Covariant energy density functionals: the assessment of global performance across the nuclear landscape

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Abstract. The assessment of the global performance of the state-of-the-art covariant energy density functionals and related theoretical uncertainties in the description of ground state observables has recently been performed. Based on these results, the correlations between global description of binding energies and nuclear matter properties of covariant energy density functionals have been studied in this contribution.

INTRODUCTION

The global performance of the covariant energy density functionals (CEDF’s) in the description of ground state observables has been assessed in Refs. [1, 2, 3] employing the state-of-the-art functionals NL3*, DD-ME2, DD-MEδ, and DD-PC1. They represent three classes of functionals which differ by basic model assumptions and fitting protocols. The available experimental data on ground state properties of even-even nuclei such as binding energies, charge radii, neutron skin thicknesses as well as two-proton and two-neutron separation energies and the positions of two-proton and two-neutron drip lines have been confronted with the results of the calculations. For the first time, theoretical systematic uncertainties in the prediction of physical observables have been investigated on a global scale for relativistic functionals. Special attention has been paid to the propagation of these uncertainties towards the neutron-drip line [2] and the sources of these uncertainties [3]. Since the details of these studies are easily accessible, I will focus in this contribution on the relations between global description of masses and nuclear matter properties of underlying functionals.

THE COMPARISON OF DIFFERENT FUNCTIONALS

In Fig. 1 the map of theoretical uncertainties $\Delta E(Z,N)$ in the description of binding energies is shown. The comparison of this figure with Fig. 1 in Ref. [1] (which presents experimentally known nuclei in the nuclear chart), shows that the spreads in the predictions of binding energies stay within 5-6 MeV for the known nuclei. These spreads are even smaller (typically around 3 MeV) for the nuclei in the valley of beta-stability. However, theoretical systematic uncertainties for the masses increase drastically when approaching the neutron-drip line and in some nuclei they reach 15 MeV. This is a consequence of poorly defined isovector properties of many CEDF’s.

The fitting protocols of employed functionals always contain data on finite nuclei and nuclear matter properties (see Sect. II in Ref. [2] for more details). The data on finite nuclei includes binding energies, charge radii and occasionally neutron skin thicknesses. The isovector properties of the functionals are affected by their nuclear matter properties. However, it is not always possible to find one-to-one correspondence between the differences in nuclear matter properties of two functionals and the differences in their description of masses. This can be illustrated by the comparison of binding energy spreads for the pairs of the functionals (Fig. 2) with their nuclear matter properties (Table 1). The smallest difference in the predictions of binding energies exists for the DD-ME2/DD-MEδ pair of the functionals (see Fig. 9 in Ref. [2]); for almost half of the $Z \leq 104$ nuclear landscape their predictions differ by less than 1.5 MeV and only in a few points of nuclear landscape the difference in binding energies of two functionals exceeds 5 MeV. The nuclear matter properties of these two functionals are similar with some minor differences existing only
for the incompressibility $K_\infty$ and Lorentz effective mass $m^*/m$ (Table 1). However, there is an opposite example of the pair of the DD-ME2 and DD-PC1 functionals for which substantial differences in the mass predictions (Fig. 2c) exist for quite similar nuclear matter properties (Table 1). Note that these differences in mass predictions are larger than the ones for the NL3*/DD-PC1 pair of the functionals (Fig. 2a) which are characterized by a substantial difference in the energy per particle ($E/A$), symmetry energy $J$ and its slope $L$ (Table 1).

![Binding energy spread ΔE [MeV]](image)

**FIGURE 1.** The binding energy spreads $\Delta E(Z,N)$ as a function of proton and neutron number. $\Delta E(Z,N) = |E_{\text{max}}(Z,N) - E_{\text{min}}(Z,N)|$, where $E_{\text{max}}(Z,N)$ and $E_{\text{min}}(Z,N)$ are the largest and the smallest binding energies for each $(N,Z)$ nucleus obtained with the NL3*, DD-ME2, DD-MEδ and DD-PC1 functionals. From Ref. [2].

It is clear that the part of the difference in mass predictions is coming from the use of different data on finite nuclei in fitting protocols; the binding energies of these nuclei provide the normalization of the energy for the functional. The most similar fitting protocols exist in the case of the NL3* and DD-ME2 functionals which were fitted to the same 12 spherical nuclei [4, 5]. The comparison of Figs. 1a,b of Ref. [2] with Fig. 2b in the present manuscript clearly illustrates that the difference in binding energies is minimal for these two functionals in the gray band region of Fig. 2b which overlaps with the nuclei used in the fitting protocol. Fig. 2 also illustrate the fact that most rapid increase of the differences in the predicted binding energies takes place not in the direction of isospin but in the direction which is perpendicular to the gray band of similar energies. These differences are due in part to different nuclear matter properties of these two functionals.

