

What is *ab initio*?

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Abstract. Microscopic nuclear theory is based on the tenet that atomic nuclei can be accurately described as collections of point-like nucleons interacting via two- and many-body forces obeying nonrelativistic quantum mechanics – and the concept of the *ab initio* approach is to calculate nuclei accordingly. The forces are fixed in free-space scattering and must be accurate. We will critically review the history of this approach from the early beginnings until today. An analysis of current *ab initio* calculations reveals that some mistakes of history are being repeated today. The ultimate goal of nuclear theory are high-precision *ab initio* calculations which, as it turns out, may be possible only at the fifth order of the chiral expansion. Thus, for its fulfillment, nuclear theory is still facing an enormous task.

1 Introduction

The tenet of microscopic nuclear theory is that atomic nuclei can be accurately described as collections of point-like nucleons interacting via two- and many-body forces obeying nonrelativistic quantum mechanics – the forces being fixed in free-space scattering.

The microscopic or *ab initio* approach to nuclear structure and reactions is then defined as calculating the properties of nuclei in accordance with the tenet.

It is the purpose of this note to discuss how consistent or inconsistent the fundamental model of nuclear theory has been pursued through the history of nuclear physics and to provide an outlook for the future.

2 Early History of the Microscopic Approach

The microscopic approach to nuclear structure is almost as old as nuclear physics itself. Brueckner and co-workers introduced Brueckner theory as early as 1954 [1] and performed the first semi-realistic microscopic nuclear matter calculation in 1958 [2]. Already that same year, Brueckner discussed finite nuclei proposing the local density approximation [3].

In the second half of the 1960's, one of the hottest topics in nuclear structure physics was calculating the properties of finite nuclei without recourse through nuclear matter using Brueckner-Hartree-Fock (BHF) theory. The Oak Ridge National Laboratory (ORNL) with its computer power played a leading role in this effort that was guided by Thomas Davies and Michel Baranger [4, 5]. BHF

(and coupled cluster) calculations of finite nuclei continued into the early 1970s with work by the Bochum [6] and the Bonn-Jülich groups [7].

In parallel to the above developments, research on the microscopic derivation of the shell-model effective interaction was conducted (again, applying Brueckner theory) that had been kicked off by Kuo and Brown in 1966 [8].

Applying the nucleon-nucleon (NN) potentials available at the time, the BHF approach reproduced about one half of the binding energies of closed-shell nuclei which, in the early phase, was seen as a great success [4], but in the long run did not satisfy demands for more quantitative predictions. Therefore, a departure from the microscopic approach happened around 1973 as reflected most notably in a lead-talk by Michel Baranger at the International Conference on Nuclear Physics in Munich in 1973 [9].

The shell-model effective interaction suffered a similar fate at the International Conference on Effective Interactions and Operators in Nuclei in Tucson, Arizona, in 1975, organized by Bruce Barrett [10].

And so it happened that in the early 1970s, the microscopic approach was abandoned and replaced by phenomenological effective interactions (also known as mean-field models): the Skyrme interaction [11] as revived by Vautherin and co-workers [12, 13], the Gogny force [14, 15], and the relativistic mean-field model of Walecka [16, 17].

Ironically, the calculations with those effective interactions continued to be called “microscopic”, for which John Negele had provided the (debatable) justification in his Ph.D. thesis of 1970 [18]. Before calculating finite nuclei in the local density approximation, Negele had adjusted the insufficient binding of nuclear matter provided by the Reid soft-core potential [19] (11 MeV per nucleon) by hand to the presumed empirical value of 15.68 MeV making “the assumption that when higher-order corrections have been evaluated carefully, nuclear-matter theory will indeed produce the correct binding” [18]. Negele had many followers [20–22].

However, the true “deeper reason” for those effective interactions was much simpler: “To get better results!” [23]. Clearly, the trends that won popularity in the early 1970s were a setback for the fundamental research in nuclear structure.

Nuclear structure theory at its basic level is not about fitting data to get “good” results. Fundamental nuclear structure theory is about answering the question:

Do the same nuclear forces that explain free-space scattering experiments also explain the properties of finite nuclei and nuclear matter when applied in nuclear many-body theory?

