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Nuclear Density Functional Theory (DFT): perspectives and *ab initio*-based functionals

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Nuclear Density Functional Theory (DFT) is widely used to predict global properties of nuclei throughout the isotope chart. Despite many successes, it is not obvious how to make further progress and improve the predictive power of this theory. Among the different attempts, in this contribution we discuss our investigation on constructing nuclear Energy Density Functionals (EDFs) based on the *ab initio* nuclear theory.

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1. Introduction

The most widely used approaches in nuclear structure studies are *ab initio* methods [1, 2], the nuclear Shell Model (SM) [3], and Density Functional Theory (DFT) [4, 5]. These have different pros and cons. The *ab initio* approach is characterized by employing realistic nuclear interactions and solving the many-nucleon problem with exact or systematically improvable methods, thus allowing in principle to estimate the uncertainty on the theoretical predictions. In spite of indubitable progress, *ab initio* approaches still fail short of describing several emergent nuclear properties, and the quality of agreement with the experiment is somewhat dependent on the specific Hamiltonian. At the other extreme, the SM is an excellent tool for "precision" nuclear structure (notably, nuclear spectroscopy) but it calls for phenomenological input specific to the mass region under study. Finally, DFT aims at a description of global properties of nuclei throughout the mass table in a unified manner. The concept of the Energy Density Functional (EDF) lies at the heart of DFT.

While in principle a unique, exact EDF exists, in practice several approximations thereof have been developed. The different EDFs that exist on the market are based on some phenomenological ansatz and have been optimized with a focus on different nuclear properties. Their predictive power tends to decrease when going far from well-known, stable nuclei. There are several proposals, or attempts, to remedy this: among them, considering richer functional forms, or employing advanced statistical methods like Bayesian inference [6] or machine learning. In this contribution, we focus in particular on the idea of grounding EDF on *ab initio* calculations.

In the case of electronic systems, which are governed by the well-known Coulomb Hamiltonian, EDF models, the simplest of which is the Local Density Approximation (LDA), can be grounded on rigorous numerical calculations of the electron gas performed e.g. with Quantum Monte Carlo or coupled cluster (CC). In this sense, electronic DFT is considered an *ab initio* approach. There have been only a few attempts to connect nuclear DFT and *ab initio* [7–10]. Our strategy [11, 12] tries to stick to the spirit of the "Jacob's ladder" [13] program of electronic DFT, which aims at constructing a hierarchy of EDFs of increasing complexity and accuracy and favors the use of exact properties and model systems over fitting on empirical data. LDA is the first rung of the ladder, where an EDF that depends on the density alone (without gradients) is derived from the equations of state (EoS) of uniform matter. The second rung, called gradient approximation (GA), introduces the gradients of the density into the EDF. *Ab initio* calculations of uniform matter subject to a weak external perturbation can be used to constrain the GA rung [14]. The purpose of this paper is to report on our attempts to derive *ab initio*-based nuclear EDFs.

2. Methods

2.1 *Ab initio*-based EDFs

The simplest way to build an EDF is the LDA scheme. In it, one assumes that the same expression of the potential energy density valid in infinite matter also holds for non-uniform densities $\rho_q(\mathbf{x})$, where q distinguishes neutrons and protons. The only input for LDA is the Equation of State (EoS) of homogeneous matter, and thus information on infinite matter is directly mapped to finite systems.

Following Refs. [11, 12], we write the energy per particle $e(\rho_0, \beta)$, where $\rho_0 = \rho_n + \rho_p$ is the total density and $\beta = (\rho_n - \rho_n)/\rho_0$ is the local isospin asymmetry, as the sum of the kinetic energy per particle of the Fermi gas $t(\rho_0, \beta)$ and of a potential term $v(\rho_0, \beta)$: $e(\rho_0, \beta) = t(\rho_0, \beta) + v(\rho_0, \beta)$. We assume a quadratic dependence on β and that the EoS can be represented by a power series in the Fermi momentum $q_F \sim \rho_0^{1/3}$. Accordingly,

$$v(\rho_0, \beta) = \sum_{\gamma=1/3\ldots6/3} c_\gamma(\beta)\rho_0^\gamma = \sum_{\gamma=1/3\ldots6/3} \left[c_{\gamma,0} + c_{\gamma,1}\beta^2\right] \rho_0^\gamma, \tag{1}$$

