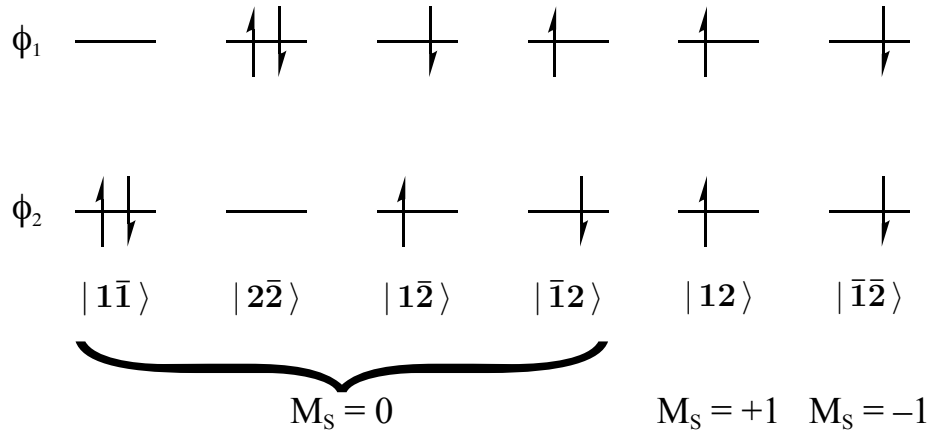
(a) Multiconfigurational + Multireference Approach



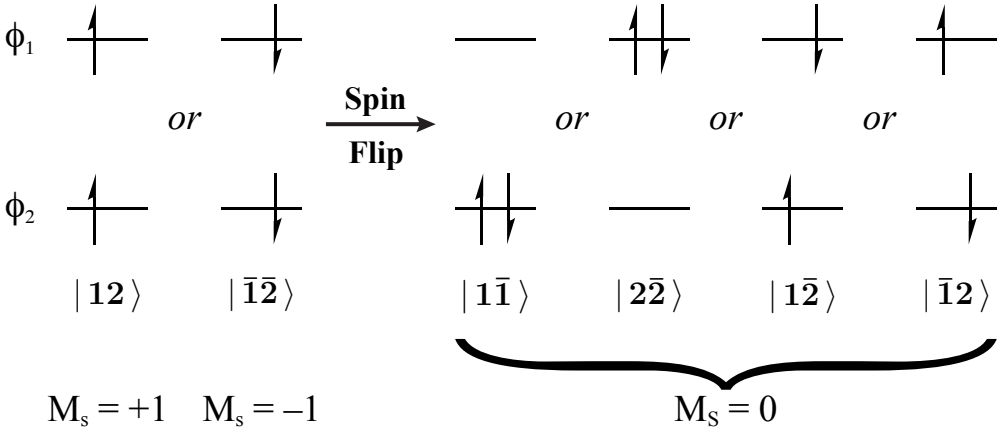
SALCs

$$\Psi_{+}^{TCS} = |1\bar{1}\rangle + |2\bar{2}\rangle$$
$$\Psi_{-}^{TCS} = |1\bar{1}\rangle - |2\bar{2}\rangle$$
$$\Psi^{OSS} = |1\bar{2}\rangle - |\bar{1}2\rangle$$
$$\Psi_{M_s=0}^{T} = |1\bar{2}\rangle + |\bar{1}2\rangle$$
$$\Psi_{M_s=+1}^{T} = |12\rangle$$
$$\Psi_{M_s=-1}^{T} = |\bar{1}\bar{2}\rangle$$

(i) Electronic Configurations & Reference Active Spaces: ROHF/UHF

(ii-iii) Electronic States: MCSCF + MR

(b) Spin-Flip Approach



SALCs

$$\Psi_{+}^{TCS} = |1\bar{1}\rangle + |2\bar{2}\rangle$$
$$\Psi_{-}^{TCS} = |1\bar{1}\rangle - |2\bar{2}\rangle$$
$$\Psi^{OSS} = |1\bar{2}\rangle - |\bar{1}2\rangle$$
$$\Psi_{M_s=0}^{T} = |1\bar{2}\rangle + |\bar{1}2\rangle$$
$$\Psi_{M_s=+1}^{T} = |12\rangle$$
$$\Psi_{M_s=-1}^{T} = |\bar{1}\bar{2}\rangle$$

(i) Reference Determinant: UHF/ROHF or UKS/ROKS

(ii) Excited Determinants: EOM-SF-CC or SF-TDDFT

(iii) Electronic States: Correlated "for free"