New developments in nuclear energy-density-functional models

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F-91191 Gif-sur-Yvette, France

I. PROBLEMATIC

The Energy Density Functional (EDF) method is a powerful tool to study medium-mass and heavy nuclei in a systematic manner [1]. The assumption underlying this class of models is that the effects of quantum many-body correlations can be absorbed, to various degrees, in an effective energy functional, allowing a description of the nucleus in terms of a reduced set of simplified auxiliary wave functions.

Nuclei are self-bound systems exhibiting signatures of superfluidity, spontaneous rotational symmetry breaking and collective shape fluctuations in their low-energy spectra. Different EDF-based many-body schemes, from single-reference (SR) to multi-reference (MR) calculations [1–4] and its quasiparticle random-phase approximation (QRPA) [5–8], or collective-Hamiltonian-based approximations [9, 10], access various ranges of observables. Still, the formal underpinnings of the theory are an open area of development [11–15].

Improving the accuracy and predictive power of EDF models is a permanent concern. However, increasingly sophisticated strategies for optimizing their parameters [16–18] have revealed the limits of currently-used analytical forms. Establishing a connection with the underlying physics of high-precision vacuum potentials, e.g. by building functionals through the density matrix expansion [19–21], may seem promising. However, issues with MR-EDF calculations [22–25] have recently put the focus on models based on antisymmetrized, density-independent effective interaction operators or "pseudo-potentials" [26] containing two-, three- and possibly four-body operators [27], higher orders in gradients [28], or an explicit finite range [29]. Therefore, the field seems to split into different approaches which vary in their range of applicability, and possibly, performance.

The parameters of empirical functionals are typically determined by fitting to a set of measured observables which are easily computable, enough to be incorporated in an iterative optimization algorithm. Beyond the commonly-used masses, charge radii, single-particle spectra and homogeneous matter properties, quantities requiring symmetry-breaking [16, 17] or multi-reference calculations [30, 31] are now being considered, thanks to the progress in available computing power. Similarly, ab-initio calculations of infinite matter are being put on a more solid footing thanks to the development of chiral effective field theory (EFT) [32, 33], while computations of finite systems are being extended to medium-mass nuclei [34–36] and neutron drops [37], which overlaps with the range of applicability of EDF models, offering opportunities for comparisons and benchmarks.

Another concern is that, in the case of semi-local functionals containing gradient terms, some regions of the parameter space yield functionals exhibiting instabilities in the self-consistent iterations [38], and need to be detected and excluded [39, 40].

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Given a set of input data, the determination of functional parameters requires to decide on, then optimize, an objective measure of the agreemeent between data and theory. The empirical nature of the models we are dealing with implies that the resulting parameter set is affected by both statistical and systematic uncertainties. The propagation of errors to calculated observables is then a concern, especially when extrapolating the models to exotic nuclei and nuclear matter [41–44].

II. GOALS OF THE WORKSHOP

In our exchanges with the community, it appeared that a few years had elapsed since the last gathering of practitioners interested in developing EDF models, and that the ESNT would be an appropriate setting for a restart of these events. In summary, the goals of the workshop are to gather the community and allow us to:

1. discuss issues of conceptual foundations, formal development and construction strategies,
2. compare progress in various approaches and exchange ideas,
3. find synergies and spur further collaboration.

In order to facilitate the understanding and involvement of young theorists and experimentalists, two lectures on (i) the historical development of energy density functional models and (ii) the reasons for going back to pseudopotential-based functionals will be included at the beginning of the workshop.

