
Unitary Group Adapted Iterative Configuration Expansion(ICE): Implementation and Applications

Vijay Gopal Chilkuri*¹ and Frank Neese²

¹Max-Planck-Institut für Kohlenforschung (coal research) – Allemagne

²Max Planck Institut für Kohlenforschung – Allemagne

Résumé

We present a novel implementation of selected CI (ICE) including non-abelian SU(2) symmetry with an emphasis on efficiency. A detailed comparison of the SU(2) adapted selected CI with the usual determinant based CI and DMRG is performed in order to assess the efficiency and accuracy of the ICE method. Finally, we present a few case studies which demonstrate the power of the SU(2) adaptation as opposed to the determinant representation. Our method seems especially effective for describing the wavefunction of molecules containing a number of transition metal atoms interacting via a strong anti-ferromagnetic coupling.

Mots-Clés: selected CI, non-abelian symmetry, SU(2), magnetic molecules

*Intervenant