

I. EXPRESSIONS FOR \bar{H} (UP TO TRIPLE COMMUTATORS)

A. E_{gr}

The ground state energy comprises the Hartree-Fock energy and the correlation energy. The latter is the fully contracted part of \bar{H} . We collect all contributions up to triple commutators for E_{gr} . $[O, \sigma]$ can yield a fully contracted contribution only when O is non-diagonal. The expression for E_{gr} is given by

$$E_{gr} = E_{\text{HF}} + \left(\sum_{ijab} \frac{1}{8} \langle ij || ab \rangle \sigma_{ij}^{ab} + \sum_{ijab} \frac{1}{12} \langle ij || ab \rangle \sigma_i^a \sigma_j^b + h.c. \right) \quad (1)$$

$$+ \left(- \sum_{ijklabcd} \frac{1}{12} (\sigma_{kl}^{cd})^* \langle ij || ab \rangle \sigma_{ik}^{ac} \sigma_{jl}^{bd} - \sum_{ijklabcd} \frac{1}{24} (\sigma_{kl}^{cd})^* \langle ij || ab \rangle \sigma_{ij}^{ac} \sigma_{kl}^{bd} \right. \\ \left. - \sum_{ijklabcd} \frac{1}{24} (\sigma_{kl}^{cd})^* \langle ij || ab \rangle \sigma_{ik}^{ab} \sigma_{jl}^{cd} - \sum_{ijklabcd} \frac{1}{96} (\sigma_{kl}^{cd})^* \langle ij || ab \rangle \sigma_{ij}^{cd} \sigma_{kl}^{ab} + h.c. \right) \quad (2)$$

$$+ \left(\sum_{ijklabc} \frac{1}{4} (\sigma_{jl}^{bc})^* \langle ik || aj \rangle \sigma_i^a \sigma_{kl}^{bc} - \sum_{ijkabcd} \frac{1}{4} (\sigma_{jk}^{cd})^* \langle ic || ab \rangle \sigma_i^a \sigma_{jk}^{bd} \right. \\ + \sum_{ijklabc} \frac{1}{2} (\sigma_{il}^{bc})^* \langle kj || ai \rangle \sigma_j^b \sigma_{lk}^{ca} - \sum_{ijkabcd} \frac{1}{2} (\sigma_{jk}^{cd})^* \langle ic || ab \rangle \sigma_j^b \sigma_{ik}^{ad} \\ + \sum_{ijklabc} \frac{1}{12} (\sigma_{il}^{bc})^* \langle jk || ia \rangle \sigma_l^c \sigma_{kj}^{ab} - \sum_{ijkabcd} \frac{1}{12} (\sigma_{jk}^{cd})^* \langle ic || ab \rangle \sigma_k^d \sigma_{ij}^{ab} \\ \left. + \sum_{ijklabc} \frac{1}{8} (\sigma_{il}^{cb})^* \langle kj || ia \rangle \sigma_l^a \sigma_{kj}^{cb} - \sum_{ijkabcd} \frac{1}{8} (\sigma_{jk}^{dc})^* \langle ci || ab \rangle \sigma_i^d \sigma_{kj}^{ab} + h.c. \right) \quad (3)$$

$$+ \left(- \sum_{ijkabc} \frac{1}{12} (\sigma_k^c)^* \langle ij || ab \rangle \sigma_i^a \sigma_{jk}^{bc} - \sum_{ijkabc} \frac{1}{12} (\sigma_k^c)^* \langle ij || ab \rangle \sigma_i^c \sigma_{jk}^{ba} \right. \\ - \sum_{ijkabc} \frac{1}{12} (\sigma_k^c)^* \langle ij || ab \rangle \sigma_k^a \sigma_{ij}^{cb} - \sum_{ijkabc} \frac{1}{3} (\sigma_{ik}^{bc})^* \langle jb || ai \rangle \sigma_j^c \sigma_k^a \\ - \sum_{ijklab} \frac{1}{12} (\sigma_{ij}^{ab})^* \langle kl || ij \rangle \sigma_k^a \sigma_l^b - \sum_{ijabcd} \frac{1}{12} (\sigma_{ij}^{cd})^* \langle cd || ab \rangle \sigma_j^b \sigma_i^a + h.c. \left. \right) \quad (4)$$

$$+ \left(+ \sum_{ijkab} \frac{1}{3} (\sigma_k^b)^* \langle ij || ak \rangle \sigma_i^a \sigma_j^b - \sum_{ijabc} \frac{1}{3} (\sigma_j^a)^* \langle ai || bc \rangle \sigma_j^b \sigma_i^c + h.c. \right). \quad (5)$$

B. \bar{H}_{ai}

$$\bar{H}_{ai}^{[1]} = \sum_{jb} \langle aj||ib \rangle \sigma_j^b + \sum_{jb} \frac{1}{2} (\sigma_j^b)^* \langle ab||ij \rangle + \sum_{jbc} \frac{1}{2} \langle aj||cb \rangle \sigma_{ij}^{cb} - \sum_{jkb} \frac{1}{2} \langle kj||ib \rangle \sigma_{jk}^{ba}. \quad (6)$$

$$\begin{aligned} \bar{H}_{ai}^{[2]} = & \left(\sum_{jbc} \langle aj||cb \rangle \sigma_j^b \sigma_i^c - \sum_{jkb} \langle kj||ib \rangle \sigma_j^b \sigma_k^a + \sum_{jbc} \frac{1}{2} (\sigma_j^b)^* \langle ab||cj \rangle \sigma_i^c - \sum_{jkb} \frac{1}{2} (\sigma_j^b)^* \langle kb||ij \rangle \sigma_k^a \right. \\ & \left. + \sum_{jbc} \frac{1}{2} (\sigma_j^c)^* \langle ac||ib \rangle \sigma_j^b - \sum_{jkb} \frac{1}{2} (\sigma_j^b)^* \langle ak||ij \rangle \sigma_k^b \right) \end{aligned} \quad (7)$$

$$\begin{aligned} & + \left(\sum_{jkbc} \frac{5}{12} \langle jk||bc \rangle \sigma_j^b \sigma_{ik}^{ac} - \sum_{jkbc} \frac{1}{3} \langle jk||bc \rangle \sigma_k^a \sigma_{ij}^{cb} - \sum_{jkbc} \frac{1}{3} \langle jk||bc \rangle \sigma_i^c \sigma_{jk}^{ba} \right. \\ & - \sum_{jkbc} \frac{1}{2} (\sigma_k^c)^* \langle cj||ib \rangle \sigma_{jk}^{ba} - \sum_{jkbc} \frac{1}{2} (\sigma_k^c)^* \langle aj||kb \rangle \sigma_{ij}^{cb} - \sum_{jkbc} \frac{1}{3} (\sigma_{jk}^{cb})^* \langle ab||ij \rangle \sigma_k^c \\ & - \sum_{jkbc} \frac{1}{6} (\sigma_{jk}^{bc})^* \langle bc||ji \rangle \sigma_k^a - \sum_{jkbc} \frac{1}{6} (\sigma_{jk}^{bc})^* \langle ab||kj \rangle \sigma_i^c + \sum_{jbcd} \frac{1}{4} (\sigma_j^c)^* \langle ac||bd \rangle (\sigma_{ij}^{bd})^* \\ & \left. + \sum_{jklb} \frac{1}{4} (\sigma_k^b)^* \langle jl||ik \rangle (\sigma_{jl}^{ab})^* \right) \end{aligned} \quad (8)$$

