Multi-reference Energy Density Functional calculations for nuclei

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Multi-reference Energy Density Functional (MR-EDF) calculations along the lines of the Generator Coordinate Method [1] are becoming a standard tool in nuclear structure physics [2]. Such calculations allows one to incorporate correlations associated with large amplitude collective motion and the restoration of symmetries that are broken at the single-reference level. In the harmonic limit, the random phase approximation is recovered from the MR-EDF method [3].

Multi-reference calculations rely on the extension of a basic energy functional, computed from a single symmetry-breaking product state, to non-diagonal energy kernels involving a pair of product states. There is no rigorous constructive framework for this extension so far. The commonly accepted way proceeds by formal analogy with the expression obtained when applying the generalized Wick theorem [4] to the non-diagonal matrix element of a Hamilton operator between two non-orthogonal product states. It will be pointed out that this procedure is ill-defined when extended to EDF calculations and is responsible for the appearance of spurious divergences and steps in MR-EDF energies, as was recently observed [5] in calculations restoring good particle number or angular momentum. A method to regularize non-diagonal energy kernels such that divergences and steps are removed from MR-EDF energies will be discussed [6]. Although applicable to any symmetry or generator coordinate, the regularization method will be illustrated for particle number symmetry where it restores sum-rules over positive (physical) particle numbers (irreducible representations of $U(1)$). If time allows, further constraints on non-diagonal energy kernels based on group-theory considerations will be discussed [7].

References

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