III. LECTURERS

1. J.-P. Ebran, *Origins and evolution of nuclear energy density functional models*
2. T. Duguet, *Why go back to pseudo-potential-based models ?*

IV. LIST OF SPEAKERS

1. DFT/EDF Formalism
   - B. G. Giraud, CEA Saclay/IPhT, *Radial-density functional theory*
   - J. Messud, CENBG Bordeaux and CGG Veritas, *Internal-density functional theory and center-of-mass correlations*
   - T. Lesinski, CEA Saclay/SPhN, *Density-functional theory with spatial-symmetry breaking and configuration mixing*
   - M. Grasso, IPN Orsay, *Renormalizability of the Skyrme pseudo-potential beyond the mean field*
2. Analytical form of functionals/pseudo-potentials
   - M. Bender, CENBG Bordeaux, *Towards a predictive Skyrme pseudo-potential-based energy density functional*
   - D. Peña Arteaga, CEA Bruyères-le Châtel, *Development of the Gogny effective interaction*
   - K. Bennaceur, U. of Lyon and U. of Jyväskylä, *Skyrme pseudo-potentials with 2-, 3- and 4-body terms: the SLyMR family*
   - J. Dobaczewski, U. of Warsaw and U. of Jyväskylä, *New family of finite-range pseudo-potential-based energy density functionals*
3. Optimization, sensitivity analysis, extrapolation
   - S. M. Wild, Argonne National Laboratory, *Derivative-free optimization for parameter estimation in computational nuclear physics*
   - P.-G. Reinhard, U. Erlangen, *Optimization and theoretical uncertainties*
   - E. M. Kortelainen, U. of Jyväskylä, *Optimization and sensitivity analysis for the UNEDF family of functionals*

4. Data, pseudodata, ab-initio inputs and other constraints

- D. Lacroix, IPN Orsay, *Strategies for constructing energy density functionals beyond mean-field*
- S. Hilaire, CEA Bruyères-le-Châtel, *Optimization at the multi-reference level*
- T. Krüger, TU Darmstadt, *Neutron matter from chiral effective field theory interactions*
- V. Somà, CEA Saclay/SPhN, *Ab-initio calculations of mid-mass nuclei*
- D. Davesne, U. of Lyon, *Nuclear matter response functions: principles and applications*
- A. Pastore, ULB Brussels, *Linear response theory in asymmetric nuclear matter for Skyrme functionals*

V. PROGRAM

The workshop will start on Monday, November 24th at 10h00 in room 135.
A conference dinner will be held on Tuesday, *"Chez Fernand"*, 127 Bd. du Montparnasse, Paris.

<table>
<tr><td rowspan="2">09h00</td><td>Mon. 24</td><td>Tue. 25</td><td>Wed. 26</td><td>Thu. 27</td><td>Fri. 28</td></tr>
<tr><td rowspan="2">09h45</td><td rowspan="2"></td><td rowspan="2">T. Duguet</td><td>M. Bender</td><td>D. Lacroix</td><td>T. Krüger</td></tr>
<tr><td rowspan="2">10h30</td><td rowspan="2">Welcome (10h00)</td><td>D. Peña Arteaga</td><td>S. Hilaire</td><td>V. Somà</td></tr>
<tr><td rowspan="3">11h00</td><td rowspan="3">J.-P. Ebran</td><td>Break</td><td>Break</td><td>Break</td><td>Break</td></tr>
<tr><td rowspan="2">11h45</td><td>B. Giraud</td><td>K. Bennaceur</td><td>D. Davesne</td><td rowspan="2">Discussion</td></tr>
<tr><td>J. Messud</td><td>J. Dobaczewski</td><td>A. Pastore</td></tr>
<tr><td>12h30</td><td>Lunch</td><td>Lunch</td><td>Lunch</td><td>Lunch</td><td>Lunch</td></tr>
<tr><td rowspan="2">14h15</td><td>P.-G. Reinhard</td><td>M. Grasso</td><td rowspan="2">Discussion</td><td rowspan="4">10 years
of the ESNT</td><td rowspan="4"></td></tr>
<tr><td rowspan="2">15h00</td><td>S. M. Wild</td><td>T. Lesinski</td></tr>
<tr><td rowspan="2">15h45</td><td>Break</td><td rowspan="3"></td><td rowspan="3"></td></tr>
<tr><td rowspan="2">16h15</td><td>M. Kortelainen</td></tr>
<tr><td>17h00</td><td></td><td></td></tr>
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