To which extent can strong correlation be treated by single reference perturbation theory?

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Single-reference many-body perturbation theory, performed in the basis of either canonical or some localized orbitals, is a standard tool for the estimation of the electronic correlation energy in molecular systems. However, it usually fails when applied in the strong correlation regime. This failure can be manifested in improper low-order contributions as well as in the divergence of the perturbation series. Multi-reference perturbation theory is an obvious remedy, but it requires a complicated formalism, may get expensive for large reference spaces, and sometimes violates the extensivity requirement.

Therefore, interest remains in investigating less-standard formulations and techniques of single reference perturbation theories which may treat strongly correlated electronic systems to some extent. We shall consider two different possibilities:

1. Replacing the standard Fockian of Møller-Plesset partitioning by an alternative one-body zero-order Hamiltonian

2. Applying some kind of resummation techniques in divergent cases.

As to 1, we shall discuss the so-called *Dyson partitioning*[1] in which the canonical orbital energies in the denominators are replaced by correlated ionization potentials emerging from, e.g., the Dyson equation, and the *Knowles partitioning*[2], in which special equations are solved for obtaining a better one-electron zero order Hamiltonian prior to computing the perturbation corrections. As to 2, we shortly discuss analytic continuation methods including extrapolation[3,4] with quadratic Padé approximants and the so-called inverse boundary problem[5] technique.

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