$$\begin{aligned} & + \left(- \sum_{jklbc} \frac{1}{2} (\sigma_{jk}^{bc})^* \langle al||ik \rangle \sigma_{jl}^{bc} + \sum_{jkbcd} \frac{1}{2} (\sigma_{jk}^{bd})^* \langle ad||ic \rangle \sigma_{jk}^{bc} - \sum_{jklbc} (\sigma_{jk}^{bc})^* \langle bl||ji \rangle \sigma_{kl}^{ca} \right. \\ & + \sum_{jkbcd} (\sigma_{jk}^{bc})^* \langle ab||dj \rangle \sigma_{ki}^{cd} - \sum_{jklbc} \frac{1}{4} (\sigma_{jk}^{bc})^* \langle bl||jk \rangle \sigma_{il}^{ac} + \sum_{jkbcd} \frac{1}{4} (\sigma_{jk}^{bd})^* \langle bd||jc \rangle \sigma_{ik}^{ac} \\ & \left. + \sum_{jklbc} \frac{1}{4} (\sigma_{jk}^{bd})^* \langle bd||ic \rangle \sigma_{jk}^{ca} - \sum_{jkbcd} \frac{1}{4} (\sigma_{jk}^{bc})^* \langle al||jk \rangle \sigma_{il}^{cb} \right). \end{aligned} \quad (9)$$

$$\begin{aligned} \bar{H}_{ai}^{[3]} = & \left(- \sum_{jkbc} \frac{7}{12} \langle jk||bc \rangle \sigma_j^a \sigma_i^b \sigma_k^c + \sum_{jklb} \frac{1}{2} (\sigma_l^b)^* \langle jk||il \rangle \sigma_k^b \sigma_j^a + \sum_{jbcd} \frac{1}{2} (\sigma_j^b)^* \langle ab||cd \rangle \sigma_j^d \sigma_i^c \right. \\ & - \sum_{jkbc} \frac{1}{3} (\sigma_k^c)^* \langle jk||bi \rangle \sigma_j^b \sigma_k^a - \sum_{jkbc} \frac{1}{3} (\sigma_k^c)^* \langle ja||bk \rangle \sigma_j^b \sigma_i^c - \sum_{jkbc} \frac{1}{6} (\sigma_k^c)^* \langle jc||bk \rangle \sigma_i^b \sigma_j^a \\ & \left. + \sum_{jkbc} \frac{1}{6} (\sigma_k^c)^* \langle ja||bi \rangle \sigma_j^c \sigma_k^b + \sum_{jkbc} \frac{1}{2} (\sigma_k^c)^* \langle jc||bi \rangle \sigma_j^a \sigma_k^b + \sum_{jkbc} \frac{1}{2} (\sigma_k^c)^* \langle ja||bk \rangle \sigma_j^c \sigma_i^b \right) \end{aligned}$$

$$\begin{aligned}
& + \sum_{jklbc} \frac{1}{8} (\sigma_k^c)^* (\sigma_j^b)^* \langle bc || ji \rangle \sigma_k^a - \sum_{jklbc} \frac{1}{8} (\sigma_k^c)^* (\sigma_j^b)^* \langle ab || kj \rangle \sigma_i^c + \sum_{jklbc} \frac{1}{6} (\sigma_k^b)^* (\sigma_j^c)^* \langle ab || ij \rangle \sigma_k^c \Big) \quad (10) \\
& + \left(\sum_{jklbc} \frac{1}{12} (\sigma_l^c)^* \langle jk || bl \rangle \sigma_{ij}^{ab} \sigma_k^c - \sum_{jklbcd} \frac{1}{12} (\sigma_k^c)^* \langle jc || bd \rangle \sigma_{ij}^{ab} \sigma_k^d + \sum_{jklbc} \frac{1}{6} (\sigma_l^c)^* \langle jk || bl \rangle \sigma_{ij}^{cb} \sigma_k^a \right. \\
& - \sum_{jklbcd} \frac{1}{6} (\sigma_k^c)^* \langle jc || bd \rangle \sigma_{jk}^{ba} \sigma_i^d + \sum_{jklbc} \frac{1}{6} (\sigma_l^c)^* \langle jk || bi \rangle \sigma_{jl}^{ba} \sigma_k^c + \sum_{jklbcd} \frac{1}{6} (\sigma_k^d)^* \langle ja || bc \rangle \sigma_{ij}^{db} \sigma_k^c \\
& + \sum_{jklbc} \frac{1}{12} (\sigma_l^c)^* \langle jk || bl \rangle \sigma_{ki}^{ca} \sigma_j^b - \sum_{jklbcd} \frac{1}{12} (\sigma_k^c)^* \langle jc || bd \rangle \sigma_{ki}^{da} \sigma_j^b + \sum_{jklbc} \frac{1}{12} (\sigma_l^c)^* \langle jk || bl \rangle \sigma_{jk}^{ac} \sigma_i^b \\
& - \sum_{jklbcd} \frac{1}{12} (\sigma_k^c)^* \langle jc || bd \rangle \sigma_{ik}^{bd} \sigma_j^a - \sum_{jklbc} \frac{1}{12} (\sigma_l^c)^* \langle jk || bi \rangle \sigma_{kj}^{ac} \sigma_l^b + \sum_{jklbcd} \frac{1}{12} (\sigma_k^d)^* \langle ja || bc \rangle \sigma_{ik}^{cb} \sigma_j^d \\
& + \sum_{jklbc} \frac{1}{6} (\sigma_{kl}^{cb})^* \langle jb || kl \rangle \sigma_j^a \sigma_i^c - \sum_{jklbcd} \frac{1}{6} (\sigma_{kj}^{bc})^* \langle bc || dj \rangle \sigma_k^a \sigma_i^d - \sum_{jklbc} \frac{1}{3} (\sigma_{kl}^{bc})^* \langle jb || ik \rangle \sigma_j^a \sigma_l^c \\
& + \sum_{jklbcd} \frac{1}{3} (\sigma_{jk}^{bd})^* \langle ab || cj \rangle \sigma_i^c \sigma_k^d + \sum_{jklbc} \frac{1}{3} (\sigma_{kl}^{bc})^* \langle jb || ik \rangle \sigma_j^c \sigma_l^a - \sum_{jklbcd} \frac{1}{3} (\sigma_{jk}^{bd})^* \langle ab || cj \rangle \sigma_k^c \sigma_i^d \\
& + \sum_{jklbc} \frac{1}{6} (\sigma_{kl}^{cb})^* \langle ja || lk \rangle \sigma_j^b \sigma_i^c + \sum_{jklbcd} \frac{1}{6} (\sigma_{jk}^{bc})^* \langle bc || di \rangle \sigma_j^d \sigma_k^a \\
& + \sum_{jklbc} \frac{1}{2} (\sigma_k^c)^* (\sigma_l^b)^* \langle jb || kl \rangle \sigma_{ij}^{ac} - \sum_{jklbcd} \frac{1}{2} (\sigma_k^b)^* (\sigma_j^c)^* \langle bc || dj \rangle \sigma_{ik}^{ad} + \sum_{jklbc} \frac{1}{4} (\sigma_k^b)^* (\sigma_l^c)^* \langle jb || ik \rangle \sigma_{jl}^{ac} \\
& - \sum_{jklbcd} \frac{1}{4} (\sigma_k^d)^* (\sigma_j^b)^* \langle ab || cj \rangle \sigma_{ik}^{cd} + \sum_{jklbc} \frac{1}{4} (\sigma_k^b)^* (\sigma_l^c)^* \langle ja || ki \rangle \sigma_{jl}^{bc} - \sum_{jklbcd} \frac{1}{4} (\sigma_k^d)^* (\sigma_j^b)^* \langle ab || ic \rangle \sigma_{jk}^{cd} \Big) \quad (11) \\
& + \left(- \sum_{jklbcd} \frac{1}{8} (\sigma_l^d)^* \langle jk || bc \rangle \sigma_{ij}^{ab} \sigma_{kl}^{cd} - \sum_{jklbcd} \frac{1}{24} (\sigma_l^d)^* \langle jk || bc \rangle \sigma_{kj}^{ca} \sigma_{li}^{db} + \sum_{jklbcd} \frac{1}{48} (\sigma_l^d)^* \langle jk || bc \rangle \sigma_{ik}^{bc} \sigma_{lj}^{da} \right. \\
& - \sum_{jklbcd} \frac{1}{6} (\sigma_j^b)^* \langle kl || cd \rangle \sigma_{ik}^{bc} \sigma_{lj}^{da} + \sum_{jklbcd} \frac{1}{24} (\sigma_l^d)^* \langle jk || bc \rangle \sigma_{il}^{bc} \sigma_{kj}^{da} \\
& - \sum_{jklmbc} \frac{1}{12} (\sigma_{lm}^{cb})^* \langle jk || il \rangle \sigma_{jk}^{bc} \sigma_m^a - \sum_{jklbcd} \frac{1}{12} (\sigma_{jk}^{eb})^* \langle ab || cd \rangle \sigma_{kj}^{dc} \sigma_i^e + \sum_{jklmbc} \frac{1}{6} (\sigma_{lm}^{bc})^* \langle jk || li \rangle \sigma_{jk}^{ba} \sigma_m^c \\
& + \sum_{jklbcd} \frac{1}{6} (\sigma_{kj}^{eb})^* \langle ab || cd \rangle \sigma_{ij}^{cd} \sigma_k^e + \sum_{jklmbc} \frac{5}{24} (\sigma_{ml}^{cb})^* \langle jk || lm \rangle \sigma_{ki}^{ca} \sigma_j^b + \sum_{jklbcd} \frac{5}{24} (\sigma_{jk}^{bc})^* \langle bc || de \rangle \sigma_{ik}^{ae} \sigma_j^d \\
& + \sum_{jklmbc} \frac{1}{2} (\sigma_{lm}^{bc})^* \langle jk || il \rangle \sigma_{mk}^{cb} \sigma_j^a + \sum_{jklbcd} \frac{1}{2} (\sigma_{jk}^{be})^* \langle ab || cd \rangle \sigma_{jk}^{de} \sigma_i^c - \sum_{jklmbc} \frac{1}{6} (\sigma_{ml}^{cb})^* \langle jk || lm \rangle \sigma_{ik}^{bc} \sigma_j^a \\
& - \sum_{jklbcd} \frac{1}{6} (\sigma_{jk}^{bc})^* \langle bc || ed \rangle \sigma_{jk}^{ad} \sigma_i^e + \sum_{jklmbc} (\sigma_{lm}^{bc})^* \langle jk || il \rangle \sigma_{jm}^{ac} \sigma_k^b + \sum_{jklbcd} (\sigma_{jk}^{be})^* \langle ab || cd \rangle \sigma_{ik}^{ce} \sigma_j^d
\end{aligned}$$

