Open-shell Symmetry-Adapted Perturbation Theory

- The SAPT0 interaction energy terms are:

$$E_{int} = E_{elst}^{(10)} + E_{exch}^{(10)} + E_{ind}^{(20)} + E_{exch-ind}^{(20)} + E_{disp}^{(20)} + E_{exch-disp}^{(20)} + \ldots$$

Where intramonomer correlation and terms beyond second-order are neglected.

The induction term can include orbital relaxation through CPHF and becomes:

$$E_{ind,r}^{(20)} + E_{exch-ind,r}^{(20)}$$

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The exchange terms are often expressed through the single-exchange approximation:

$$E_{exch}^{(10)}(S^2),\ E_{exch-ind}^{(20)}(S^2),\ E_{exch-disp}^{(20)}(S^2)$$

Each term exists in second-quantized formalism (valid for DCBS only) or density matrix formalism (generally valid).

USAPT0: SAPT0 with UHF reference. Terms currently implemented:

$$E_{elst}^{(10)},\ E_{exch}^{(10)}\ \text{(full)},\ E_{exch}^{(10)}(S^2)\ \text{(second-quantized formalism)},$$
$$E_{exch}^{(10)}(S^2)\ \text{(density matrix formalism)}$$

$$E_{ind}^{(20)},\ E_{exch-ind}^{(20)}(S^2)\ \text{(second-quantized formalism)}$$
$$E_{ind,r}^{(20)},\ E_{exch-ind,r}^{(20)}(S^2)\ \text{(second-quantized formalism)}$$

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USAPT0: SAPT0 with UHF reference. Terms implemented in the more or less near future:

$$E_{disp}^{(20)},\ E_{exch-disp}^{(20)}(S^2)\ \text{(second-quantized formalism)}$$

$$E_{exch-ind}^{(20)}(\text{full}),\ E_{exch-ind,r}^{(20)}(\text{full}),\ E_{exch-disp}^{(20)}(\text{full})$$

USAPT0 is now a plugin, so proper merging with existing SAPT code is on the agenda as well.