where $c_{\gamma,0} \equiv c_\gamma(\beta = 0)$ and $c_{\gamma,1} \equiv c_\gamma(\beta = 1) - c_\gamma(\beta = 0)$. To determine how many terms and which powers should enter the potential, we perform a model selection procedure [11]. Then, the LDA EDF reads $E_{LDA} = E_{kin} + E_{bulk} + E_{Coul}$, with the bulk energy given by

$$E_{bulk}\left[\rho_0(\mathbf{x}), \beta(\mathbf{x})\right] = \int d\mathbf{x}\, \rho_0(\mathbf{x}) v\left[\rho_0(\mathbf{x}), \beta(\mathbf{x})\right]. \tag{2}$$

It is known that the inclusion of density gradients as well as spin-orbit contributions are essential for a realistic description of nuclei. Empirical EDFs directly use experimental data of stable nuclei to constrain these terms. Our alternative path [12] consists in using perturbed nuclear matter results from *ab initio* calculations to fix the GA EDFs, which have the form $E_{GA} = E_{LDA} + E_{surf}$, where

$$E_{surf} = \int d\mathbf{x} \left[\sum_{t=0,1} \left(C_t^{\Delta\rho} \rho_t \Delta\rho_t + C_t^{\nabla J} \rho_t \nabla \cdot \mathbf{J}_t\right)\right]. \tag{3}$$

Here, $\rho_1 = \rho_n - \rho_p$ and similarly for the spin-orbit density $\mathbf{J}_0$, $\mathbf{J}_1$. The parameters $C_t^{\Delta\rho}$, $C_t^{\nabla J}$ are assumed to be density-independent constants.

2.2 *Ab initio* methods

We have focused on two *ab initio* methods (see [11, 12] and references therein): Auxiliary field diffusion Monte Carlo (AFDMC) and Self-Consistent Green's functions (SCGF). In AFDMC [15], the exact many-body ground state (g.s.) is determined by evolving an initial state in imaginary time. A crucial speed-up is achieved by using Monte Carlo stochastic techniques to sample both the spatial coordinates and the spin-isospin amplitudes of the nucleons. Infinite nuclear matter is simulated by using a finite number of particles confined in a finite box and subject to periodic boundary conditions (PBCs) [12, 16]. AFDMC is well-suited for studying both the EoS and the static response, as it provides a natural way of treating the effect of external density perturbations. On the other hand, some types of realistic interactions are difficult to employ in AFDMC. Also, additional complexity and systematic uncertainties are induced by the need to control the Fermion sign problem inherent to diffusion methods.

SCGF methods [17] are rooted in the solution of the Dyson equations for the propagator, from which it is possible to evaluate the g.s. energy and one-body properties. The algebraic diagrammatic construction (ADC) [17] is a state-of-the-art approximation to the self-energy entering the Dyson equations, and has been successfully applied to nuclear matter in Refs. [18, 19] in conjunction with chiral interactions. In particular, ADC at third order incorporating CC amplitudes, dubbed ADC(3)-D, is used to determine the EoS in Sec. 3.1.

2.3 Static response theory

In response theory, the goal is to determine how a many-particle system reacts when an external perturbing potential is applied [12, 16, 20]. We consider a homogeneous system with density ρ_0 and a sinusoidal (monochromatic) potential coupled to the total density, $v(\mathbf{x}) = 2v_q \cos(qz)$, where q is the momentum carried by the external potential, taken along the $\hat{\mathbf{z}}$ direction, and v_q is the strength of the perturbation. The energy of the perturbed system is expected to be quadratic in the external potential when the perturbation is small,

$$\delta e_v = e_v - e_0 = \frac{\chi(q)}{\rho_0} v_q^2. \tag{4}$$

e_v denotes the energy per particle with momentum q and strength v_q, and the static response function $\chi(q)$ has been introduced. PBCs force q to be an integer multiple of $q_{min} = \frac{2\pi}{L}$, with $L = (A/\rho_0)^{1/3}$ being the box size [16].