One can think of many reasons why the basic tenet should be wrong. According to the EMC effect, nucleons swell when inserted into nuclei which might affect the force between nucleons [24]. Meson exchange in the nuclear medium may be different than in free-space for various reasons [25–27]. The excitation of resonances, e. g. $\Delta(1232)$ isobars, within the nucleon-nucleon interaction

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process is subject to changes when happening in a nuclear medium [28–31]. And many more ideas have been advanced, like e. g., Brown-Rho scaling [32]. In fact, in the 1970s, a popular believe was that medium effects on the NN interaction may be the solution to the problem of lacking saturation [33].

Thus, it is a good question to ask whether medium modifications of nuclear forces show up in a noticeable way and/or are even needed for quantitative nuclear structure predictions. But when we re-adjust the free-space forces arbitrarily to get “good” results, then we will never find out. Note also that at some (high) energy and high density, the picture of point-like nucleons is bound to break down [34]. So, the issue behind the nuclear theory tenet is: Are the energies typically involved in conventional nuclear structure physics low enough to treat nucleons as structure-less objects?

To come back to history: the renunciation of the truly microscopic approach lasted about two decades (essentially the 1970s and 80s). Then, in the early 1990s, the microscopic theory was revived by the Argonne-Urbana group [35, 36]. The crucial element in those new microscopic calculations was the inclusion of a three-nucleon force (3NF). The idea of a nuclear 3NF was not new. In fact, it is almost as old as meson theory itself [37]. But for years it had been considered just an academic topic, too difficult to incorporate into actual calculations, anyhow. But the persistent failure to saturate nuclear matter at reasonable energies and densities, as well as the underbinding of nuclei, finally compelled nuclear structure physicists to take a serious look at the 3NF issue, as explained in the exemplary Comment by Ben Day [38] based upon first test calculations by the Urbana group [39]. The 3NF definitely improved nuclear saturation and the properties of light nuclei, even though nothing was perfect [36].

3 Recent History

After the year of 2000, two changes occurred. First, the term ‘microscopic’ was increasingly replaced by the term ‘*ab initio*’ [40] – for reasons nobody knows (but nothing to worry about because both mean the same). Second and more importantly, nuclear forces based upon chiral effective field theory (EFT) entered the picture [41, 42]. This development was of great advantage. Note that for a microscopic approach to be truly microscopic, the free-space forces need to be accurate. But with phenomenological or meson-theoretic forces it was difficult to define what sufficiently accurate means, since the errors in those theories are unknown. However, in the framework of an EFT, the theoretical uncertainty can be determined and, thus, related with the accuracy of the predictions. Hence, in the framework of an EFT:

Accurate free-space forces are forces that predict experiment within the theoretical uncertainty of the EFT at the given order.

After 2000, it also became well established that predictive nuclear structure must include 3NFs, besides the usual two-nucleon force (2NF) contribution. An-

other advantage of chiral EFT is then that it generates 2NFs and multi-nucleon forces simultaneously and on an equal footing. In the Δ -less theory [43, 44], 3NFs occur for the first time at next-to-next-to-leading order (NNLO) and continue to have additional contributions in higher orders. If an explicit Δ -isobar is included in chiral EFT (Δ -full theory [45–48]), then 3NF contributions start already at next-to-leading order (NLO).

In the initial phase, the 3NFs were typically adjusted in $A = 3$ and/or the $A = 4$ systems and the *ab initio* calculations were driven up to the oxygen region [49]. It turned out that for $A \lesssim 16$ the ground-state energies and radii are predicted about right, no matter what type of chiral or phenomenological potentials were applied (local, nonlocal, soft, hard, etc.) and what the details of the 3NF adjustments to few-body systems were [49–54].

However, around the year of 2015, the picture changed, when the many-body practitioners were able to move up to medium-mass nuclei (e. g., the calcium or even the tin regions). Large variations of the predictions now occurred depending on what forces were used, and cases of severe underbinding [55] as well as of substantial overbinding [56] were observed. Ever since, the nuclear structure community understands that accurate *ab initio* explanations of intermediate and heavy nuclei is an outstanding problem.