$$\begin{aligned}
& - \sum_{jklbcd} \frac{1}{6} (\sigma_{kl}^{cd})^* \langle jc || bi \rangle \sigma_{kl}^{ad} \sigma_j^b - \sum_{jklbcd} \frac{1}{6} (\sigma_{kl}^{cd})^* \langle ja || bk \rangle \sigma_{il}^{cd} \sigma_j^b - \sum_{jklbcd} \frac{1}{3} (\sigma_{kl}^{cd})^* \langle jc || bk \rangle \sigma_{jl}^{ba} \sigma_i^d \\
& - \sum_{jklbcd} \frac{1}{3} (\sigma_{kl}^{cd})^* \langle jc || bk \rangle \sigma_{ji}^{bd} \sigma_l^a - \sum_{jklbcd} \frac{1}{3} (\sigma_{kl}^{cd})^* \langle jc || bi \rangle \sigma_{jk}^{ba} \sigma_l^d - \sum_{jklbcd} \frac{1}{3} (\sigma_{kl}^{cd})^* \langle ja || bk \rangle \sigma_{ij}^{cb} \sigma_l^d \\
& - \sum_{jklbcd} \frac{1}{3} (\sigma_{kl}^{cd})^* \langle ja || bk \rangle \sigma_{jl}^{bd} \sigma_i^c - \sum_{jklbcd} \frac{1}{3} (\sigma_{kl}^{cd})^* \langle jc || bi \rangle \sigma_{jl}^{bd} \sigma_k^a + \sum_{jklbcd} \frac{1}{2} (\sigma_{kl}^{cd})^* \langle ja || bi \rangle \sigma_{jl}^{cd} \sigma_k^b \\
& + \sum_{jklbcd} \frac{1}{3} (\sigma_{kl}^{cd})^* \langle ja || bi \rangle \sigma_{kl}^{bd} \sigma_j^c + \sum_{jklbcd} \frac{1}{3} (\sigma_{il}^{cd})^* \langle jc || bi \rangle \sigma_{kl}^{bd} \sigma_j^a + \sum_{jklbcd} \frac{1}{2} (\sigma_{kl}^{cd})^* \langle ja || bk \rangle \sigma_{jl}^{cd} \sigma_i^b \\
& - \sum_{jklbcd} \frac{2}{3} (\sigma_{kl}^{cd})^* \langle jc || bk \rangle \sigma_{jl}^{ad} \sigma_i^b + \sum_{jklbcd} \frac{2}{3} (\sigma_{kl}^{cd})^* \langle jc || bk \rangle \sigma_{il}^{bd} \sigma_j^a + \sum_{jklbcd} (\sigma_{kl}^{cd})^* \langle jc || bi \rangle \sigma_{jl}^{ad} \sigma_k^b \\
& + \sum_{jklbcd} (\sigma_{kl}^{cd})^* \langle ja || bk \rangle \sigma_{li}^{db} \sigma_j^c - \sum_{jklbcd} \frac{1}{2} (\sigma_{kl}^{cd})^* \langle jc || bi \rangle \sigma_{kl}^{ab} \sigma_j^d - \sum_{jklbcd} \frac{1}{2} (\sigma_{kl}^{cd})^* \langle ja || bk \rangle \sigma_{ij}^{cd} \sigma_l^b \\
& + \sum_{jklbcd} \frac{5}{12} (\sigma_{kl}^{cd})^* \langle jc || bk \rangle \sigma_{ij}^{ad} \sigma_l^b + \sum_{jklbcd} \frac{5}{12} (\sigma_{kl}^{cd})^* \langle jc || bk \rangle \sigma_{il}^{ab} \sigma_j^d \\
& + \sum_{jklbcd} \frac{1}{16} (\sigma_j^b)^* (\sigma_{kl}^{cd})^* \langle bc || ji \rangle \sigma_{kl}^{ad} \Bigg) \tag{12} \\
& + \left(- \sum_{jklmbcd} \frac{1}{24} (\sigma_{ml}^{dc})^* \langle jk || bl \rangle \sigma_{jk}^{bc} \sigma_{mi}^{da} + \sum_{jklbcde} \frac{1}{24} (\sigma_{kl}^{ce})^* \langle jc || bd \rangle \sigma_{jk}^{bd} \sigma_{li}^{ea} + \sum_{jklmbcd} \frac{1}{12} (\sigma_{lm}^{cd})^* \langle jk || bl \rangle \sigma_{jk}^{ba} \sigma_{im}^{cd} \right. \\
& - \sum_{jklbcde} \frac{1}{12} (\sigma_{kl}^{ce})^* \langle jc || bd \rangle \sigma_{ij}^{db} \sigma_{kl}^{ae} - \sum_{jklmbcd} \frac{1}{4} (\sigma_{lm}^{cd})^* \langle jk || bl \rangle \sigma_{ji}^{ba} \sigma_{km}^{cd} + \sum_{jklbcde} \frac{1}{4} (\sigma_{kl}^{ce})^* \langle jc || bd \rangle \sigma_{ij}^{ab} \sigma_{kl}^{de} \\
& + \sum_{jklmbcd} \frac{1}{3} (\sigma_{ml}^{dc})^* \langle jk || bi \rangle \sigma_{lj}^{ab} \sigma_{km}^{cd} - \sum_{jklbcde} \frac{1}{3} (\sigma_{lk}^{ed})^* \langle ja || bc \rangle \sigma_{ji}^{bd} \sigma_{kl}^{ce} - \sum_{jklmbcd} \frac{2}{3} (\sigma_{lm}^{cd})^* \langle jk || bi \rangle \sigma_{jl}^{bc} \sigma_{km}^{ad} \\
& + \sum_{jklbcde} \frac{2}{3} (\sigma_{kl}^{de})^* \langle ja || bc \rangle \sigma_{jk}^{bd} \sigma_{il}^{ce} - \sum_{jklmbcd} (\sigma_{lm}^{cd})^* \langle jk || bl \rangle \sigma_{ij}^{cb} \sigma_{km}^{ad} - \sum_{jklbcde} (\sigma_{kl}^{ce})^* \langle jc || bd \rangle \sigma_{jk}^{ba} \sigma_{il}^{de} \\
& - \sum_{jklmbcd} \frac{1}{2} (\sigma_{ml}^{dc})^* \langle jk || bl \rangle \sigma_{jm}^{bd} \sigma_{ik}^{ac} + \sum_{jklbcde} \frac{1}{2} (\sigma_{kl}^{ce})^* \langle jc || bd \rangle \sigma_{jl}^{be} \sigma_{ik}^{ad} \\
& + \sum_{jklmbcd} \frac{1}{2} (\sigma_{lm}^{cd})^* \langle jk || bl \rangle \sigma_{jm}^{ba} \sigma_{ik}^{dc} - \sum_{jklbcde} \frac{1}{2} (\sigma_{kl}^{ce})^* \langle jc || bd \rangle \sigma_{ji}^{be} \sigma_{kl}^{da} + \sum_{jklmbcd} \frac{1}{2} (\sigma_{lm}^{cd})^* \langle jk || bl \rangle \sigma_{im}^{bd} \sigma_{jk}^{ac} \\
& - \sum_{jklmbcd} \frac{1}{2} (\sigma_{kl}^{ce})^* \langle jc || bd \rangle \sigma_{jl}^{ae} \sigma_{ik}^{bd} - \sum_{jklmbcd} \frac{1}{8} (\sigma_{lm}^{cd})^* \langle jk || bl \rangle \sigma_{im}^{ab} \sigma_{jk}^{dc} + \sum_{jklmbcd} \frac{1}{8} (\sigma_{ml}^{ec})^* \langle jc || bd \rangle \sigma_{ij}^{ae} \sigma_{ml}^{bd} \\
& - \sum_{jklmbcd} \frac{1}{6} (\sigma_{ml}^{dc})^* \langle jk || bi \rangle \sigma_{jk}^{ca} \sigma_{ml}^{db} + \sum_{jklbcde} \frac{1}{6} (\sigma_{lk}^{ed})^* \langle ja || bc \rangle \sigma_{jl}^{de} \sigma_{ik}^{cb} + \sum_{jklmbcd} \frac{1}{12} (\sigma_{ml}^{dc})^* \langle jk || bi \rangle \sigma_{jk}^{dc} \sigma_{lm}^{ab}
\end{aligned}$$

