OMP2

1. Build h_p^q and $\overline{g}_{pq}^{rs}$ in the Hartree-Fock spin-orbital basis.

2. Build an empty array of amplitudes, $t_{ab}^{ij} = 0$.

3. Build the Fock matrix.

$$f_p^q = h_p^q + \overline{g}_{pi}^{qi} \tag{1}$$

4. Build the off-diagonal Fock matrix and the orbital energies.

$$\epsilon_p = f_p^p \qquad\qquad f'^q_p = (1 - \delta_p^q) f_p^q \tag{2}$$

5. Update the amplitudes.

$$t_{ab}^{ij} = (\mathcal{E}_{ab}^{ij})^{-1} \left(\overline{g}_{ab}^{ij} + P_{(a/b)} f'^c_a t_{cb}^{ij} - P^{(i/j)} f'^i_k t_{ab}^{kj} \right) \tag{3}$$

6. Build the one- and two-particle density matrices.

$$\gamma_q^p = \tilde{\gamma}_q^p + \mathring{\gamma}_q^p \qquad\qquad \gamma_{rs}^{pq} = \tilde{\gamma}_{rs}^{pq} + P_{(r/s)}^{(p/q)} \tilde{\gamma}_r^p \mathring{\gamma}_s^q + P_{(r/s)} \mathring{\gamma}_r^p \mathring{\gamma}_s^q \tag{4}$$

$$\tilde{\gamma}_b^a = \tfrac{1}{2} t_{ij}^{ac*} t_{bc}^{ij} \qquad \tilde{\gamma}_j^i = -\tfrac{1}{2} t_{jk}^{ab*} t_{ab}^{ik} \qquad \tilde{\gamma}_{ij}^{ab} = t_{ij}^{ab*} \qquad \tilde{\gamma}_{ab}^{ij} = t_{ab}^{ij} \qquad \mathring{\gamma}_q^p = \begin{cases} \delta_j^i & \text{for } p = i,\ q = j \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

7. Compute the Newton-Raphson step.

$$x_a^i = \frac{(\mathbf{F} - \mathbf{F}^\dagger)_a^i}{\epsilon_i - \epsilon_a} \qquad\qquad (\mathbf{F})_p^q \equiv h_p^r \gamma_r^q + \tfrac{1}{2} \overline{g}_{pr}^{st} \gamma_{st}^{qr} \tag{6}$$

8. Build the Newton-Raphson orbital rotation matrix.

$$\mathbf{U} = \exp(\mathbf{X} - \mathbf{X}^\dagger) \qquad\qquad \mathbf{X}_{\text{vo}} = [x_a^i] \tag{7}$$

9. Rotate the spin-orbital coefficients.

$$\mathbf{C} \leftarrow \mathbf{CU} \tag{8}$$

10. Transform the one- and two-electon integrals to the spin-orbital basis using the new coefficient matrix.

$$h_p^q = \sum_{\mu\nu} C_{\mu p}^* \, h_{\mu\nu} \, C_{\nu q} \qquad\qquad \overline{g}_{pq}^{rs} = \sum_{\mu\nu\rho\sigma} C_{\mu p}^* \, C_{\nu q}^* \, \langle \mu\nu || \rho\sigma \rangle C_{\rho r} C_{\sigma s} \tag{9}$$

11. Evaluate the energy.

$$E = h_p^q \gamma_q^p + \tfrac{1}{4} \overline{g}_{pq}^{rs} \gamma_{rs}^{pq} \tag{10}$$

12. If the energy is converged, quit. Otherwise, return to step 3.