

2.2 Algebraic equations

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

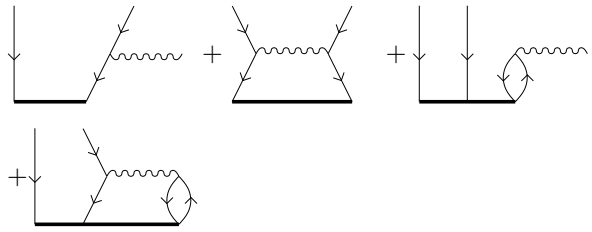
$$\begin{aligned}\left(\bar{H}R\right)_{i}^{abc} = {} & P(ab)P(ac)I_{e}^{bci}r^{ae} + P(ac)P(bc)I_{e}^{c}r_{i}^{abe} - P(ac)P(bc)I_{m}^{i}r_{m}^{abc} \\ & + \frac{1}{2}P(ac)P(bc)I_{ef}^{ab}r_{i}^{efc} + P(ac)P(bc)I_{me}^{ci}r_{m}^{abe} \end{aligned} \tag{2.2.2}$$

(2.2.3)

3 Two particle removed EOM CCSD

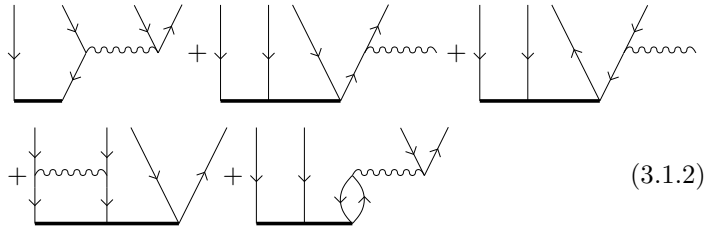
3.1 Diagram equations

$\left(\bar{H}R\right)^{ab}$ =



(3.1.1)

$\left(\bar{H}R\right)_{i}^{abc}$ =



(3.1.2)

3.2 Algebraic equations

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

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

(3.2.3)