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Erratum

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Erratum: "The Variationally Orbital-Adapted Configuration Interaction Singles (VOA-CIS) Approach to Electronically Excited States"

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Equation 16 should be:

$$\mathcal{M}(D, A, B, C) \equiv D\cdot(AB^{\mathrm{T}}C + CB^{\mathrm{T}}A)$$

The third equation in eq 17 of our paper should read:

$$\begin{aligned}\langle\Psi^{\tilde{I}JK}|H|\Psi^{\tilde{I}'J'K'}\rangle &= \sum_{abij}\theta_{bj}^{\tilde{I}J}\theta_{ai}^{\tilde{I}'J'}\langle\Psi^{K}|a_j^{\dagger}a_bHa_a^{\dagger}a_i|\Psi^{K'}\rangle\\ &= +(t^K\cdot t^{K'})(\theta^{\tilde{I}J}\cdot\theta^{\tilde{I}'J'})E_{\mathrm{HF}}\\ &\quad +(t^K\cdot\theta^{\tilde{I}'J'})(\theta^{\tilde{I}J}\cdot t^{K'})E_{\mathrm{HF}}\\ &\quad -\mathcal{M}(\theta^{\tilde{I}J},\theta^{\tilde{I}'J'},t^K,t^{K'})E_{\mathrm{HF}}\\ &\quad +(t^K\cdot\mathcal{F}(t^{K'}))(\theta^{\tilde{I}J}\cdot\theta^{\tilde{I}'J'})\\ &\quad +(t^K\cdot t^{K'})(\theta^{\tilde{I}J}\cdot\mathcal{F}(\theta^{\tilde{I}'J'}))\\ &\quad +(t^K\cdot\theta^{\tilde{I}'J'})(\theta^{\tilde{I}J}\cdot\mathcal{F}(t^{K'}))\\ &\quad +(\theta^{\tilde{I}'J'}\cdot\mathcal{F}(t^K))(\theta^{\tilde{I}J}\cdot t^{K'})\\ &\quad -\mathcal{M}(\theta^{\tilde{I}J},\theta^{\tilde{I}'J'},t^K,\mathcal{F}(t^{K'}))\\ &\quad -\mathcal{M}(\theta^{\tilde{I}J},t^{K'},t^K,\mathcal{F}(\theta^{\tilde{I}'J'}))\\ &\quad -\mathcal{M}(\theta^{\tilde{I}J},\theta^{\tilde{I}'J'},\mathcal{L}_{vo}^{vo}(t^K),t^{K'})\\ &\quad -\mathcal{M}(t^K,t^{K'},\mathcal{L}_{vo}^{vo}(\theta^{\tilde{I}J}),\theta^{\tilde{I}'J'})\\ &\quad +\theta^{\tilde{I}J}\cdot(\mathcal{K}_{vv}(t^{K'},t^K)\theta^{\tilde{I}'J'})\\ &\quad -\theta^{\tilde{I}J}\cdot(\theta^{\tilde{I}'J'}\mathcal{K}_{oo}(t^{K'},t^K))\\ &\quad +\theta^{\tilde{I}J}\cdot(\mathcal{K}_{vv}(\theta^{\tilde{I}'J'},t^K)t^{K'})\\ &\quad -\theta^{\tilde{I}J}\cdot(t^{K'}\mathcal{K}_{oo}(\theta^{\tilde{I}'J'},t^K))\end{aligned}$$

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