

orbital relaxation pt.1



TCC:

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$\Psi_{cc}$

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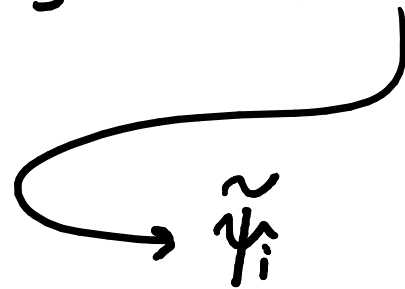
$$\Psi_{CC} = \exp(T_1 + T_2 + T_3 + \dots) \mathbb{E}$$

$$= \exp(T_2 + T_3 + \dots) \tilde{\mathbb{E}}$$

TCC:

$$\Psi_{CC} = \exp(T_1 + T_2 + T_3 + \dots) \Phi$$


$$= \exp(T_2 + T_3 + \dots) \tilde{\Phi}$$



TCC:

$$\Psi_{CC} = \exp(T_1 + T_2 + T_3 + \dots) \Xi$$

$$= \exp(T_2 + T_3 + \dots) \tilde{\Xi}$$



$$\tilde{\psi}_i = \psi_i + \sum_a t_a^i \psi_a$$



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$$= \exp(T_2 + T_3 + \dots) \tilde{\Phi}$$


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$T_1$  is big when  $\Phi$  is bad

$\tilde{\Phi} = \exp(T_1) \Phi$  is intermediately  
normalized

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$$\tilde{\Phi} = \exp(T_1 - T_1^\dagger) \Phi \quad \text{is normalized}$$



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"optimized orbitals"