There have been several attempts to predict the properties of medium-mass nuclei with more accuracy. Of the various efforts, we will now list four cases, which are representative for the status, and will denote each case with a short label for ease of communication. We restrict ourselves to cases, where the properties of medium-mass nuclei *and* nuclear matter have been calculated, because the simultaneous description of both systems is part of the problem.¹

- **“Magic”** [60, 61]: A seemingly successful interaction for the intermediate mass region commonly denoted by “1.8/2.0(EM)” (sometimes dubbed “the Magic force”). It is a similarity renormalization group (SRG) evolved version of the N^3LO 2NF of Ref. [42] complemented by a NNLO 3NF adjusted to the triton binding energy and the point charge radius of ^4He . With this force, the ground-state energies all the way up to the tin isotopes are reproduced perfectly – but with charge radii being on the smaller side [62, 63]. Nuclear matter saturation is also reproduced reasonably well, but at a slightly too high saturation density [60].
- **“GO”** [64, 65]: A family of Δ -full NNLO potentials constructed by the Göteborg/Oak Ridge (GO) group. The authors claim to obtain “accurate binding energies and radii for a range of nuclei from $A = 16$ to $A = 132$, and provide accurate equations of state for nuclear matter” [65].
- **“Hoppe”** [58, 66]: Recently developed soft chiral 2NFs [67] at NNLO and N^3LO complemented with 3NFs at NNLO and N^3LO , respectively, to fit

¹Other interesting cases are the models by Soma *et al.* [57] and Maris *et al.* [54] for which, however, presently no nuclear matter results are available.

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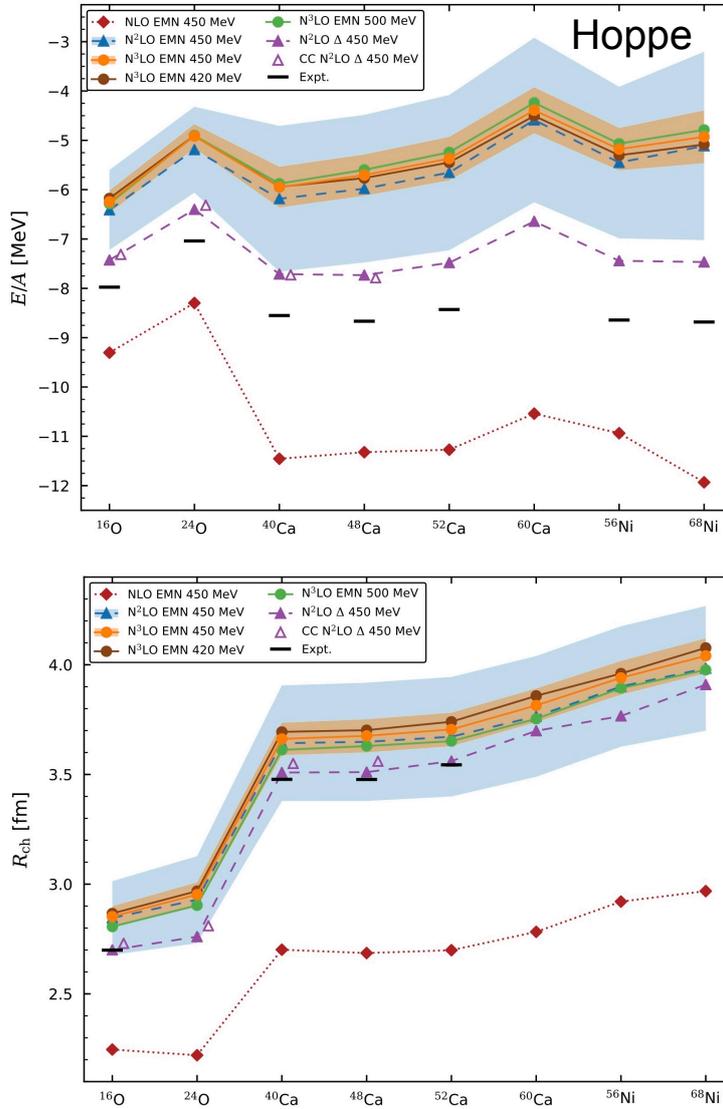


Figure 1. Upper panel: Ground-state energies per nucleon, E/A , of selected closed-shell oxygen, calcium, and nickel isotopes as obtained in the “Hoppe” case [58]. Results are shown for various chiral interactions as denoted. The blue and orange bands give the NNLO and N^3LO uncertainty estimates, respectively. $\Lambda = 450$ MeV in all cases except the green curve. Black bars indicate experimental data. Lower panel: Same as upper panel, but for charge radii. (Reproduced from Ref. [58] with permission.)

