

Closed-shell EOM-CCSD Equations

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October 20, 2021

output,level=2

EOM-CCSD singles contribution of the matrix vector multiplication $\langle \tilde{\psi}_i^a | \exp(-\mathbf{T}_2) \mathbf{H} \exp(\mathbf{T}_2) \mathbf{u}_1 | 0 \rangle$ equation with $\exp(\mathbf{T}_1)$ -similarity transformed \mathbf{H} :

$$\begin{aligned}
 & \left\langle \tilde{\Phi}_i^a \left| \mathbf{H} \left(1 + \mathbf{T}_2 + \frac{1}{2} \mathbf{T}_2 \mathbf{T}_2 \right) (\mathbf{u}_1 + \mathbf{u}_2) \right| 0 \right\rangle_C = \\
 & 4 * 1 \sum_{jkb c} (jb|kc) T_{ba}^{ji} u_c^k + 2 * 1 \sum_{jb} f_{jb} u_{ba}^{ji} + (-2 * 1) \sum_{jj_1 b_1} (ji|j_1 b_1) u_{ab_1}^{jj_1} \\
 & + (-2 * 1) \sum_{jj_1 b c} (jb|j_1 c) T_{ba}^{jj_1} u_c^i + (-2 * 1) \sum_{jkb b_1} (jb|kb_1) T_{bb_1}^{ji} u_a^k + 2 * 1 \sum_{jb} (jb|ai) u_b^j \\
 & + 2 * 1 \sum_{jbb_1} (jb|ab_1) u_{bb_1}^{ji} + (-2 * 1) \sum_{jkb_1 c} (jb_1|kc) T_{ab_1}^{ji} u_c^k + (-2 * 1) \sum_{jkb c} (jc|kb) T_{ba}^{ji} u_c^k \\
 & + (-1) \sum_j f_{ji} u_a^j + (-1) \sum_{jb_1} f_{jb_1} u_{ab_1}^{ji} + \sum_b f_{ab} u_b^i + \sum_{jj_1 b} (ji|j_1 b) u_{ba}^{jj_1} \\
 & + (-1) \sum_{jb} (ji|ab) u_b^j + \sum_{jj_1 b_1 c} (jb_1|j_1 c) T_{ab_1}^{jj_1} u_c^i + \sum_{jkb b_1} (jb_1|kb) T_{bb_1}^{ji} u_a^k \\
 & + (-1) \sum_{jbb_1} (jb_1|ab) u_{bb_1}^{ji} + \sum_{jkb_1 c} (jc|kb_1) T_{ab_1}^{ji} u_c^k
 \end{aligned} \tag{1}$$

Doubles contributions

$$\begin{aligned}
& \left\langle \tilde{\Phi}_{ij}^{ab} \right| \mathbf{H} \left(1 + \mathbf{T}_2 + \frac{1}{2} \mathbf{T}_2 \mathbf{T}_2 \right) (\mathbf{u}_1 + \mathbf{u}_2) | 0 \rangle_C = \\
& (4 * 1 + 4 * \mathcal{P}(ijab, jiba)) \sum_{klcd} (kc|ld) T_{ca}^{ki} u_{db}^{lj} + (-2 * 1 \\
& - 2 * \mathcal{P}(ijab, jiba)) \sum_{klcd} (ki|ld) T_{ab}^{kj} u_d^l + (-2 * 1 - 2 * \mathcal{P}(ijab, jiba)) \sum_{kk_1cd} (kc|k_1d) T_{ca}^{kk_1} u_{db}^{ij} \\
& + (-2 * 1 - 2 * \mathcal{P}(ijab, jiba)) \sum_{klc} (kc|li) T_{cb}^{kj} u_a^l + (-2 * 1 \\
& - 2 * \mathcal{P}(ijab, jiba)) \sum_{klcc_1} (kc|lc_1) T_{cc_1}^{ki} u_{ab}^{lj} + (-2 * 1 \\
& - 2 * \mathcal{P}(ijab, jiba)) \sum_{klcd_1} (kc|ld_1) T_{ca}^{ki} u_{bd_1}^{lj} + (2 * 1 + 2 * \mathcal{P}(ijab, jiba)) \sum_{kc} (kc|ai) u_{cb}^{kj} \\
& + (2 * 1 + 2 * \mathcal{P}(ijab, jiba)) \sum_{kcd} (kc|ad) T_{cb}^{kj} u_d^i + (-2 * 1 \\
& - 2 * \mathcal{P}(ijab, jiba)) \sum_{klc_1d} (kc_1|ld) T_{ac_1}^{ki} u_{db}^{lj} + (-2 * 1 \\
& - 2 * \mathcal{P}(ijab, jiba)) \sum_{klcd} (kd|lc) T_{ca}^{ki} u_{db}^{lj} + (-2 * 1 \\
& - 2 * \mathcal{P}(ijab, jiba)) \sum_{kl_1dd_1} (kd|l_1d_1) T_{ab}^{kj} u_{dd_1}^{il_1} + (-2 * 1 \\
& - 2 * \mathcal{P}(ijab, jiba)) \sum_{ll_1cd_1} (lc|l_1d_1) T_{cb}^{ij} u_{ad_1}^{ll_1} + (2 * 1 + 2 * \mathcal{P}(ijab, jiba)) \sum_{lcd} (ld|ac) T_{cb}^{ij} u_d^l \\
& + (-1 - \mathcal{P}(ijab, jiba)) \sum_k f_{ki} u_{ab}^{kj} + (-1 - \mathcal{P}(ijab, jiba)) \sum_{kd} f_{kd} T_{ab}^{kj} u_d^i + (-1 \curvearrowright
\end{aligned} \tag{2}$$

