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Quantification of Uncertainties in Nuclear Density Functional Theory

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Reliable predictions of nuclear properties are needed as much to answer fundamental science questions as in applications such as reactor physics or data evaluation. Nuclear density functional theory is currently the only microscopic, global approach to nuclear structure that is applicable throughout the nuclear chart. In the past few years, a lot of effort has been devoted to setting up a general methodology to assess theoretical uncertainties in nuclear DFT calculations. In this paper, we summarize some of the recent progress in this direction. Most of the new material discussed here will be be published in separate articles.

I. INTRODUCTION

The rapid development of leadership class computing facilities throughout the world, accompanied by targeted programs from funding agencies to foster the use of high-performance computing methods in science, have opened new opportunities in theoretical nuclear structure [1]. It has become possible to address important questions of nuclear science using microscopic approaches to structure and reaction rooted in the knowledge of effective nuclear forces and standard methods of quantum mechanics. Recent examples include the explanation of the anomalously long half-life of ^{14}C isotope used in carbon-dating [2], predictions of neutrino-nucleus currents relevant to physics beyond the standard model [3], or of light ion fusion reactions relevant to the National Ignition Facility [4], to name but a few.

In parallel, there has been an increasing need for accurate and precise data, whether from measurements or simulations, in areas as diverse as nuclear astrophysics [5, 6], reactor physics [7] or data evaluation [8]. In the past, the cost of using standard methods of statistics to estimate theoretical uncertainties in such microscopic approaches was often prohibitive, but this limitation has slowly been disappearing.

Among the few microscopic theories of nuclear structure, density functional theory (DFT) plays a special role, since it is the only one to be applicable across the entire nuclear chart, from the lightest to the heaviest elements. Therefore, DFT is the tool of choice to study phenomena such as nuclear fission [9] or superheavy element predictions [10], but has also seen applications in tests of fundamental symmetries [11, 12] or the search for neutrino-less double beta-decay [13].

In this proceeding, we briefly present some of the challenges and methodologies used in nuclear DFT to estimate theoretical uncertainties. This topic is covered in greater details in an invited contribution to a Focus Issue of the Journal of Physics G: Nuclear and Particle Physics on "Enhancing the Interaction Between Nuclear Experiment and Theory Through Information and Statistics" [14–16]. In Sect. II, we recall the main components of nuclear DFT. In Sect. III, we summarize some of the recent results in uncertainty quantification and error propagation, before we conclude in Sect. IV.

II. NUCLEAR DENSITY FUNCTIONAL THEORY

Density functional theory (DFT) is a general approach to the quantum many-body system. It is based on a series of theorems by Kohn and Sham, who have shown that it is theoretically possible to find the exact ground-state energy of a system of N interacting electrons by solving a system of equations characteristic of an independent particle system [17, 18]. This existence theorem was later extended to the context of nuclear physics [19]. Nuclear DFT is a reformulation of the traditional self-consistent mean-field (SCMF) theory of nuclear structure, which has been very successful in predicting a broad range of nuclear properties.

The essential component of both the SCMF theory and nuclear DFT is the energy density functional (EDF), which encapsulates all information about the system (in principle). The EDF is a functional of the density of neutrons and protons, as well as of the pairing density [20].

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In nuclear DFT, the EDF is treated at the Hartree-Fock-Bogoliubov (HFB) approximation [21]; in the SCMF, the EDF is often related to an underlying two-body Hamiltonian, and the HFB approximation may be only the first step of a series of calculations [22]. In any case, the EDF is characterized by a number of coupling constants which are not given by any underlying theory and must therefore be adjusted to some experimental data.

One must emphasize that the Kohn-Sham theorem is only an existence theorem: there is no magic recipe to determine the one EDF that will give the exact energy of the nucleus. In addition, in-medium nuclear forces are poorly known and should in principle be derived from quantum chromodynamics. This is in contrast to electronic DFT, where the Coulomb force is known exactly. For these reasons, one should, therefore, consider nuclear DFT (and the SCMF) as inherently imperfect models of the nucleus: this is the first, major source of errors in DFT, which we will refer to as "model errors". Let us denote by $\boldsymbol{x} = (x_1, \ldots, x_{n_x})$ the parameters of the EDF, aka the model. Typically, $n_x \approx 10 - 20$. These parameters will be fitted on some n_d data points y_i. There could be different types of data: atomic masses, r.m.s. charge radii, mass differences, excitation energies of isomers, etc. It is clear that, given a specific EDF, the choice of the experimental data will impact the overall predictive power of DFT: this is the second source of errors in DFT, which we will label "fitting errors". Finally, there is a third source of errors, "implementation errors", caused by the need to solve the DFT equations numerically. These various sources of uncertainties are discussed in more details in [14]. In this proceeding, we focus only on selected aspects of fitting errors.