$$+ \sum_{jklmbcd} \frac{1}{12} (\sigma_{kl}^{de})^* \langle ja||bc \rangle \sigma_{ij}^{de} \sigma_{lk}^{bc} \rangle. \quad (13)$$

C. $\bar{H}_{ab,ij}$

$$\begin{aligned} \bar{H}_{ab,ij}^{[1]} = & \sum_c f_{ac} \sigma_{ij}^{cb} - \sum_k f_{ki} \sigma_{kj}^{ab} - P(ab) \sum_k \langle ka||ji \rangle \sigma_k^b + P(ij) \sum_c \langle ab||ic \rangle \sigma_j^c + \sum_{kl} \frac{1}{2} \langle kl||ij \rangle \sigma_{kl}^{ab} \\ & + \sum_{cd} \frac{1}{2} \langle ab||cd \rangle \sigma_{ij}^{cd} + P(ij) P(ab) \sum_{kc} \langle ak||ic \rangle \sigma_{jk}^{bc}. \end{aligned} \quad (14)$$

$$\begin{aligned} \bar{H}_{ab,ij}^{[2]} = & \left(P(ab) \sum_{kl} \frac{1}{2} \langle kl||ij \rangle \sigma_k^a \sigma_l^b - P(ij) P(ab) \sum_{kc} \langle ak||cj \rangle \sigma_i^c \sigma_k^b + P(ij) \sum_{cd} \frac{1}{2} \langle ab||cd \rangle \sigma_i^c \sigma_j^d \right. \\ & \left. - P(ab) \sum_{kc} \frac{1}{3} (\sigma_k^c)^* \langle ac||ij \rangle \sigma_k^b - P(ij) \sum_{kc} \frac{1}{3} (\sigma_k^c)^* \langle ab||ik \rangle \sigma_j^c \right) \end{aligned} \quad (15)$$

$$\begin{aligned} & + \left(-P(ij) \sum_{klc} (\sigma_l^c)^* \langle ck||lj \rangle \sigma_{ik}^{ab} + P(ab) \sum_{lcd} (\sigma_l^c)^* \langle bc||dl \rangle \sigma_{ij}^{ad} + P(ij) \sum_{lcd} \frac{1}{2} (\sigma_l^c)^* \langle ab||id \rangle \sigma_{jl}^{dc} \right. \\ & - P(ab) \sum_{klc} \frac{1}{2} (\sigma_l^c)^* \langle ak||ij \rangle \sigma_{kl}^{bc} + \sum_{klc} (\sigma_l^c)^* \langle ck||ji \rangle \sigma_{kl}^{ab} + P(ij) P(ab) \sum_{klc} (\sigma_l^c)^* \langle bk||li \rangle \sigma_{jk}^{ca} \\ & - P(ij) P(ab) \sum_{lcd} (\sigma_l^c)^* \langle ac||dj \rangle \sigma_{il}^{db} - \sum_{lcd} (\sigma_l^c)^* \langle ab||dl \rangle \sigma_{ij}^{dc} - P(ij) \sum_{klc} \langle kl||cj \rangle \sigma_k^c \sigma_{il}^{ab} \\ & + P(ab) \sum_{kcd} \langle kb||cd \rangle \sigma_k^c \sigma_{ij}^{ad} - P(ij) P(ab) \sum_{klc} \langle kl||cj \rangle \sigma_l^b \sigma_{ik}^{ac} + P(ij) P(ab) \sum_{kcd} \langle kb||cd \rangle \sigma_j^d \sigma_{ik}^{ac} \\ & \left. + P(ij) \frac{1}{2} \sum_{klc} \langle kl||ci \rangle \sigma_j^c \sigma_{kl}^{ba} - P(ab) \frac{1}{2} \sum_{kcd} \langle ka||cd \rangle \sigma_k^b \sigma_{ij}^{dc} \right) \end{aligned} \quad (16)$$

