Configuration Interaction Singles with Spin-Orbit Coupling: Constructing Spin-Adiabatic States and Their Analytical Nuclear Gradients

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There is a sign error in Eq. 41. The correct expression for $Y_{ck}$ should be:

$$Y_{ck} \equiv - \sum_{\mu\nu\lambda\gamma} C_{\lambda c} C_{\gamma k} \left( B_{\mu\nu} + B_{\nu\mu} \right) \Pi_{\mu\lambda\nu\gamma}$$

$$+ \sum_{j\mu\nu\lambda\gamma} C_{\nu j} C_{\mu k} \left( X_{cj} R_{\gamma\lambda} + X_{cj}^* R_{\gamma\lambda}^* \right) \Pi_{\mu\lambda\nu\gamma}$$

$$- \sum_{b\mu\nu\lambda\gamma} C_{\nu c} C_{\mu b} \left( R_{\gamma\lambda} X_{bk}^* + R_{\gamma\lambda}^* X_{bk} \right) \Pi_{\mu\lambda\nu\gamma}$$

(41)