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:

$$\begin{aligned} Y_{\mathbf{ck}} \equiv & -\sum_{\boldsymbol{\mu\nu\lambda\gamma}} C_{\boldsymbol{\lambda}\mathbf{c}} C_{\boldsymbol{\gamma}\mathbf{k}} \left(B_{\boldsymbol{\mu\nu}} + B_{\boldsymbol{\nu\mu}}\right) \Pi_{\boldsymbol{\mu\lambda\nu\gamma}} \\ & + \sum_{\mathbf{j}\boldsymbol{\mu\nu\lambda\gamma}} C_{\boldsymbol{\nu}\mathbf{j}} C_{\boldsymbol{\mu}\mathbf{k}} \left(X^*_{\mathbf{cj}} R_{\boldsymbol{\gamma\lambda}} + X_{\mathbf{cj}} R^*_{\boldsymbol{\gamma\lambda}}\right) \Pi_{\boldsymbol{\mu\lambda\nu\gamma}} \\ & - \sum_{\mathbf{b}\boldsymbol{\mu\nu\lambda\gamma}} C_{\boldsymbol{\nu}\mathbf{c}} C_{\boldsymbol{\mu}\mathbf{b}} \left(R_{\boldsymbol{\gamma\lambda}} X^*_{\mathbf{bk}} + R^*_{\boldsymbol{\gamma\lambda}} X_{\mathbf{bk}}\right) \Pi_{\boldsymbol{\mu\lambda\nu\gamma}} \end{aligned} \tag{41}$$