$$\begin{aligned}
& -\mathcal{P}(ijab, jiba)) \sum_{lc} f_{lc} T_{cb}^{ij} u_a^l + (1 + \mathcal{P}(ijab, jiba)) \sum_c f_{ac} u_{cb}^{ij} + \sum_{kk_1} (ki|k_1j) u_{ab}^{kk_1} \\
& + (1 + \mathcal{P}(ijab, jiba)) \sum_{kk_1d} (ki|k_1d) T_{ab}^{kk_1} u_d^j + (1 + \mathcal{P}(ijab, jiba)) \sum_{klc} (ki|lc) T_{cb}^{kj} u_a^l + (1 \\
& + \mathcal{P}(ijab, jiba)) \sum_{klc_1} (ki|lc_1) T_{ac_1}^{kj} u_b^l + (-1 - \mathcal{P}(ijab, jiba)) \sum_{kc} (ki|ac) u_{cb}^{kj} + (-1 \\
& - \mathcal{P}(ijab, jiba)) \sum_k (ki|bj) u_a^k + (-1 - \mathcal{P}(ijab, jiba)) \sum_{kc_1} (ki|bc_1) u_{ac_1}^{kj} + (1 \\
& + \mathcal{P}(ijab, jiba)) \sum_{kk_1c_1d} (kc_1|k_1d) T_{ac_1}^{kk_1} u_{db}^{ij} + (1 + \mathcal{P}(ijab, jiba)) \sum_{klc_1} (kc_1|li) T_{bc_1}^{kj} u_a^l + (1 \\
& + \mathcal{P}(ijab, jiba)) \sum_{klc_1} (kc_1|lc) T_{cc_1}^{ki} u_{ab}^{lj} + (1 + \mathcal{P}(ijab, jiba)) \sum_{klc_1d_1} (kc_1|ld_1) T_{ac_1}^{ki} u_{bd_1}^{lj} \\
& + (-1 - \mathcal{P}(ijab, jiba)) \sum_{kc_1} (kc_1|ai) u_{bc_1}^{kj} + (-1 - \mathcal{P}(ijab, jiba)) \sum_{kc_1d} (kc_1|ad) T_{bc_1}^{kj} u_d^i \\
& + \sum_{kk_1dd_1} (kd|k_1d_1) T_{ab}^{kk_1} u_{dd_1}^{ij} + (1 + \mathcal{P}(ijab, jiba)) \sum_{kld} (kd|li) T_{ab}^{kj} u_d^l + (1 \\
& + \mathcal{P}(ijab, jiba)) \sum_{klc_1d} (kd|lc_1) T_{ac_1}^{ki} u_{db}^{lj} + (1 + \mathcal{P}(ijab, jiba)) \sum_{kldd_1} (kd|ld_1) T_{ab}^{kj} u_{dd_1}^{li} + (1 \\
& + \mathcal{P}(ijab, jiba)) \sum_{kl_1cd} (kd|l_1c) T_{ca}^{ki} u_{db}^{jl_1} + (1 + \mathcal{P}(ijab, jiba)) \sum_{kl_1c_1d} (kd|l_1c_1) T_{ac_1}^{kj} u_{db}^{il_1} \\
& + (-1 - \mathcal{P}(ijab, jiba)) \sum_{kcd} (kd|ac) T_{cb}^{kj} u_d^i + (-1 - \mathcal{P}(ijab, jiba)) \sum_{kc_1d} (kd|ac_1) T_{bc_1}^{ki} u_d^j \\
& + \sum_{ll_1cc_1} (lc|l_1c_1) T_{cc_1}^{ij} u_{ab}^{ll_1} + (1 + \mathcal{P}(ijab, jiba)) \sum_{ll_1cd} (lc|l_1d) T_{cb}^{ij} u_{da}^{ll_1} + (-1 \\
& - \mathcal{P}(ijab, jiba)) \sum_{lcc_1} (lc|ac_1) T_{cc_1}^{ji} u_b^l + (-1 - \mathcal{P}(ijab, jiba)) \sum_{lcd} (lc|ad) T_{cb}^{ij} u_d^l + (1 \\
& + \mathcal{P}(ijab, jiba)) \sum_c (ai|bc) u_c^j + \sum_{cc_1} (ac|bc_1) u_{cc_1}^{ij}
\end{aligned} \tag{3}$$