spin-Generator Coordinate Method

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Löwdin's dilemma states that artifical symmetry breaking in variational mean field theories can result in lower energies, however at the cost of a symmetry broken wave-function and related quantum number. I will present the spin-Generator Coordinate Method (spin-GCM), in which the artificial symmetry can be broken in a controled way via a constrained Hartree-Fock computation, and restored within a non-orthogonal configuration approach, capturing additional correlation energy. Joint work with Ghent Quantum Chemistry Group and Hugh Burton.