III. QUANTIFYING AND PROPAGATING ERRORS IN NUCLEAR DENSITY FUNCTIONAL THEORY

As already mentioned above, we will only discuss uncertainties pertaining to the determination of model parameters. We thus assume we have an energy density functional, which is characterized by the n_x unknown parameters $\boldsymbol{x}$. We are trying to determine the best way to obtain an optimal set of parameters $\boldsymbol{x}$ and, in the same time, to quantify the uncertainties associated with this procedure.

We recall that there is a very large amount of experimental data that potentially could be used to fit the few parameters of an EDF. However, different data types may have very different impacts on specific model parameters. For example, it was pointed out using a singular value decomposition analysis that only a few of the eight parameters of a standard Skyrme EDF are really relevant to reproduce nuclear masses [23] or single-particle energies [24]. In order to constrain every coupling constant of the EDF, it thus appears necessary to introduce different types of data. In practice, the determination of EDF parameters is thus made by minimizing the composite χ^2 function

$$\chi^2(\boldsymbol{x}) = \frac{1}{n_d - n_x} \sum_{t=1}^{n_T} \sum_{j=1}^{n_t} \left(\frac{y_{tj}(\boldsymbol{x}) - d_{tj}}{\sigma_t} \right)^2 , \qquad (1)$$

with n_T the number of different data types, n_t the number of data points for type t, and $n_d = \sum_t n_t$ the total number of data points over all types. The calculated value of data point number j of type t is denoted by y_{tj}, with d_{tj} the corresponding experimental value. Because there are different types of data, relative distances must be properly normalized by the quantity σ_t, which represents an estimate of the theoretical error on data type t. This strategy was followed in a series of paper by the UNEDF collaboration [25–27].

The minimization of the χ^2 function gives access to the "optimal" parametrization of the EDF. Obviously, one should bear in mind that this optimal choice is strongly dependent on (i) the choice of the types t of experimental data, (ii) the number of data points for each type t, (iii) the weight σ_t chosen for each type. In addition, the quality of the optimization is contingent of the algorithm used and depends on the starting point. Bearing in mind these caveats, it is possible to estimate the covariance matrix by assuming normally distributed errors and approximate linear variations of the χ^2 function under variations of model parameters [28]. This approximation has often been used to propagate model errors [29–32].

Very recently, alternative approaches to uncertainty quantification based on Bayesian statistics have been investigated for semi-microscopic nuclear mass models based [33]. In the context of nuclear DFT, such approaches are appealing since they treat model parameters as intrinsically random variables, the true value of which can not be known with certainty. This perspective is particularly adapted to nuclear structure theory, since the nuclear many-problem is unsolvable exactly: only approximations are available (DFT is one of them), and, therefore, uncertainties are unavoidable and should be quantified. Mathematical details on how posterior distributions can be generated in the context of nuclear DFT are discussed in details in [16]; a paper currently being finalized by our group also uses Bayesian posteriors to analyze theoretical uncertainties for the prediction of neutron-drip lines and fission barriers in actinides [34].

We show in Fig. 1 one of the first examples of a Bayesian posterior distribution corresponding to the UNEDF1 χ^2 function of [27]. The red dots correspond to the UNEDF1 solution itself. Obtaining such distributions requires first to set up intervals of variations $[x_i^{\min}, x_i^{\max}]$ for each of the DFT parameters. These intervals define a 12-d hypercube in parameter space from which the prior distribution is sampled. In the case shown in Fig. 1, the interval for each parameter x_i was defined as $[x_i^* - 3\sigma_i, x_i^* + 3\sigma_i]$, with x_i^* the UNEDF1 value and σ_i its standard deviation; see [26]. Since this work is still exploratory, we chose a uniform prior distribution. Because of the significant cost of running the DFT calcula-