Hartree-Fock Orbital Space and Filling

Inactive virtual orbitals

Active orbital subspace

$a_{3\uparrow}^{\dagger}|vac\rangle$

$a_{2\uparrow}^{\dagger}a_{2\downarrow}^{\dagger}|vac\rangle$

$a_{1\uparrow}^{\dagger}a_{1\downarrow}^{\dagger}|vac\rangle$

Inactive filled orbitals
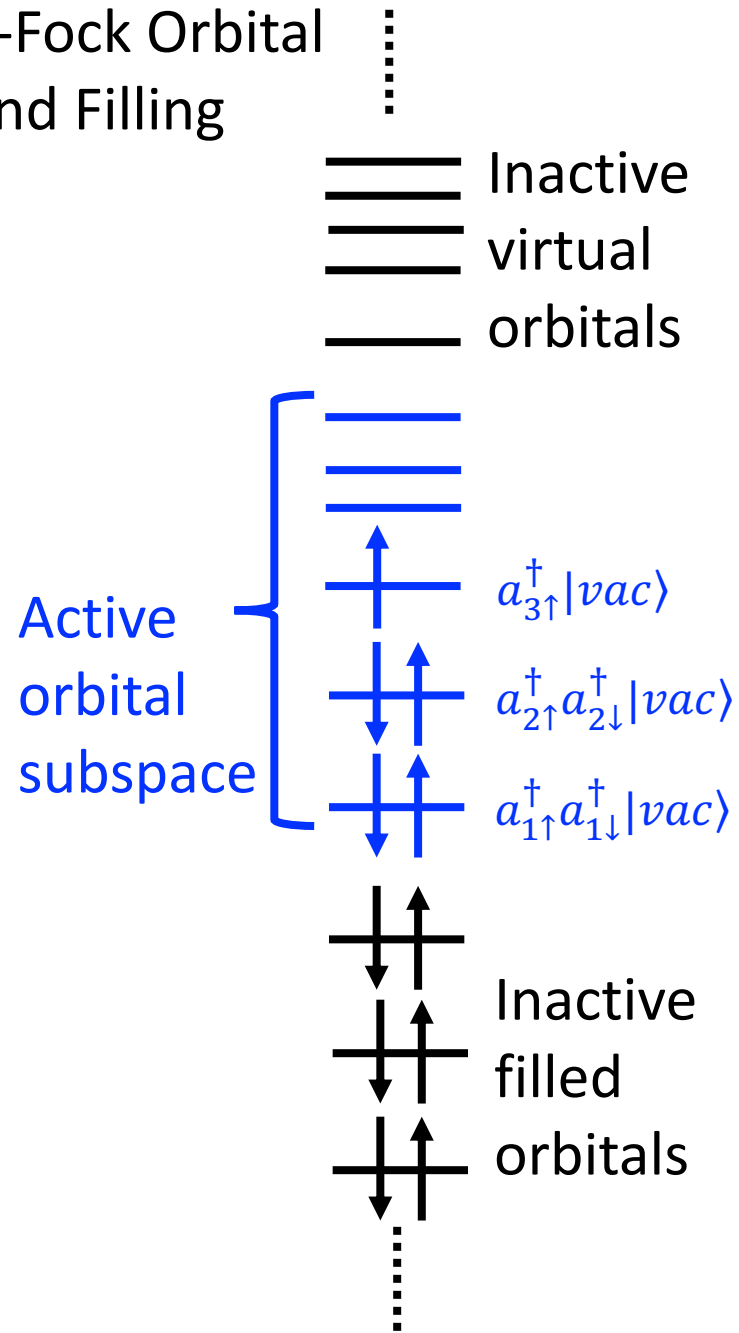
Initial guesses for ground-state and excited state configurations

$$|\Psi_{gs}^{guess}\rangle = a_{3\uparrow}^{\dagger}a_{2\uparrow}^{\dagger}a_{2\downarrow}^{\dagger}a_{1\uparrow}^{\dagger}a_{1\downarrow}^{\dagger}|vac\rangle$$

$$|\Psi_{excited}^{guess}\rangle = c_1 a_{4\uparrow}^{\dagger}a_{2\uparrow}^{\dagger}a_{2\downarrow}^{\dagger}a_{1\uparrow}^{\dagger}a_{1\downarrow}^{\dagger}|vac\rangle$$
$$+ c_2 a_{5\uparrow}^{\dagger}a_{2\uparrow}^{\dagger}a_{2\downarrow}^{\dagger}a_{1\uparrow}^{\dagger}a_{1\downarrow}^{\dagger}|vac\rangle$$
$$+ \ldots$$