I. CCSD

Defining some quantities
ERIs, which notation?

$$v_{qs}^{pr} = (pq|rs) \tag{1}$$

$$w_{ab}^{ij} = 2v_{ab}^{ij} - v_{ba}^{ij} \tag{2}$$

CCSD energy equation

$$E = \langle \Phi_0 | H e^{T_1+T_2} | \Phi_0 \rangle \tag{3}$$

$$E_{\text{CCSD}} = 2\sum_{i,a} f_a^i t_i^a + \sum_{i,j,a,b} w_{ab}^{ij} t_i^a t_j^b + \sum_{i,j,a,b} w_{ab}^{ij} t_{ij}^{ab} \tag{4}$$

Defining the T_1 transformed operators

$$\hat{O} = e^{-T_1} O e^{T_1} \tag{5}$$

The CCSD amplitude equations with transformed operators

$$\langle \Phi_i^a \big| \hat{H} + \left[\hat{H}, T_2\right] \big| \Phi_0 \rangle = 0 \tag{6}$$

$$\left\langle \Phi_{ij}^{ab} \middle| \hat{H} + \left[\hat{H}, T_2\right] + \frac{1}{2}\left[\left[\hat{H}, T_2\right], T_2\right] \middle| \Phi_0 \right\rangle = 0 \tag{7}$$

T_1 amplitude equation

$$\begin{aligned} 0 =& f_i^a - 2\sum_{k,c} f_c^k t_k^a t_i^c + \sum_c \kappa_c^a t_i^c - \sum_k \kappa_i^k t_k^a \\ &+ \sum_{k,c} \kappa_c^k \left(2t_{ki}^{ca} - t_{ik}^{ca}\right) + \sum_{k,c} \kappa_c^k t_i^c t_k^a + \sum_{k,c} w_{ic}^{ak} t_k^c \\ &+ \sum_{k,c,d} w_{cd}^{ak} t_{ik}^{cd} + \sum_{k,c,d} w_{cd}^{ak} t_i^c t_k^d - \sum_{k,l,c} w_{ic}^{kl} t_{kl}^{ac} \\ &- \sum_{k,l,c} w_{ic}^{kl} t_k^a t_l^c \end{aligned} \tag{8}$$

T_2 Amplitude Equations

$$\begin{aligned} 0 =& v_{ab}^{ij} + \sum_{k,l} \chi_{ij}^{kl} t_{kl}^{ab} + \sum_{k,l} \chi_{ij}^{kl} t_k^a t_l^b + \sum_{c,d} \chi_{cd}^{ab} t_{ij}^{cd} \\ &+ \sum_{c,d} \chi_{cd}^{ab} t_i^c t_j^d + P\sum_c \lambda_c^a t_{ij}^{cb} - P\sum_k \lambda_i^k t_{kj}^{ab} \\ &+ P\sum_c \left(v_{ic}^{ab} - \sum_k v_{ic}^{kb} t_k^a\right) t_j^c - P\sum_k \left(v_{ij}^{ak} + \sum_c v_{ic}^{ak} t_j^c\right) t_k^b \\ &+ P\sum_{k,c} \left(2\chi_{ic}^{ak} - \chi_{ci}^{ak}\right) t_{kj}^{cb} - P\sum_{k,c} \chi_{ic}^{ak} t_{kj}^{bc} \\ &- P\sum_{k,c} \chi_{ci}^{bk} t_{kj}^{ac} \end{aligned} \tag{9}$$

Intermediates

$$\kappa_i^k = f_i^k + \sum_{l,c,d} w_{cd}^{kl} t_{il}^{cd} + \sum_{l,c,d} w_{cd}^{kl} t_i^c t_l^d \tag{10}$$

$$\kappa_c^a = f_c^a - \sum_{k,l,d} w_{cd}^{kl} t_{kl}^{ad} - \sum_{k,l,d} w_{cd}^{kl} t_k^a t_l^d \tag{11}$$

$$\kappa_c^k = f_c^k + \sum_{l,d} w_{cd}^{kl} t_l^d \tag{12}$$

$$\lambda_i^k = \kappa_i^k + \sum_c f_c^k t_i^c + \sum_{l,c} w_{ic}^{kl} t_l^c \tag{13}$$

$$\lambda_c^a = \kappa_c^a - \sum_k f_c^k t_k^a + \sum_{k,d} w_{cd}^{ak} t_k^d \tag{14}$$

$$\chi_{ij}^{kl} = v_{ij}^{kl} + \sum_c v_{ic}^{kl} t_j^c + \sum_c v_{cj}^{kl} t_i^c + \sum_{c,d} v_{cd}^{kl} t_{ij}^{cd} + \sum_{l,d} v_{dc}^{lk} t_i^d t_l^a \tag{15}$$

