# Pertinent ingredients for MR EDF calculations

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### I. PROBLEMATIC

For more than forty years, the Energy Density Functional (EDF) method [1, 2] has proven to be a useul tool to study low-energy nuclear structure and reactions. In particular, its Multi-Reference (MR) formulation allows the study of complex phenomena that emerge in the strongly-correlated finite quantal system that is the atomic nucleus. Over the last few years, the full-fledged MR-EDF method and its derivatives (e.g. the quasiparticle random-pase approximation [3] (QRPA), the microscopic collective Hamiltonian [4, 5], the Lipkin method [6], . . . ) have been subject to important developments, both regarding their theoretical foundations and their applications. On the formal side, efforts are being made to design parametrizations of the (off-diagonal) energy kernel that are consistent with the MR methodology [2, 7–11]. As for applications, the horizon has immensely widen over the years and now concern topics as diverse as the spectroscopy of even and odd-mass nuclei [12–19], the estimation of $\beta$ decay rates [19–21], the calculations of nuclear matrix elements for neutrinoless double-$\beta$ decay [22–24], the study of giant resonances [25–28], the investigation of fission dynamics [29, 30], or the analysis of clusterization in light nuclei [31–33], just to give a few examples.

From a technical point of view, this large-scale availability of MR-EDF calculations is made possible by the advances in scientific computing and the access to ever-growing computational resources. Indeed, the most advanced MR-EDF methods that combine symmetry restorations and/or configuration mixing are computationally demanding and require large-scale computing facilities. This has to be contrasted with the picturesque idea of EDF approaches as low-cost computing methods. The difficulty comes from the fact that MR calculations represent a multi-dimensional problem that rapidly grows as one includes more (collective or non-collective) degrees of freedom into it. Consequently, even with the future increase in computational resources and the advent of exascale computing, it may not be possible to solve for the most general MR scheme, including variationally all possible degrees of freedom. To overcome those hardware limitations, one has to cleverly select the degrees of freedom that must be taken into account. The problem is thus to determine, for a given observable and a specified accuracy, which correlations are mandatory to be treated explicitly, and which MR schemes are the most efficient to achieve this. This is not an easy task for several reasons.

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First, the EDF method relies on the use of an effective parameterization of the off-diagonal energy kernel, which itself accounts for correlations that, qualitatively speaking, vary smoothly with nucleon number. The analytical form of this energy kernel is traditionally postulated with essentially no underlying rooting or systematic argument, except for symmetry ones, while its parameters are fitted to reproduce a biased set of (experimental or theoretical) data on the basis of the diagonal part of the kernel only. The fact that there is little control on what the energy kernel itself accounts (should account) for makes difficult to characterize the modes and the MR scheme that constitute the optimal compromise in the calculation of a given set of nuclear observables.

Second, the manner one optimizes the reference states that are mixed in a full-fledged MR-EDF calculation impacts the actual result and the numerical cost. A typical example relates to symmetry-breaking and restoration MR schemes where two variants can be considered, i.e. (i) the Variation-After-Projection (VAP) approach where one variationally searches for the reference state that gives the lowest energy after the symmetry restoration, and (ii) the Projection-After-Variation (PAV) approach where one variationally searches for the reference state that gives the lowest energy before symmetry restoration. While the VAP approach is computationally more demanding than the PAV approach it is better from a variational viewpoint. Still, it is not clear to which extent this statement remains true when only a subset of the symmetries are treated in a VAP scheme while the others rely on a PAV scheme, as different symmetry restorations may favor reference states with different intrinsic configurations.

A third difficulty resides in the fact that, contrarily to what one may intuitively hope for, the various (collective and non-collective) modes whose dynamics can be explicitly treated at the MR level are usually not independent from one another. Consequently, disentangling the merit of various modes and concluding on the superiority of incorporating a particular one in the description of a certain phenomenon requires a thorough and systematic multi-dimensional analysis that could not been conducted until now.

Fourth, the computation of observables besides the energy is traditionally performed with bare, e.g. one-body, operators. On the one hand, the use of bare nucleonic parameters (e.g. electric charge and $g$ factor) is motivated by the fact that the dynamics of all nucleons is explicitly treated in the EDF method. On the other hand, the omitted internal structure of the nucleons and the inherent truncation of the many-body Hilbert space explicitly spanned within the (SR- and MR-) EDF method, should allow for the use of many-body operators on the one hand and of possibly effective nucleonic parameters (i.e. low energy coupling constant) on the other when considering the calculations of, e.g. electromagnetic, observables besides the energy.

