POSTER ABSTRACT

The Algebraic Diagrammatic Construction scheme for the particle-particle propagator: Access to excitation energies for $N \pm 2$-electron states

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Theoretical methods for the calculation of excited states based on propagator theory have established a versatile toolkit in computational chemistry. Following this theory, the Algebraic Diagrammatic Construction scheme[1] based on the work of J. Schimer et al.[2] has introduced an approach for the calculation of excited states following the perturbative treatment of the underlying propagator. The p-p (particle-particle) propagator establishes access to the compuataion of electron excitations with final $N \pm 2$-electron states.
This work presents an implementation for the computation of excitation energies for doubly-ionized (N-2) and doubly-electronically attached (N+2) species in the framework of the Algebraic Diagrammatic Construction scheme. Schemes for DIP-ADC(1) (2h/2h block in first order pertubation theory), DIP-ADC(2) (see figure) and the extended DIP-ADC(2)-x scheme (p3h/p3h block expanded to first order pertubation theory) as well as their DEA-ADC equivalents are included.

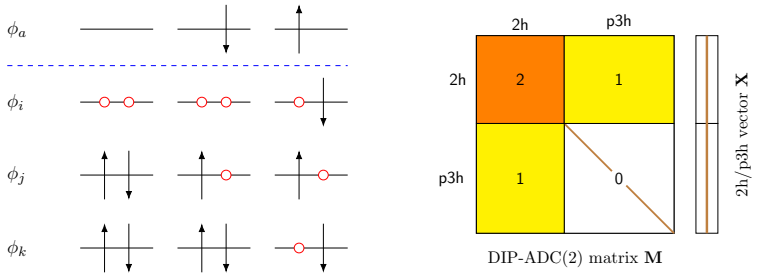

Figure 1. Left side: Examples of 2h and p3h configurations. Right side: Second-order DIP-ADC scheme, the number in the blocks is the order of pertubation theory applied (diagonal form for zeroth order). Excitation energies ω are the solutins of the eingenvalue equation $\mathbf{MX} = \omega\mathbf{X}$.

References

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[2] J. Schirmer and A. Barth, Zeitschr. f. Physik A Atoms and Nuclei **317** (3), 267–279 (1984).

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