$$\chi_{cd}^{ab} = v_{cd}^{ab} - \sum_k v_{cd}^{ak} t_k^b - \sum_k v_{cd}^{kb} t_k^a \tag{16}$$

$$\begin{aligned}\chi_{ic}^{ak} = v_{ic}^{ak} &- \sum_l v_{ic}^{lk} t_l^a + \sum_d v_{dc}^{ak} t_i^d - \frac{1}{2} \sum_{l,d} v_{dc}^{lk} t_{il}^{da} \\ &- \sum_{l,d} v_{dc}^{lk} t_i^d t_l^a + \frac{1}{2} \sum_{l,d} w_{dc}^{lk} t_{il}^{ad}\end{aligned} \tag{17}$$

$$\begin{aligned}\chi_{ci}^{ak} = v_{ci}^{aj} &- \sum_l v_{ci}^{lk} t_l^a + \sum_d v_{cd}^{ak} t_i^d - \frac{1}{2} \sum_{l,d} v_{cd}^{lk} t_{il}^{da} \\ &- \sum_{l,d} v_{cd}^{lk} t_i^d t_l^a\end{aligned} \tag{18}$$

II. CC2

The doubles equations are approximated to first order.

The CC2 doubles amplitude equations with transformed operators

$$\left\langle \Phi_{ij}^{ab} \middle| [F, T_2] + \hat{H} \middle| \Phi_0 \right\rangle = 0 \tag{19}$$

Note that F doesn't have a hat!

Current implementation of T_2 amplitude equations

$$\begin{aligned}0 = v_{ab}^{ij} &+ \sum_{k,l} \chi_{ij}^{kl} t_k^a t_l^b + \sum_{c,d} \chi_{cd}^{ab} t_i^c t_j^d + P \sum_c \lambda_c^a t_{ij}^{cb} - P \sum_k \lambda_i^k t_{kj}^{ab} \\ &+ P \sum_c \left(v_{ic}^{ab} - \sum_k v_{ic}^{kb} t_k^a \right) t_j^c - P \sum_k \left(v_{ij}^{ak} + \sum_c v_{ic}^{ak} t_j^c \right) t_k^b\end{aligned} \tag{20}$$

Intermediates

$$\kappa_i^k = f_i^k \tag{21}$$

$$\kappa_c^a = f_c^a \tag{22}$$

$$\lambda_i^k = \kappa_i^k + \sum_c f_c^k t_i^c \tag{23}$$

$$\lambda_c^a = \kappa_c^a - \sum_k f_c^k t_k^a \tag{24}$$

$$\chi_{ij}^{kl} = v_{ij}^{kl} + \sum_c v_{ic}^{kl} t_j^c + \sum_c v_{cj}^{kl} t_i^c + \sum_{l,d} v_{dc}^{lk} t_i^d t_l^a \tag{25}$$

$$\chi_{cd}^{ab} = v_{cd}^{ab} - \sum_k v_{cd}^{ak} t_k^b - \sum_k v_{cd}^{kb} t_k^a \tag{26}$$

$$\tag{27}$$

T_1 transform

$$X_{\alpha i} = C_{\alpha i} \tag{28}$$

$$X_{\alpha a} = C_{\alpha a} - \sum_i C_{\alpha i} t_i^a \tag{29}$$

$$Y_{\alpha i} = C_{\alpha i} + \sum_a C_{\alpha a} t_i^a \tag{30}$$

$$Y_{\alpha a} = C_{\alpha a} \tag{31}$$

T_1 transformed two-electron integral

$$(p\hat{q}|rs) = \sum_{\mu\nu\lambda\sigma} X_{\mu p} Y_{\nu q} X_{\lambda r} Y_{\sigma s} (\mu\nu|\lambda\sigma) \tag{32}$$

Doubles amplitude

$$t_{ij}^{ab} = \frac{(ai\hat{|}bj)}{\varepsilon_i - \varepsilon_a + \varepsilon_j - \varepsilon_b} \tag{33}$$

III. EOMEE

Original Barlett Paper

$$\left\langle a^\dagger b \right\rangle = \rho_{ab} = r_0 \left[t_m^b l_a^m + \frac{1}{2} t_{mn}^{eb} l_{ea}^{mn} \right] + r_m^b l_a^m + \frac{1}{2} r_{mn}^{eb} l_{ea}^{mn} + t_n^b r_m^e l_{ea}^{mn} \tag{34}$$