3. Results

3.1 Local density approximation

In Fig. 1 (left), the EoS for the ΔNNLO$_{\rm go}$(394) interaction [21] has been determined using ADC-SCGF, and results have been interpolated with Eq. (1) using powers 1/3, 4/3, 5/3, 6/3, or (1,4,5,6) for short. In the right panel, the difference between the predictions of the LDA EDF and experiment, for binding energies per nucleon (top) and charge radii (bottom), is shown in the case of selected closed-shell nuclei. "GA" refers to GA EDFs whose coefficients have been tuned to improve the agreement with these experimental data. LDA overbinds nuclei and produces too small radii, while GA corrects these deficiencies to a certain extent, However, these EDFs perform worse than those based on the NNLO$_{\rm sat}$ potential [22] (see [11]), which was fit also on medium-mass nuclei, in contrast to ΔNNLO$_{\rm go}$(394).

In Fig. 2, the EoS has been computed with AFDMC and the AV4′+UIX$_c$ force. In SNM, calculations have been performed with either $A = 76$ or $A = 132$. The agreement of LDA with the experiment is in this case worse, probably in connection to the SNM EoS saturating at large density and low binding energy [11].

3.2 *Ab initio* static response and gradient-approximation EDFs

We now present AFDMC calculations of perturbed nuclear matter, and discuss their use as pseudo-data to tune the gradient terms of the GA EDFs (built on top of the LDA of Sec. 3.1). SNM and PNM are studied separately as they are sensitive to $C_0^{\Delta\rho}$ and $C_0^{\nabla J}$, and to $C_{PNM}^{\Delta\rho} = C_0^{\Delta\rho} + C_1^{\Delta\rho}$ and $C_{PNM}^{\nabla J} = C_0^{\nabla J} + C_1^{\nabla J}$, respectively. The shorthand notation $C^{\Delta\rho}$, $C^{\nabla J}$ will be used in the following, and we require $C^{\Delta\rho} < 0$, as the density-gradient terms should provide a repulsive contribution. The AV4′+UIX$_c$ potential is used throughout this section. For each combination of q and v_q a full AFDMC computation has been performed. To mitigate the sign problem, we have used the constrained propagation technique, which is deemed accurate for this interaction [12]. The trial wave function is a Slater determinant of Mathieu orbitals, on top of which central correlations, as well as linear correlations for the operators $\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}$, $\boldsymbol{\tau}\cdot\boldsymbol{\tau}$ and $(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma})(\boldsymbol{\tau}\cdot\boldsymbol{\tau})$, are included.

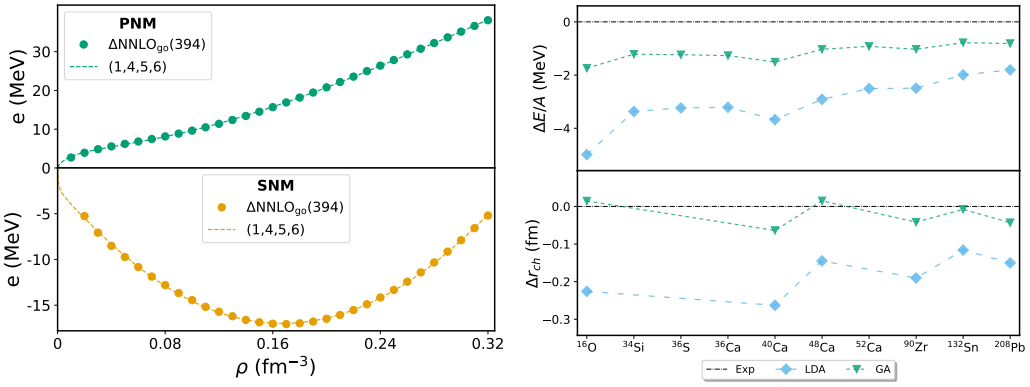

Figure 1: Left: EoS in PNM with $N = 66$ neutrons (top) and SNM (bottom) with $A = 132$ nucleons (circles). Calculations have been performed using the ΔNNLO$_{\rm go}$(394) interaction and the ADC(3)-D method. Dashed lines denote fits (see the main text). Right: difference between the predicted energies per nucleon (top) and charge radii (bottom) with experimental values.