**TABLE 1.** Properties of symmetric nuclear matter at saturation for the covariant energy density functionals: the density $\rho_0$, the energy per particle $E/A$, the incompressibility $K_\infty$, the symmetry energy $J$ and its slope $L$, and the Lorentz effective mass $m^*/m$ [6] of a nucleon at the Fermi surface. The quantities which are located beyond the limits of the SET2b constraint set of Ref. [7] are shown in bold. The last column shows the rms deviations $\Delta E_{\text{rms}}$ between calculated and experimental binding energies. For first four functionals, they are defined in Ref. [2] with respect of 640 measured masses presented in the AME2012 compilation [8]. For PC-PK1 they are defined with respect of 575 masses in Ref. [9].

| CEDF         | $\rho_0$ [fm$^{-3}$] | $E/A$ [MeV] | $K_\infty$ [MeV] | $J$ [MeV] | $L$ [MeV] | $m^*/m$ | $\Delta E_{\text{rms}}$ [MeV] |
|--------------|----------------------|--------------|------------------|-----------|-----------|--------|------------------|
| NL3* [4]     | 0.150                | -16.31       | 258              | 38.68     | 122.6     | 0.67   | 2.96             |
| DD-ME2 [5]   | 0.152                | -16.14       | 251              | 32.40     | 49.4      | 0.66   | 2.39             |
| DD-MEδ [10]  | 0.152                | -16.12       | 219              | 32.35     | 52.9      | 0.61   | 2.29             |
| DD-PC1 [11, 12] | 0.152             | -16.06       | 230              | 33.00     | 68.4      | 0.66   | 2.01             |
| PC-PK1 [12]  | 0.154                | -16.12       | 238              | 35.6      | 113       | 0.65   | 2.58             |
The question to which extent nuclear matter constraints are important (and how strictly they have to be imposed) for the definition of the properties of covariant energy density functionals still remains not fully answered. Definitely, the equation of state (EOS) relating pressure, energy density, and temperature at a given particle number density is essential for modeling neutron stars, core-collapse supernovae, mergers of neutron stars and the processes (such as nucleosynthesis) taking place in these environments. However, the properties of finite nuclei are in addition defined by the underlying shell structure which depends sensitively on the single-particle features [13].

Recent analysis of the 263 relativistic functionals with respect of nuclear matter constraints has been performed in Ref. [7]. Note that only around ten of these functionals have been used in a more or less systematic studies of the properties of finite nuclei; the performance of other functionals with respect of the description of finite nuclei (apart of few spherical nuclei used in the fitting protocols) is not known. Three different sets of constraints related to symmetric nuclear matter, pure neutron matter, symmetry energy and its derivatives were employed in the analysis of Ref. [7]. Among these 263 functionals only 4 and 3 satisfy nuclear matter constraint sets called SET2a and SET2b, respectively. However, these functionals have never been used in the studies of finite nuclei. Thus, it is impossible to verify whether
good nuclear matter properties of the functional will translate into good global description of binding energies, charge radii, deformations etc. Removing isospin incompressibility constraint increases the number of functionals which satisfy SET2a and SET2b constraints to 35 and 30, respectively [7]. Again the performance of absolute majority of these functionals in finite nuclei is not known. However, among those are the FSUGold and DD-MEδ covariant energy density functionals the global performance of which has been studied in the RMF+BCS and RHB models in Refs. [14, 2], respectively. FSUGold is characterized by the largest rms deviations from experiment for binding energies (6.5 MeV) among all CEDF’s the global performance of which is known [2]. Although the DD-MEδ functional provides quite reasonable description of the binding energies (Table 1), it generates unrealistically low inner fission barriers in superheavy elements [15].

The analysis of Refs. [2, 16, 17, 15] clearly indicates that the NL3*, DD-ME2, PC-PK1 and DD-PC1 CEDF’s represent better and well-rounded functionals as compared with FSUGold and DD-MEδ. They are able to describe not only ground state properties but also the properties of excited states. This is despite the fact that first three functionals definitely fail to describe some of the nuclear matter properties (see Table 1 and Ref. [7]). It is not clear whether that is also a case for DD-PC1 since it was not analyzed in Ref. [7]. As a result, one can conclude that the functionals, which provide good nuclear matter properties, do not necessary well describe finite nuclei. Such a possibility has already been mentioned in Ref. [7].

CONCLUSIONS

The correlations between global description of masses and nuclear matter properties of the underlying functionals has been discussed based on the results of recent assessment of global performance of covariant energy density functionals presented in Refs. [1, 2, 3]. It was concluded that the strict enforcement of the limits on the nuclear matter properties defined in Ref. [7] will not necessary (i) lead to the functionals with good description of masses and (ii) substantially decrease the uncertainties in the description of masses in neutron-rich systems. This is quite likely related to the mismatch of phenomenological content, existing in all modern functionals, related to nuclear matter physics and the physics of finite nuclei; the later being strongly affected by underlying shell effects.

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