$$\begin{aligned} & + \left(P(ij) P(ab) \sum_{klcd} \frac{1}{3} \langle kl||cd \rangle \sigma_{ik}^{ac} \sigma_{jl}^{bd} + \sum_{klcd} \frac{1}{6} \langle kl||cd \rangle \sigma_{ij}^{cd} \sigma_{kl}^{ab} - P(ab) \sum_{klcd} \frac{1}{3} \langle kl||cd \rangle \sigma_{ij}^{ad} \sigma_{kl}^{cb} \right. \\ & - P(ij) \sum_{klcd} \frac{1}{3} \langle kl||cd \rangle \sigma_{il}^{ab} \sigma_{jk}^{dc} + P(ij) P(ab) \sum_{klcd} \frac{1}{3} (\sigma_{kl}^{cd})^* \langle ad||il \rangle \sigma_{jk}^{bc} + \sum_{klcd} \frac{1}{12} (\sigma_{kl}^{cd})^* \langle cd||ij \rangle \sigma_{kl}^{ab} \\ & + \sum_{klcd} \frac{1}{12} (\sigma_{kl}^{cd})^* \langle ab||kl \rangle \sigma_{ij}^{cd} - P(ab) \sum_{klcd} \frac{1}{6} (\sigma_{kl}^{cd})^* \langle ad||ij \rangle \sigma_{kl}^{cb} - P(ij) \sum_{klcd} \frac{1}{6} (\sigma_{kl}^{cd})^* \langle ab||il \rangle \sigma_{jk}^{dc} \\ & \left. - P(ij) \sum_{klcd} \frac{1}{6} (\sigma_{kl}^{cd})^* \langle cd||kj \rangle \sigma_{il}^{ab} - P(ab) \sum_{klcd} \frac{1}{6} (\sigma_{kl}^{cd})^* \langle bc||lk \rangle \sigma_{ij}^{ad} \right). \end{aligned} \quad (17)$$

$$\begin{aligned}
\bar{H}_{ab,ij}^{[3]} = & \left(P(ij)P(ab) \sum_{klc} \langle kl||ic \rangle \sigma_k^a \sigma_j^c \sigma_l^b - P(ij)P(ab) \sum_{kcd} \langle ak||dc \rangle \sigma_k^b \sigma_j^c \sigma_i^a \right. \\
& + P(ij)P(ab) \sum_{klc} \frac{1}{3} (\sigma_l^c)^* \langle ka||jl \rangle \sigma_k^b \sigma_i^c - P(ij) \sum_{kcd} \frac{1}{3} (\sigma_k^d)^* \langle ab||kc \rangle \sigma_j^c \sigma_i^d \\
& \left. + P(ab) \sum_{klc} \frac{1}{3} (\sigma_l^c)^* \langle kc||ji \rangle \sigma_k^b \sigma_i^a - P(ij)P(ab) \sum_{kcd} \frac{1}{3} (\sigma_k^d)^* \langle bd||ci \rangle \sigma_k^a \sigma_j^c \right) \\
& + \left(- P(ab) \sum_{klcd} \frac{7}{12} \langle kl||cd \rangle \sigma_{ij}^{ac} \sigma_k^b \sigma_l^d - P(ij) \sum_{klcd} \frac{7}{12} \langle kl||cd \rangle \sigma_{ik}^{ab} \sigma_j^c \sigma_l^d \right. \\
& - P(ij)P(ab) \sum_{klcd} \frac{3}{4} \langle kl||cd \rangle \sigma_{il}^{ad} \sigma_j^c \sigma_k^b + P(ab) \sum_{klcd} \frac{3}{8} \langle kl||cd \rangle \sigma_{ij}^{cd} \sigma_k^a \sigma_l^b \\
& + P(ij) \sum_{klcd} \frac{3}{8} \langle kl||cd \rangle \sigma_{kl}^{ab} \sigma_i^c \sigma_j^d \\
& - P(ij) \sum_{klmc} \frac{1}{6} (\sigma_m^c)^* \langle kl||mj \rangle \sigma_{kl}^{ab} \sigma_i^c - P(ab) \sum_{kcde} \frac{1}{6} (\sigma_k^c)^* \langle bc||de \rangle \sigma_{ji}^{de} \sigma_k^a \\
& + P(ij) \sum_{klmc} (\sigma_m^c)^* \langle kl||mi \rangle \sigma_{lj}^{ab} \sigma_k^c + P(ab) \sum_{kcde} (\sigma_k^c)^* \langle ac||de \rangle \sigma_{ij}^{db} \sigma_k^e \\
& + P(ij)P(ab) \sum_{klmc} (\sigma_m^c)^* \langle kl||im \rangle \sigma_{lj}^{cb} \sigma_k^a + P(ij)P(ab) \sum_{kcde} (\sigma_k^c)^* \langle ac||de \rangle \sigma_{kj}^{eb} \sigma_i^d \\
& + P(ab) \sum_{klmc} \frac{1}{2} (\sigma_m^c)^* \langle kl||ij \rangle \sigma_{lm}^{bc} \sigma_k^a + P(ij) \sum_{kcde} \frac{1}{2} (\sigma_k^e)^* \langle ab||cd \rangle \sigma_{kj}^{ed} \sigma_i^c \\
& - \sum_{klmc} \frac{2}{3} (\sigma_m^c)^* \langle kl||ij \rangle \sigma_{lm}^{ba} \sigma_k^c - \sum_{kcde} \frac{2}{3} (\sigma_k^e)^* \langle ab||cd \rangle \sigma_{ij}^{ed} \sigma_k^c \\
& - P(ij)P(ab) \sum_{klcd} \frac{1}{3} (\sigma_l^d)^* \langle ka||cl \rangle \sigma_{jk}^{bc} \sigma_i^d - P(ij)P(ab) \sum_{klcd} \frac{1}{3} (\sigma_l^d)^* \langle kd||ci \rangle \sigma_{jk}^{bc} \sigma_i^a \\
& - P(ab) \sum_{klcd} \frac{1}{3} (\sigma_l^d)^* \langle kb||cl \rangle \sigma_{ij}^{ad} \sigma_k^c - P(ij) \sum_{klcd} \frac{1}{3} (\sigma_l^d)^* \langle kd||cj \rangle \sigma_{il}^{ab} \sigma_k^c \\
& - P(ij) \sum_{klcd} \frac{2}{3} (\sigma_l^d)^* \langle kd||cl \rangle \sigma_{kj}^{ab} \sigma_i^c - P(ab) \sum_{klcd} \frac{2}{3} (\sigma_l^d)^* \langle kd||cl \rangle \sigma_{ij}^{cb} \sigma_k^a \\
& + P(ij)P(ab) \sum_{klcd} \frac{2}{3} (\sigma_l^d)^* \langle ka||ci \rangle \sigma_{jk}^{bd} \sigma_i^c + P(ij)P(ab) \sum_{klcd} \frac{2}{3} (\sigma_l^d)^* \langle ka||ci \rangle \sigma_{jl}^{bc} \sigma_k^d \\
& \left. - P(ij)P(ab) \sum_{klcd} \frac{1}{2} (\sigma_l^d)^* \langle ka||ci \rangle \sigma_{kl}^{bd} \sigma_j^c - P(ij)P(ab) \sum_{klcd} \frac{1}{2} (\sigma_l^d)^* \langle ka||ci \rangle \sigma_{jl}^{cd} \sigma_k^b \right)
\end{aligned} \tag{18}$$