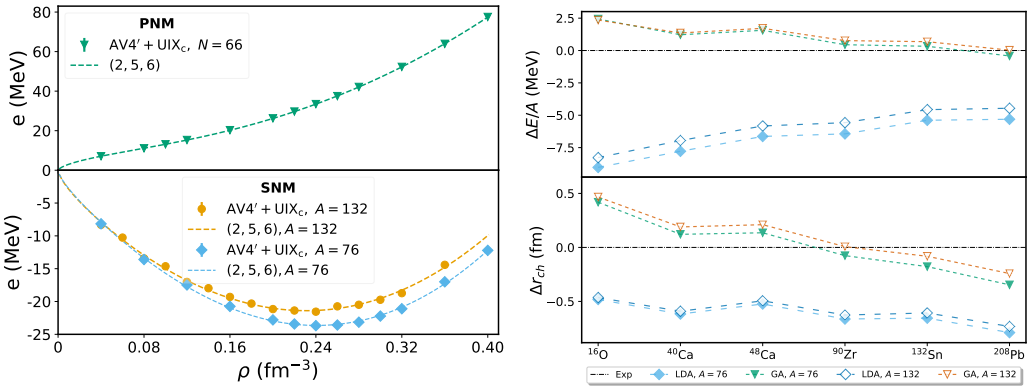

Figure 2: Same as Fig. 1, but using the LDA and GA EDFs based on the AV4′+UIX$_c$ EoS. Predictions based on employing $A = 76$ or $A = 132$ for SNM are compared.

To determine the optimal parameters of the GA EDF, we minimize a least-squares cost function that accounts for the difference between the DFT calculations of inhomogeneous matter [16] and the AFDMC results. We aim at reproducing relative energies rather than absolute energies and define the cost function as

$$\chi^2(\mathbf{C}) = \sum_i \left(\frac{\delta e(x_i, \mathbf{C}) - \delta e_i}{\sigma_i} \right)^2 . \tag{5}$$

Here, δe_i denotes the difference between perturbed energies and the unperturbed energy in the *ab initio* data; $x_i = (N_i, Z_i, \rho_{0,i}, q_i, v_{q,i})$, where N_i, Z_i are the neutron and proton numbers, $\rho_{0,i}$ the unperturbed densities, and $q_i, v_{q,i}$ the momenta and strengths of the external potential, respectively; $\mathbf{C} = \left(C^{\Delta\rho}, C^{\nabla J}\right)$; and $\delta e(x_i, \mathbf{C})$ refers to the prediction of the EDF with parameters $\mathbf{C}$. A uniform error $\sigma_i = 100$ keV is chosen to account for AFDMC systematic uncertainties. $\chi^2(\mathbf{C})$ is optimized using the Migrad algorithm of Minuit [23].

AFDMC energies (solid markers) and the predictions of the best GA EDF (empty markers) are reported for $\rho_0 = 0.16\,\text{fm}^{-3}$ in the left panel of Fig. 3. Fits to the energies are performed with Eq. (4)

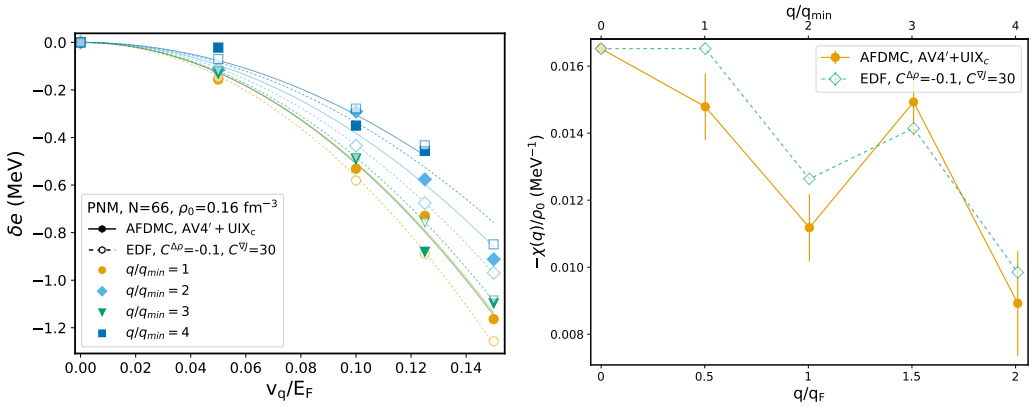

Figure 3: Left: AFDMC energies (solid markers) and predictions by the best-fit GA EDF (empty markers) in PNM at $\rho_0 = 0.16$ fm^{-3} as a function of v_q/E_F for different values of the momentum q/q_{min}. Solid (dashed) lines: fits of the AFDMC (EDF) perturbed energies using Eq. (4). Right: static response $-\chi(q)/\rho_0$ extracted from the AFDMC (solid symbols) and EDF (empty) calculations as a function of q [in units of q_F (bottom) and q_{min} (top)]. For $q/q_{min} \geq 1$, the response has been obtained with Eq. (4). The response at $q = 0$ has been obtained from the EoS using the compressibility sum rule (see [16], App. E). Lines are a guide to the eye.

