A hierarchical decomposition of Hilbert space based on excitations and seniorities

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Full Configuration Interaction (FCI) is the special case of CI where we include all the possible Slater determinants (or configurations) in the variational procedure to obtain the electronic energies. There have been multiple established procedures to reduce these number of Slater determinants in the variational procedure based on excitation (e.g., CID, CISD, CISDT) and seniorities (e.g., DOCI). To achieve the same (and following a recent proposal by Loos et al.), we use a hierarchical parameter 'h' which has two weights α_1 and α_2 measuring the importance of excitation (e) and seniority (s) contributions to the wavefunctions according to:

$h= \alpha_1 * e + \alpha_2 * s$

Standard, excitation-level CI (CISD, CISDT, etc.) corresponds to $\alpha_1=1$ and $\alpha_2=0$. Seniority-based CI, on the other hand, corresponds to $\alpha_1=0$ and $\alpha_2=1$. In his work, Loos only considers $\alpha_1=0.5$ and $\alpha_2=0.25$. The question is then: can we find other ways to generate partitions of the Hilbert space? We vary α_1 and α_2 values in the [- 1, 1] interval in order to partition the Hilbert space. The key idea is to see how the interplay between excitation and seniority leads to descriptions of systems where dynamic or static correlation is dominant (and, hopefully, identifying a regime that provides a balanced description of both correlation types). These new CI hierarchies were implemented in our Fanpy package, and tested on model systems.