$$\begin{aligned}
& + P(ij)P(ab) \sum_{klcd} (\sigma_l^d)^* \langle kd || ci \rangle \sigma_{ij}^{cb} \sigma_k^a + P(ij)P(ab) \sum_{klcd} (\sigma_l^d)^* \langle ka || cl \rangle \sigma_{jk}^{bd} \sigma_i^c \\
& + P(ij) \sum_{klcd} (\sigma_l^d)^* \langle kd || ci \rangle \sigma_{kj}^{ab} \sigma_l^c + P(ab) \sum_{klcd} (\sigma_l^d)^* \langle ka || cl \rangle \sigma_{ij}^{cb} \sigma_k^d \\
& + P(ij) \sum_{klcd} (\sigma_l^d)^* \langle kd || ci \rangle \sigma_{kl}^{ba} \sigma_j^c + P(ab) \sum_{klcd} (\sigma_l^d)^* \langle ka || cl \rangle \sigma_{ij}^{dc} \sigma_k^b \\
& - P(ij)P(ab) \sum_{klcd} \frac{1}{4} (\sigma_{kl}^{cd})^* \langle bc || jk \rangle \sigma_i^d \sigma_l^a + P(ij) \sum_{klcd} \frac{1}{8} (\sigma_{kl}^{cd})^* \langle ab || kl \rangle \sigma_i^c \sigma_j^d \\
& + P(ab) \sum_{klcd} \frac{1}{8} (\sigma_{kl}^{cd})^* \langle cd || ij \rangle \sigma_l^b \sigma_k^a - P(ij) \sum_{klcd} \frac{1}{4} (\sigma_{kl}^{cd})^* \langle ab || lj \rangle \sigma_k^c \sigma_i^d \\
& - P(ab) \sum_{klcd} \frac{1}{4} (\sigma_{kl}^{cd})^* \langle bd || ji \rangle \sigma_l^a \sigma_k^c + P(ij)P(ab) \sum_{klcd} \frac{1}{2} (\sigma_k^d)^* (\sigma_l^c)^* \langle ad || il \rangle \sigma_{kj}^{cb} \\
& - P(ij) \sum_{klcd} \frac{1}{8} (\sigma_k^c)^* (\sigma_l^d)^* \langle ab || lj \rangle \sigma_{ki}^{cd} - P(ab) \sum_{klcd} \frac{1}{8} (\sigma_k^c)^* (\sigma_l^d)^* \langle db || ij \rangle \sigma_{lk}^{ac} \\
& + \sum_{klcd} \frac{1}{4} (\sigma_k^c)^* (\sigma_j^d)^* \langle cd || ij \rangle \sigma_{kl}^{ab} + \sum_{klcd} \frac{1}{4} (\sigma_k^c)^* (\sigma_l^d)^* \langle ab || kl \rangle \sigma_{ij}^{cd} \\
& - P(ij) \sum_{klcd} \frac{7}{24} (\sigma_k^c)^* (\sigma_l^d)^* \langle cd || kj \rangle \sigma_{li}^{ba} - P(ab) \sum_{klcd} \frac{7}{24} (\sigma_k^c)^* (\sigma_l^d)^* \langle bc || lk \rangle \sigma_{ij}^{ad} \Big) \quad (19) \\
& + \left(- P(ij)P(ab) \sum_{klmcd} \frac{2}{3} (\sigma_m^d)^* \langle kl || cm \rangle \sigma_{ik}^{ac} \sigma_{jl}^{bd} + P(ij)P(ab) \sum_{klcde} \frac{2}{3} (\sigma_l^d)^* \langle kd || ce \rangle \sigma_{ik}^{ac} \sigma_{jl}^{be} \right. \\
& - P(ij)P(ab) \sum_{klmcd} \frac{1}{2} (\sigma_m^d)^* \langle kl || cj \rangle \sigma_{ik}^{ac} \sigma_{lm}^{bd} + P(ij)P(ab) \sum_{klcde} \frac{1}{2} (\sigma_l^e)^* \langle kb || cd \rangle \sigma_{ik}^{ac} \sigma_{jl}^{de} \\
& - P(ij) \sum_{klmcd} \frac{1}{2} (\sigma_m^d)^* \langle kl || cj \rangle \sigma_{il}^{ab} \sigma_{km}^{cd} + P(ab) \sum_{klcde} \frac{1}{2} (\sigma_l^e)^* \langle bk || cd \rangle \sigma_{ij}^{ac} \sigma_{kl}^{de} \\
& + P(ij) \sum_{klmcd} \frac{2}{3} (\sigma_m^d)^* \langle kl || ic \rangle \sigma_{km}^{ab} \sigma_{jl}^{dc} + P(ij)P(ab) \sum_{klmcd} \frac{2}{3} (\sigma_m^d)^* \langle kl || jc \rangle \sigma_{ik}^{ad} \sigma_{ml}^{bc} \\
& - P(ij)P(ab) \sum_{klcde} \frac{2}{3} (\sigma_l^e)^* \langle kb || cd \rangle \sigma_{il}^{ad} \sigma_{kj}^{ce} - P(ab) \sum_{klcde} \frac{2}{3} (\sigma_l^e)^* \langle ka || cd \rangle \sigma_{ij}^{de} \sigma_{kl}^{cb} \\
& + P(ij) \sum_{klmcd} \frac{2}{3} (\sigma_m^d)^* \langle kl || cm \rangle \sigma_{il}^{ab} \sigma_{jk}^{dc} - P(ab) \sum_{klcde} \frac{2}{3} (\sigma_l^e)^* \langle kc || de \rangle \sigma_{ij}^{ae} \sigma_{kl}^{db} \\
& \left. + P(ij) \sum_{klmcd} \frac{1}{4} (\sigma_m^d)^* \langle kl || ci \rangle \sigma_{kl}^{ba} \sigma_{jm}^{cd} - P(ab) \sum_{klcde} \frac{1}{4} (\sigma_l^e)^* \langle ka || dc \rangle \sigma_{ij}^{cd} \sigma_{kl}^{be} \right)
\end{aligned}$$