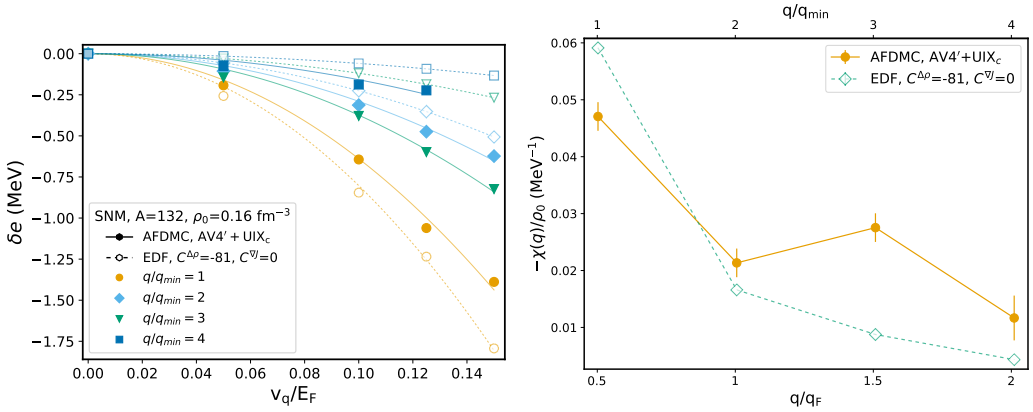

Figure 4: Same as Fig. 3, but for the AV4′+UIX$_c$ interaction in SNM at density $\rho_0 = 0.16$ fm^{-3}.

and shown as solid (dashed) lines for ADFMC (EDF). The values of $-\chi(q)/\rho_0$ that are obtained from the fits are plotted in the right panel, together with the associated uncertainties (that are negligible in the EDF case). The results are unexpected, and the EDFs we obtain have unrealistic values of the coefficients. At $\rho_0 = 0.16$ fm^{-3}, we find for the best-fit model $C^{\Delta\rho} = -0.1 \pm 3$, $C^{\nabla J} = 30 \pm 40$ (in MeV fm^5). The spin-orbit coefficient is poorly constrained. The fact that $C^{\Delta\rho}$ is compatible with zero at $\rho_0 = 0.16$ fm^{-3} contradicts the empirical knowledge from existing EDFs; also, as we have seen, LDA overbinds nuclei, and thus repulsive gradient terms are called for.

In Fig. 4, SNM results at $\rho_0 = 0.16$ fm^{-3} (with $A = 132$) are shown. To our knowledge, these are the first *ab initio* calculations of the static response in SNM. The relative simplicity of the AV4′ interaction is instrumental in this respect. Unfortunately, the agreement of the GA EDF with AFDMC is unsatisfactory. Thus, we have found similar difficulties in both PNM and SNM.

4. Conclusions

In this work, we have reported our attempts to build an *ab initio*-based nuclear EDF, inspired by the "Jacob's ladder" approach of electronic DFT. First, we have constructed LDA EDFs starting from the EoS of homogeneous nuclear matter. Two *ab initio* approaches and two Hamiltonians have been employed. The LDA results are better in the case of the EDF derived from the ΔNNLO$_{\rm go}$(394) results, compared to the case of AV4′+UIX$_c$, probably because of the more realistic saturation properties. It is interesting to note that the *ab initio* EoS calls for a richer density dependence compared to e.g. the volume part of a standard Skyrme EDF [5].

Then, we have presented our first attempts to constrain a GA-EDF using the static response of nuclear matter. Unfortunately, these have led to unsatisfactory results. We have noticed that finite-size effects, stemming from simulating infinite matter with a finite number of particles, are small on the EoS, but impact much more strongly on the response. Also, while our external field is only coupled to the density, we still need to investigate if the spin density is also impacted. Finally, studying perturbed matter may require further methodological developments (e.g. more refined AFDMC wave functions or diffusion algorithms), or may call for a more elaborated EDF to map the *ab initio* results onto.

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