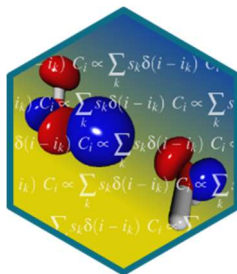


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*Perturbation Theory for strongly correlated Spin  
Systems*

Wednesday, 8 May 2024, 3 p.m.  
Pfaffenwaldring 55, Room 8.109

The study of strongly correlated systems featuring many unpaired electrons is an important task in quantum chemistry, often requiring multireference methods for accurate predictions. However, multiconfigurational simulations of such systems are typically a very expensive task due to their high dimensionality.

We have shown that this problem can be circumvented by systematic truncation of the explicitly correlated many body-basis using the criteria of partial spin expectation value and occupation number of an orbital subspace. Discarded configurations were accounted for perturbatively to yield accurate results.

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