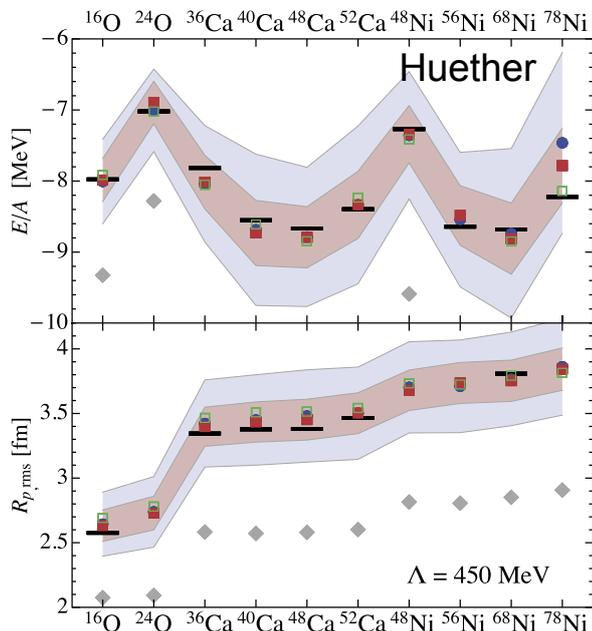


Figure 2. Ground-state energies per nucleon (top panel) and point-proton rms radii (bottom panel) for selected medium-mass isotopes as obtained in the “Hüther” case [59]. The light blue and pink bands represent the theoretical uncertainties at NNLO and $N^3\text{LO}$, respectively. $\Lambda = 450$ MeV. Black bars indicate the experimental data. (Figure courtesy of R. Roth)

the triton binding energy and nuclear matter saturation. These forces applied in in-medium similarity renormalization group (IM-SRG [68]) calculations of finite nuclei up to ^{68}Ni predict underbinding and slightly too large radii [58], see Figure 1.

- **“Hüther”** [59]: The same 2NFs used in “Hoppe”, but with the 3NFs adjusted to the triton and ^{16}O ground-state energies. The interactions so obtained reproduce accurately experimental energies and point-proton radii of nuclei up to ^{78}Ni [59], see Figure 2. However, when the 2NF plus 3NF combinations of “Hüther” are utilized in nuclear matter, then overbinding and no saturation at realistic densities is obtained [69], see Figure 3.

Obviously, in some cases, there appears to be a problem with achieving simultaneously accurate results for nuclear matter and medium-mass nuclei: In the “Hoppe” case, nuclear matter is saturated correctly, but nuclei are underbound; while in the “Hüther” case, nuclei are bound accurately, but nuclear matter is

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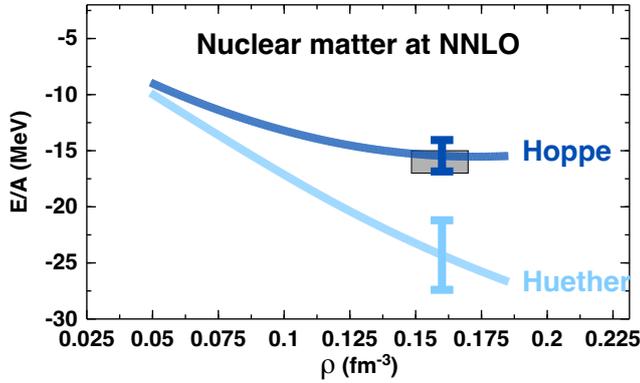