$$\begin{aligned}
& + P(ab) \sum_{klmcd} \frac{1}{3} (\sigma_m^d)^* \langle kl || cm \rangle \sigma_{ij}^{ac} \sigma_{kl}^{bd} - P(ij) \sum_{klcde} \frac{1}{3} (\sigma_l^c)^* \langle ck || de \rangle \sigma_{ik}^{ab} \sigma_{jl}^{ed} \\
& - P(ij) P(ab) \sum_{klmcd} \frac{1}{3} (\sigma_m^d)^* \langle kl || cj \rangle \sigma_{kl}^{db} \sigma_{im}^{ac} + P(ij) P(ab) \sum_{klcde} \frac{1}{3} (\sigma_l^c)^* \langle kb || cd \rangle \sigma_{jl}^{dc} \sigma_{ik}^{ae} \\
& - \sum_{klmcd} \frac{1}{3} (\sigma_m^d)^* \langle kl || cm \rangle \sigma_{ij}^{dc} \sigma_{kl}^{ba} + \sum_{klcde} \frac{1}{3} (\sigma_l^c)^* \langle kc || de \rangle \sigma_{ij}^{ed} \sigma_{kl}^{ba} \\
& + P(ab) \sum_{klmcd} \frac{1}{6} (\sigma_{ml}^{dc})^* \langle kc || ji \rangle \sigma_{ml}^{da} \sigma_k^b - P(ij) \sum_{klcde} \frac{1}{6} (\sigma_{lk}^{ed})^* \langle ab || kc \rangle \sigma_{il}^{de} \sigma_j^c \\
& - P(ij) P(ab) \sum_{klcde} \frac{1}{6} (\sigma_{kl}^{ce})^* \langle bc || jd \rangle \sigma_{kl}^{ae} \sigma_i^d + P(ij) P(ab) \sum_{klmcd} \frac{1}{6} (\sigma_{ml}^{dc})^* \langle kb || lj \rangle \sigma_{im}^{cd} \sigma_k^a \\
& - P(ij) P(ab) \sum_{klmcd} \frac{1}{3} (\sigma_{lm}^{cd})^* \langle kc || jl \rangle \sigma_{im}^{ad} \sigma_k^b + P(ij) P(ab) \sum_{klcde} \frac{1}{3} (\sigma_{kl}^{de})^* \langle bd || ck \rangle \sigma_{il}^{ae} \sigma_j^c \\
& - P(ij) P(ab) \sum_{klmcd} \frac{1}{3} (\sigma_{lm}^{cd})^* \langle ka || li \rangle \sigma_{mj}^{db} \sigma_k^c + P(ij) P(ab) \sum_{klcde} \frac{1}{3} (\sigma_{kl}^{ce})^* \langle ac || id \rangle \sigma_{lj}^{eb} \sigma_k^d \\
& - P(ab) \sum_{klmcd} \frac{1}{12} (\sigma_{lm}^{cd})^* \langle ka || ml \rangle \sigma_{ij}^{cd} \sigma_k^b + P(ij) \sum_{klcde} \frac{1}{12} (\sigma_{kl}^{dc})^* \langle cd || ei \rangle \sigma_{lk}^{ba} \sigma_j^e \\
& + \sum_{klcde} \frac{1}{6} (\sigma_{kl}^{de})^* \langle ab || kc \rangle \sigma_{ij}^{de} \sigma_l^c - \sum_{klmcd} \frac{1}{6} (\sigma_{lm}^{cd})^* \langle kc || ji \rangle \sigma_{ml}^{ba} \sigma_k^d \\
& + P(ij) \sum_{klmcd} \frac{1}{3} (\sigma_{lm}^{cd})^* \langle kc || il \rangle \sigma_{mj}^{ab} \sigma_k^d - P(ab) \sum_{klcde} \frac{1}{3} (\sigma_{kl}^{ce})^* \langle ac || dk \rangle \sigma_{ij}^{eb} \sigma_l^d \\
& + P(ab) \sum_{klmcd} \frac{1}{6} (\sigma_{lm}^{dc})^* \langle ka || ml \rangle \sigma_{ij}^{db} \sigma_k^c - P(ij) \sum_{klcde} \frac{1}{6} (\sigma_{kl}^{cd})^* \langle cd || ei \rangle \sigma_{jl}^{ba} \sigma_k^e \\
& - P(ij) \sum_{klmcd} \frac{1}{2} (\sigma_{ml}^{dc})^* \langle kc || li \rangle \sigma_{kj}^{ab} \sigma_m^d + P(ab) \sum_{klcde} \frac{1}{2} (\sigma_{kl}^{ce})^* \langle ac || dk \rangle \sigma_{ij}^{db} \sigma_l^e \\
& - P(ij) P(ab) \sum_{klmcd} \frac{1}{2} (\sigma_{ml}^{dc})^* \langle ka || li \rangle \sigma_{kj}^{cb} \sigma_m^d + P(ij) P(ab) \sum_{klcde} \frac{1}{2} (\sigma_{kl}^{ce})^* \langle ac || id \rangle \sigma_{jk}^{bd} \sigma_l^e \\
& - P(ab) \sum_{klmcd} \frac{1}{6} (\sigma_{ml}^{dc})^* \langle ka || ji \rangle \sigma_{kl}^{bc} \sigma_m^d + P(ij) \sum_{klcde} \frac{1}{6} (\sigma_{kl}^{de})^* \langle ab || ic \rangle \sigma_{jk}^{cd} \sigma_l^e \\
& - \sum_{klmcd} \frac{1}{2} (\sigma_{ml}^{dc})^* \langle kc || ji \rangle \sigma_{kl}^{ba} \sigma_m^d - \sum_{klcde} \frac{1}{2} (\sigma_{li}^{ed})^* \langle ab || kc \rangle \sigma_{ji}^{cd} \sigma_l^e \\
& + P(ij) \sum_{klmcd} \frac{1}{12} (\sigma_{ml}^{dc})^* \langle kc || ml \rangle \sigma_{kj}^{ab} \sigma_i^d - P(ab) \sum_{klcde} \frac{1}{12} (\sigma_{lk}^{cd})^* \langle cd || ek \rangle \sigma_{ji}^{be} \sigma_l^a
\end{aligned}$$

$$\begin{aligned}
& + P(ij) \sum_{klmcd} \frac{1}{2} (\sigma_{ml}^{dc})^* \langle kc || jl \rangle \sigma_{mk}^{ab} \sigma_i^d - P(ab) \sum_{klcde} \frac{1}{2} (\sigma_{lk}^{ec})^* \langle bc || dk \rangle \sigma_{ij}^{ed} \sigma_l^a \\
& + P(ij) P(ab) \sum_{klmcd} \frac{1}{2} (\sigma_{ml}^{dc})^* \langle kc || il \rangle \sigma_{jk}^{bd} \sigma_m^a - P(ij) P(ab) \sum_{klcde} \frac{1}{2} (\sigma_{lk}^{ec})^* \langle ac || dk \rangle \sigma_{lj}^{db} \sigma_i^e \\
& + P(ij) P(ab) \sum_{klmcd} \frac{1}{4} (\sigma_{ml}^{cd})^* \langle ka || ml \rangle \sigma_{jk}^{bc} \sigma_i^d - P(ij) P(ab) \sum_{klcde} \frac{1}{4} (\sigma_{kl}^{cd})^* \langle cd || ei \rangle \sigma_{kj}^{eb} \sigma_l^a \\
& + P(ij) P(ab) \sum_{klmcd} \frac{1}{2} (\sigma_{lm}^{cd})^* \langle kb || lj \rangle \sigma_{mk}^{da} \sigma_i^c - P(ij) P(ab) \sum_{klcde} \frac{1}{2} (\sigma_{kl}^{ce})^* \langle cb || dj \rangle \sigma_{il}^{de} \sigma_k^a \\
& + P(ab) \sum_{klmcd} \frac{1}{2} (\sigma_{lm}^{cd})^* \langle kc || ji \rangle \sigma_{mk}^{db} \sigma_l^a - P(ij) \sum_{klcde} \frac{1}{2} (\sigma_{km}^{de})^* \langle ab || kc \rangle \sigma_{jm}^{ce} \sigma_i^d \\
& + P(ab) \sum_{klmcd} \frac{1}{12} (\sigma_{lm}^{cd})^* \langle ka || ji \rangle \sigma_{mk}^{dc} \sigma_l^b - P(ij) \sum_{klcde} \frac{1}{12} (\sigma_{kl}^{de})^* \langle ab || ic \rangle \sigma_{kl}^{ce} \sigma_j^d \\
& + P(ij) P(ab) \sum_{klmcd} \frac{1}{4} (\sigma_{lm}^{cd})^* \langle kb || lj \rangle \sigma_{ik}^{dc} \sigma_m^a - P(ij) P(ab) \sum_{klcde} \frac{1}{4} (\sigma_{kl}^{ce})^* \langle bc || jd \rangle \sigma_{kl}^{da} \sigma_i^e \Big) (20) \\
& + \left(- P(ij) \sum_{klmnecd} \frac{1}{12} (\sigma_{mn}^{cd})^* \langle kl || im \rangle \sigma_{nj}^{dc} \sigma_{kl}^{ab} - P(ab) \sum_{klcdef} \frac{1}{12} (\sigma_{kl}^{cf})^* \langle ac || de \rangle \sigma_{ij}^{de} \sigma_{kl}^{bf} \right. \\
& + P(ij) P(ab) \sum_{klmnecd} \frac{1}{6} (\sigma_{mn}^{cd})^* \langle kl || im \rangle \sigma_{kl}^{ac} \sigma_{jn}^{bd} + P(ij) P(ab) \sum_{klcdef} \frac{1}{12} (\sigma_{kl}^{cf})^* \langle ac || de \rangle \sigma_{ik}^{de} \sigma_{lj}^{fb} \\
& - P(ij) \sum_{klmnecd} \frac{1}{12} (\sigma_{nm}^{cd})^* \langle kl || jm \rangle \sigma_{in}^{ab} \sigma_{kl}^{cd} - P(ab) \sum_{klcdef} \frac{1}{12} (\sigma_{kl}^{fc})^* \langle bc || de \rangle \sigma_{lk}^{ed} \sigma_{ij}^{af} \\
& + P(ij) \sum_{klmnecd} \frac{1}{2} (\sigma_{nm}^{cd})^* \langle kl || jm \rangle \sigma_{ik}^{ab} \sigma_{ln}^{cd} + P(ab) \sum_{klcdef} \frac{1}{2} (\sigma_{kl}^{cf})^* \langle bc || de \rangle \sigma_{kl}^{ef} \sigma_{ij}^{ad} \\
& - \sum_{klmnecd} \frac{1}{3} (\sigma_{nm}^{dc})^* \langle kl || ji \rangle \sigma_{km}^{ba} \sigma_{ln}^{cd} - \sum_{klcdef} \frac{1}{3} (\sigma_{kl}^{ef})^* \langle ab || cd \rangle \sigma_{kl}^{cf} \sigma_{ij}^{ed} \\
& + P(ab) \sum_{klmnecd} \frac{1}{2} (\sigma_{mn}^{cd})^* \langle kl || ij \rangle \sigma_{km}^{ac} \sigma_{ln}^{bd} + \sum_{klcdef} \frac{1}{2} (\sigma_{kl}^{ef})^* \langle ab || cd \rangle \sigma_{jl}^{df} \sigma_{ik}^{ce} \\
& + P(ij) P(ab) \sum_{klmnecd} \frac{2}{3} (\sigma_{mn}^{cd})^* \langle kl || mn \rangle \sigma_{ik}^{ac} \sigma_{ln}^{bd} + P(ij) P(ab) \sum_{klcdef} \frac{2}{3} (\sigma_{kl}^{cf})^* \langle cd || ef \rangle \sigma_{jl}^{df} \sigma_{ik}^{ae} \\
& - P(ij) \sum_{klmnecd} \frac{1}{6} (\sigma_{mn}^{cd})^* \langle kl || mn \rangle \sigma_{il}^{ab} \sigma_{jk}^{dc} - P(ab) \sum_{klcdef} \frac{1}{6} (\sigma_{kl}^{cd})^* \langle cd || ef \rangle \sigma_{ij}^{af} \sigma_{lk}^{be} \\
& - P(ij) \sum_{klmnecd} \frac{1}{2} (\sigma_{mn}^{cd})^* \langle kl || mi \rangle \sigma_{kj}^{cd} \sigma_{ln}^{ab} - P(ab) \sum_{klcdef} \frac{1}{2} (\sigma_{kl}^{cf})^* \langle ac || ed \rangle \sigma_{ij}^{df} \sigma_{kl}^{eb}
\end{aligned}$$