More generally, a critical analysis of mandatory correlations is inseparable from a critical analysis of the theoretical framework itself. For example, one can differentiate between MR methods according to their treatment of symmetries. On the one hand, one finds methods that break and restore symmetries [1] as a way to grasp a large part of collective correlations already at the SR level, but at the cost of the computationally demanding symmetry-restoration process at the MR level. On the other hand, one finds symmetry-conserving approaches that build a particle-hole expansion on top a reference state that carries good symmetry quantum numbers [15]. From another perspective, approaches such as QPRA [34, 35] or the Collective Hamiltonian [36, 37] are approximations to the full-fledged MR-EDF method in its most general form. As such, there applicability is not as general, e.g. QRPA only describes well systems that display a harmonic behavior with respect to collective degrees of freedom. Still, as the most general MR-EDF method is never (and may never be) applied in practice, these approximations actually give better access to specific states and observables and thus constitute optimal compromises in those cases. Even more restricted and approximate methods such as the Lipkin method [38] may grab, within a modified SR scheme, MR correlations at a severely reduced computational cost that authorizes their use on a wide scale.

A corollary of all the above is that correlations are only defined relative to an arbitrarily chosen reference and are not observable per se. As such, experimentally measurable quantities can be equally well described by expanding the many-body solution in many different ways. The non-orthogonality of the modes employed in a MR-EDF calculations and the non-additive character of the associated correlation energies as well as the possibility to employ symmetry-conserving or symmetry-broken and -restored schemes are particular manifestations of this fact. On a deeper level, even when correlations have been formally defined unambiguously within a given setting, the relative weight of "uncorrelated" and "correlated" contributions can be tuned such that absolute statements about their role must be prohibited [39, 40]. Eventually, discussing the impact of correlations on observables requires their thorough definition and the full specification of the theoretical scheme one is working with.

## II. GOALS OF THE WORKSHOP

In summary, the goals of the workshop are to:

1. gather the community of MR-EDF practitioners around a common objective.

2. identify, for a set of typical observables of interest, the most pertinent degrees of freedom to be taken into account in the calculations.

3. determine to what extent the different sources of correlations are (in)dependent from one another.

4. discuss the merits and the efficency of the different methods used to include the desired correlations, both from a conceptual and a numerical point of view.

## III. PROGRAM

| | Monday | | Tuesday | Wednesday | Thursday |
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| | | 9h30 | **Egido** | **Pillet** | **Rodríguez** |
| 10h15 | Welcome | 10h30 | Break | Break | Break |
| 10h30 | **Somà** | 11h00 | **Bender** | **Lacroix** | **Satuła** |
| 12h00 | Lunch | 12h00 | Lunch | Lunch | Lunch |
| 14h00 | **Duguet** | 14h00 | **Heenen** | **Bally** | **Péru** |
| 15h30 | Break | 15h00 | Break | Break | Break |
| 16h00 | **Dobaczewski** | 15h30 | **Nikšić** | **Colò** | **Martini** |
| 17h00 | Discussions | 16h30 | Discussions | Discussions | Final discussions |
| | | 20h00 | | Social dinner | |

### A. Introductory lectures

- V. Somà, CEA
  Many-body correlations: the relative nature of their definition and the non-observable character of their value.

- T. Duguet, CEA
  Vertical & horizontal expansions within MR EDF method

### B. List of presentations

- J. Dobaczewski, University of York and Jyväskylä
  Approximate symmetry restoration correction at the SR level with the Lipkin method

- J.L. Egido, Universidad Autónoma de Madrid, Madrid
  Are two-quasiparticle states pertinent to MR-EDF descriptions of collective states?

- M. Bender, IPNL
  Coupling of collective and single-particle degrees of freedom in symmetry-restored GCM

- P.-H. Heenen, Université Libre de Bruxelles
  Interplay between angular-momentum and parity restoration after variation

- T. Nikšić, University of Zagreb
  Comparison between collective Hamiltonian and full-fledged MR calculations using a relativistic EDF

- N. Pillet, CEA
  Second variation in the multi-particle multi-hole configuration mixing with a Gogny energy density functional

- D. Lacroix, IPNO
  Combining symmetry breaking and restoration with configuration interaction

- B. Bally, CEA
  Configuration mixing of symmetry-restored odd-quasiparticle excitations for the description of odd-mass nuclei
- G. Colò, Università degli Studi di Milano
  Multi-reference calculations in the particle-vibration coupling scheme
- T.R. Rodríguez, Universidad Autónoma de Madrid
  MR-EDF calculations of nuclear matrix elements for neutrinoless double-$\beta$ decay
- W. Satuła, University of Warsaw
  Isospin symmetry restoration for nuclear spectroscopy and the calculation of super-allowed $\beta$-decay
- S. Péru, CEA
  Quasiparticle random-phase approximation for low-lying excitations
- M. Martini, CEA
  Quasiparticle random-phase approximation calculations for charge-exchange excitations in deformed nuclei and in infinite nuclear matter

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