The SDS Family of Methods for Strongly Correlated Electrons

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Keywords: strong correlation; static-dynamic-static; SDSPT2; SDSCI; iCIPT2; SOiCI

Abstract: According to when the static and dynamic components of electron correlation are treated, the available wave function-based correlation methods can be classified into three categories, viz. "static-then-dynamic", "dynamic-then-static", and "static-dynamic-static (SDS)" [1]. Herewith we report on a *restricted* SDS framework [2], which employs *the same number* (Np; the number of target states) of primary, secondary and external states for describing the static, dynamic, and again static components of correlation. That is, the secular equation to be diagonalized is of dimension 3Np, irrespective of the numbers of correlated electrons and orbitals. Particular realizations of this framework include SDSPT2 [2,3], SDSCI [2], iCI [1], iCIPT2 [4,5], iCAS, iCISCF, SOiCI, iCISO, etc. The efficacy of such methods has been well tested against benchmark systems [9].

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