$$\begin{aligned}
& + P(ij)P(ab) \sum_{klmncd} \frac{1}{3} (\sigma_{mn}^{cd})^* \langle kl || mn \rangle \sigma_{ik}^{ac} \sigma_{jl}^{bd} + P(ij)P(ab) \sum_{klcdef} \frac{1}{3} (\sigma_{kl}^{cd})^* \langle cd || ef \rangle \sigma_{ik}^{ae} \sigma_{jl}^{bf} \\
& - P(ij)P(ab) \sum_{klmcde} \frac{1}{6} (\sigma_{ml}^{ed})^* \langle kd || cj \rangle \sigma_{ik}^{ac} \sigma_{ml}^{eb} - P(ij)P(ab) \sum_{klmcde} \frac{1}{6} (\sigma_{ml}^{ed})^* \langle kb || cl \rangle \sigma_{ik}^{ac} \sigma_{jm}^{de} \\
& - P(ij)P(ab) \sum_{klmcde} \frac{1}{3} (\sigma_{ml}^{ed})^* \langle kd || ci \rangle \sigma_{mj}^{eb} \sigma_{lk}^{ac} - P(ij)P(ab) \sum_{klmcde} \frac{1}{3} (\sigma_{ml}^{ed})^* \langle ka || cl \rangle \sigma_{ik}^{dc} \sigma_{mj}^{eb} \\
& + P(ij) \sum_{klmcde} \frac{1}{6} (\sigma_{ml}^{ed})^* \langle kd || ci \rangle \sigma_{kj}^{ce} \sigma_{lm}^{ab} + P(ab) \sum_{klmcde} \frac{1}{6} (\sigma_{ml}^{ed})^* \langle ka || cl \rangle \sigma_{km}^{cb} \sigma_{ij}^{de} \\
& - P(ij) \sum_{klmcde} \frac{1}{3} (\sigma_{ml}^{ed})^* \langle kd || cj \rangle \sigma_{mk}^{ec} \sigma_{il}^{ab} - P(ab) \sum_{klmcde} \frac{1}{3} (\sigma_{ml}^{ed})^* \langle kb || cl \rangle \sigma_{ij}^{ad} \sigma_{km}^{ce} \\
& + P(ij)P(ab) \sum_{klmcde} \frac{1}{3} (\sigma_{ml}^{ed})^* \langle ka || ci \rangle \sigma_{lj}^{cb} \sigma_{mk}^{ed} + P(ij)P(ab) \sum_{klmcde} \frac{1}{3} (\sigma_{ml}^{ed})^* \langle ka || ci \rangle \sigma_{kj}^{db} \sigma_{lm}^{ce} \\
& + P(ij) \sum_{klmcde} \frac{1}{2} (\sigma_{ml}^{ed})^* \langle kd || cj \rangle \sigma_{ik}^{ab} \sigma_{lm}^{ce} + P(ab) \sum_{klmcde} \frac{1}{2} (\sigma_{ml}^{ed})^* \langle kb || cl \rangle \sigma_{ij}^{ac} \sigma_{km}^{de} \\
& - P(ij) \sum_{klmcde} \frac{2}{3} (\sigma_{ml}^{ed})^* \langle kd || cl \rangle \sigma_{ik}^{ab} \sigma_{jm}^{ce} - P(ab) \sum_{klmcde} \frac{1}{3} (\sigma_{ml}^{ed})^* \langle kd || cl \rangle \sigma_{ij}^{ac} \sigma_{km}^{be} \\
& - P(ij)P(ab) \sum_{klmcde} \frac{2}{3} (\sigma_{ml}^{ed})^* \langle ka || ci \rangle \sigma_{jl}^{cd} \sigma_{km}^{be} + P(ij)P(ab) \sum_{klmcde} (\sigma_{ml}^{ed})^* \langle kd || cj \rangle \sigma_{il}^{ac} \sigma_{km}^{be} \\
& + P(ij)P(ab) \sum_{klmcde} (\sigma_{ml}^{ed})^* \langle kb || cl \rangle \sigma_{ik}^{ad} \sigma_{jm}^{ce} + P(ab) \sum_{klmcde} (\sigma_{ml}^{ed})^* \langle ka || cl \rangle \sigma_{ji}^{cd} \sigma_{km}^{be} \\
& + P(ij) \sum_{klmcde} (\sigma_{ml}^{ed})^* \langle kd || ci \rangle \sigma_{lk}^{ab} \sigma_{jm}^{ce} - P(ij)P(ab) \sum_{klmcde} \frac{1}{6} (\sigma_{ml}^{ed})^* \langle ka || ci \rangle \sigma_{ml}^{bc} \sigma_{jk}^{ed} \\
& - P(ij)P(ab) \sum_{klmcde} \frac{1}{2} (\sigma_{ml}^{ed})^* \langle kd || cj \rangle \sigma_{ml}^{cb} \sigma_{ik}^{ae} - P(ij)P(ab) \sum_{klmcde} \frac{1}{2} (\sigma_{ml}^{ed})^* \langle kb || cl \rangle \sigma_{jk}^{de} \sigma_{im}^{ac} \\
& + P(ij)P(ab) \sum_{klmcde} \frac{2}{3} (\sigma_{ml}^{ed})^* \langle kd || cl \rangle \sigma_{jk}^{be} \sigma_{im}^{ac} + \sum_{klmcde} \frac{2}{3} (\sigma_{ml}^{ed})^* \langle kd || cl \rangle \sigma_{ij}^{ec} \sigma_{mk}^{ab} \Bigg). \quad (21)
\end{aligned}$$