Krylov dervation

$$\gamma'_{ab} = \frac{1}{2} P_+(ab) \left(\sum_i l_i^a \tilde{\tilde{r}}_{ib} + \tilde{l}^{ab} + \sum_i Y_{ia}^1 t_i^b \right) \tag{35}$$

$$\tilde{\tilde{r}}_{ib} = r_i^b + r_0 t_i^b \tag{36}$$

$$\tilde{l}^{ab} = \frac{1}{2} \sum_{ijc} l_{ij}^{ac} \tilde{\tilde{r}}_{ij}^{bc} \tag{37}$$

$$\tilde{\tilde{r}}_{ij}^{bc} = r_{ij}^{bc} + r_0 t_{ij}^{bc} \tag{38}$$

$$\gamma'_{ab} = \frac{1}{2} P_+(ab) \left(\sum_i l_i^a r_i^b + r_0 l_i^a t_i^b + \frac{1}{2} l_{ij}^{ac} r_{ij}^{bc} + \frac{1}{2} r_0 l_{ij}^{ac} t_{ij}^{bc} + \sum_i l_{ij}^{ab} r_j^b t_i^b \right) \tag{39}$$

$$\gamma'_{ab} = \frac{1}{2} \left(\sum_i l_i^a r_i^b + r_0 l_i^a t_i^b + \frac{1}{2} l_{ij}^{ac} r_{ij}^{bc} + \frac{1}{2} r_0 l_{ij}^{ac} t_{ij}^{bc} + \sum_i l_{ij}^{ab} r_j^b t_i^b \right) \tag{40}$$

$$+ \frac{1}{2} \left(\sum_i l_i^b r_i^a + r_0 l_i^b t_i^a + \frac{1}{2} l_{ij}^{bc} r_{ij}^{ac} + \frac{1}{2} r_0 l_{ij}^{bc} t_{ij}^{ac} + \sum_i l_{ij}^{ba} r_j^a t_i^a \right) \tag{41}$$

$$Y_{ia}^1 = \sum_{jb} l_{ij}^{ab} r_j^b \tag{42}$$

IV. EOMIP

$$\gamma'_{ab} = \frac{1}{2}P_{+}(ab)\left(\tilde{l}^{ab} - \sum_{i} Y^{1}_{ia}t^{b}_{i}\right) \tag{43}$$

$$Y^{1}_{ia} = \sum_{j} l^{a}_{ij}r_{j} \tag{44}$$

$$\tilde{l}^{ab} = \frac{1}{2}\sum_{ij} l^{a}_{ij}r^{b}_{ij} \tag{45}$$

$$\gamma'_{ab} = \frac{1}{2}P_{+}(ab)\left(\frac{1}{2}\sum_{ij} l^{a}_{ij}r^{b}_{ij} - \sum_{j} l^{a}_{ij}r_{j}t^{b}_{i}\right) \tag{46}$$

$$\gamma'_{ab} = \frac{1}{2}\left(\frac{1}{2}\sum_{ij} l^{a}_{ij}r^{b}_{ij} - \sum_{ij} l^{a}_{ij}r_{j}t^{b}_{i}\right) \tag{47}$$

$$+\frac{1}{2}\left(\frac{1}{2}\sum_{ij} l^{b}_{ij}r^{a}_{ij} - \sum_{ij} l^{b}_{ij}r_{j}t^{a}_{i}\right) \tag{48}$$

V. EOMEA

$$\gamma'_{ab} = \frac{1}{2}P_{+}(ab)\left(l^{a}r^{b} + \tilde{l}_{ab}\sum_{k} Y^{1}_{ka}t^{b}_{k}\right) \tag{49}$$

$$\tilde{l}_{ab} = \sum_{kc} l^{ac}_{k}r^{bc}_{k} \tag{50}$$

$$Y^{1}_{ka} = \sum_{c} l^{ac}_{k}r^{c} \tag{51}$$

$$\gamma'_{ab} = \frac{1}{2}P_{+}(ab)\left(\sum_{i} l^{a}r^{b} + \frac{1}{2}l^{ac}_{i}r^{bc}_{i} + \sum_{m} l^{ac}_{k}r^{c}t^{b}_{k}\right) \tag{52}$$

$$\gamma'_{ab} = \frac{1}{2}\left(\sum_{i} l^{a}r^{b} + \frac{1}{2}l^{ac}_{i}r^{bc}_{i} + \sum_{k} l^{ac}_{k}r^{c}t^{b}_{k}\right) \tag{53}$$

$$+\frac{1}{2}\left(\sum_{i} l^{b}r^{a} + \frac{1}{2}l^{bc}_{i}r^{ac}_{i} + \sum_{i} l^{bc}_{k}r^{c}t^{a}_{k}\right) \tag{54}$$