Figure 3. Energy per nucleon, E/A , as a function of density, ρ , of symmetric nuclear matter as obtained in calculations with the 2NFs and 3NFs consistently at NNLO [69]. In the two cases shown, the 2NF is the same, while the 3NFs are the ones used in the calculations of finite nuclei in the “Hoppe” and “Huether” cases as denoted. $\Lambda = 450$ MeV in both cases. The error bars show the theoretical uncertainties around saturation, which is expected to occur in the area of the gray box.

overbound. Other cases seem to have solved this problem. But are they all truly *ab initio*? Our assessment:

- **“Magic”**: The construction of this force includes some inconsistencies. The 2NF is SRG evolved, while the 3NF is not. Moreover, the SRG evolved 2NF is used like an original force with the induced 3NFs omitted. Note that *ab initio* also implies that the forces are based upon some sort of theory in a consistent way. This is here not true and, thus, this case is not *ab initio*.
- **“GO”**: In Ref. [70] it has been shown that the predictions by the Δ -full NN potentials at NNLO constructed by the Göteborg-Oak Ridge (GO) group [65] are up to 40 times outside the theoretical error of chiral EFT at NNLO. So, they fail on accuracy. The reason for their favorable reproduction of the energies (and radii) of intermediate-mass nuclei, can be traced to incorrect P -wave and ϵ_1 mixing parameters [70]. Thus, this case is especially far from being *ab initio*. It is just a repetition of the mistakes of the early 1970s.
- **“Hoppe”**: In this case, the 2NF and 3NF forces are consistently chiral EFT based. Moreover, the 2NFs are accurate. Hence, “Hoppe” passes on all accounts and is, therefore, truly *ab initio*.
- **“Hüther”**: An assessment similar to “Hoppe” applies. Thus, this case is also truly *ab initio*.

The bottom line is that not all calculations, which have been published in the literature under the label of *ab initio*, are really *ab initio*. Indeed, of the cases we considered here, only 50% pass the test. But we need to point out that even in the two cases we declared *ab initio*, there are concerns. The NNLO predictions by Hoppe and H  ther for finite nuclei barely overlap within their theoretical uncertainties and, for nuclear matter, they do not overlap at all. Obviously, there are problems with the error estimates and the uncertainties are much larger than the shown ones. The true NNLO truncation errors of the Hoppe and H  ther calculations are probably as large as the differences between the two predictions. In this way, the two predictions are actually consistent with each other, in spite of their seeming discrepancy. Chiral EFT is a model-independent theory and, thus, different calculations at the same order should agree within truncation errors.

4 Summary and outlook

To summarize, let me just reiterate the main statements.

The tenet of microscopic nuclear theory is:

Atomic nuclei can be accurately described as collections of point-like nucleons interacting via two- and many-body forces obeying nonrelativistic quantum mechanics – the forces being fixed in free-space scattering.

And in the *ab initio* approach, nuclei are calculated accordingly.

We need to critically investigate if the tenet is true. To that end, we have to answer the question:

Do the same nuclear forces that explain free-space scattering experiments also explain the properties of finite nuclei and nuclear matter when applied in nuclear many-body theory?

Either way, the answer is of fundamental relevance. The correct answer can only be obtained if the free-space forces are accurate, where accurate is defined by:

Accurate free-space forces are forces that predict experiment within the theoretical uncertainty of the applied EFT at the given order.

Moreover, one would also require that the applied nuclear forces are based upon some sort of theory in a consistent way.

Without strictly adhering to these principles, the true answer to the fundamental question will not be found. Once again, the goal is not to obtain “good” results, but to understand whether there are non-negligible medium effects on nuclear forces when inserted into the nuclear many-body problem.

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In our community, the term *ab initio* is often used in a way that is too loose and many calculations that are presented as *ab initio* do not pass muster. Such calculations repeat the mistakes of history and, thus, do not move us forward.

The ultimate goal of nuclear theory should be to conduct calculations that test the tenet with high precision. There is strong evidence that this precision can only be achieved at N⁴LO of the chiral EFT expansion. Calculations of this kind, which must also include all many-body forces at that order, are very challenging, and the current status of *ab initio* calculations is far from meeting that goal.

The work that is left to do in microscopic nuclear theory is monumental.

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