Strong correlation the easy way: Spin-flip method and its applications to magnetism and spin-forbidden phenomena

Anna I. Krylov

Department of Chemistry, University of Southern California, Los Angeles, California

Strong correlation, which emerges due to electronic near-degeneracies such as small HOMO-LUMO gaps, is notoriously difficult to describe by electronic structure methods. Spin-flip (SF) family of methods offers a practical solution to this problem by utilizing a well-behaved high-spin reference state, which can be well described by a single Slater determinant, and treating multi-configurational low-spin states as excited states involving spin-flip. SF ansatz can be combined with a variety of ab initio methods, ranging from configuration interaction and coupled-cluster methods to Kohn-Sham density functional theory. It has been used to model electronic structure of di- and tri-radicals, singlet fission systems, as well as single-molecule magnets (SMMs). This lecture will describe the SF approach and highlight recent developments. The utility of the methods will be illustrated by applications to magnetic systems and spin-forbidden phenomena.

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