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AB INITIO NUCLEAR THEORY — PROGRESS AND PROSPECTS FROM QUARKS TO THE COSMOS*

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The vision of solving the nuclear many-body problem with fundamental interactions tied to QCD appears to approach reality. The goals are to preserve the predictive power of the underlying theory, to test fundamental symmetries with the nucleus as laboratory and to develop new understandings of the full range of complex nuclear phenomena. Recent progress includes the derivation, within chiral perturbation theory (ChPT), of the leading terms of the nucleon–nucleon (NN), three-nucleon (3N) and four-nucleon (4N) potentials. Additional substantial progress includes solving nuclear structure and reactions in nuclei up to mass 16 and selected heavier nuclei around closed shells using these ChPT interactions. Advances in theoretical frameworks (renormalization and many-body methods) as well as in computational resources (new algorithms and leadership-class parallel computers) signal a new generation of theory simulations that will yield valuable insights into origins of nuclear shell structure, collective phenomena and complex reaction dynamics. I outline some recent achievements and present ambitious consensus plans for a coming decade of research that will strengthen the links between nuclear theory and nuclear experiment, between nuclear physics and astrophysics, and between nuclear physics and nuclear energy applications.

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1. Introduction

The physics drivers for our field include many fundamental questions such as:

1. What controls nuclear saturation?
2. How the nuclear shell model emerges from the underlying theory?

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3. What are the properties of nuclei with extreme neutron/proton ratios?
4. Can we predict useful cross-sections that cannot be measured?
5. Can nuclei provide precision tests of the fundamental laws of nature?
6. Under what conditions do we need QCD to describe nuclear structure?

A long-standing goal of nuclear theory is to predict nuclear structure and nuclear reactions from knowledge of the underlying strong interactions. In the past, we pursued this goal with meson-theoretical nucleon–nucleon (NN) interactions that were tuned to provide high-quality descriptions of the NN scattering phase shifts and the deuteron bound state properties. We also employed three-nucleon interactions (TNI) that were derived from meson theory and then tuned to the properties of $A = 3$ nuclei. The Argonne V18 [1] plus Urbana IX [2] interactions represent popular NN and TNI forms, respectively, of this genre and we continue to use these interactions.

More recently, a concerted effort has led to development of realistic NN and TNI rooted in QCD. Chiral perturbation theory (ChPT) within effective field theory (EFT) [3] provides us with a promising bridge between QCD and the hadronic systems [4]. In this approach one works consistently with systems of increasing nucleon number [5, 6, 7] and makes use of the explicit and spontaneous breaking of chiral symmetry to systematically expand the strong interaction in terms of a dimensionless constant, the ratio of a generic small momentum divided by the chiral symmetry breaking scale taken to be about 1 GeV/c. The resulting NN and TNI interactions [8, 9] provide a high-quality fit to the NN data and the $A = 3$ ground state properties.

To solve for the properties of finite nuclei with these ChPT-derived Hamiltonians, one faces immense theoretical and computational challenges. Recently, *ab initio* approaches have been developed that preserve all the underlying symmetries and they converge to the exact result. If we limit our discussions to nuclei heavier than $A = 6$, there are two main approaches that have proven successful. The first approach, called No Core Shell Model (NCSM) [10] or No Core Full Configuration (NCFC) [11], diagonalizes the Hamiltonian in a suitable basis. The second approach, called Coupled Cluster (CC) [12] solves coupled equations that emerge from a representation of the nuclear eigenstate as a correlation operator acting on a representative Slater determinant. The primary advantages of these *ab initio* no core methods are their flexibility for choosing (1) the Hamiltonian; (2) the method of renormalization/regularization; and (3) the single-particle basis. These advantages also support the adoption of these same techniques in light-front quantum field theory [13]. We now briefly outline the first of these approaches.

2. Ab initio no core shell model (NCSM) and full configuration (NCFC) approaches

Refs. [10, 14, 15, 16] and [11, 17, 18] provide examples of the recent advances in the *ab initio* NCSM and NCFC, respectively. The NCSM adopts a renormalization method that provides an effective interaction dependent on the chosen many-body basis space cutoff (N_{max} below). The NCFC either retains the un-renormalized interaction or adopts a basis-space independent renormalization so that the exact results are obtained either by using a sufficiently large basis space or by extrapolation to the infinite matrix limit. Recent results for the NCSM employ realistic NN and TNI derived from ChPT to solve nuclei with atomic numbers 10–13 [14]. Recent results for the NCFC feature a realistic NN interaction that is sufficiently soft that binding energies and spectra from a sequence of finite matrix solutions may be extrapolated to the infinite matrix limit [18]. Experimental binding energies, spectra, magnetic moments and Gamow–Teller transition rates are well-reproduced in both the NCSM and NCFC approaches. Convergence of long range observables such as the rms charge radius and the electric quadrupole moment are more challenging.

It is important to note two recent analytical and technical advances. First, non-perturbative renormalization has been developed to accompany these basis-space methods and their success is impressive. Several schemes have emerged and current research focuses on understanding the scheme-dependence of convergence rates (different observables converge at different rates) [17]. Second, large scale calculations are performed on leadership-class parallel computers to solve for the low-lying eigenstates and eigenvectors and to evaluate a suite of experimental observables. Low-lying solutions for matrices of basis-space dimension 10-billion on 215,000 cores with a 5-hour run is the current record. However, one expects these limits to continue growing as the techniques are evolving rapidly [16] and the computers are growing dramatically. Matrices with dimensions in the several tens of billions will soon be solvable with strong interaction Hamiltonians.

In a NCSM or NCFC application, one adopts a 3-D harmonic oscillator for all the particles in the nucleus (with harmonic oscillator energy $\hbar\Omega$), treats the neutrons and protons independently, and generates a many-fermion basis space that includes the lowest oscillator configurations as well as all those generated by allowing up to N_{max} oscillator quanta of excitations. The single-particle states specify the orbital angular momentum projection and the basis is referred to as the m-scheme basis. For the NCSM one also selects a renormalization scheme linked to the basis truncation while in the NCFC the renormalization is either absent or of a type that retains an infinite matrix problem. In the NCFC case [11], one extrapolates to the continuum limit (infinite matrix result) as I now illustrate.

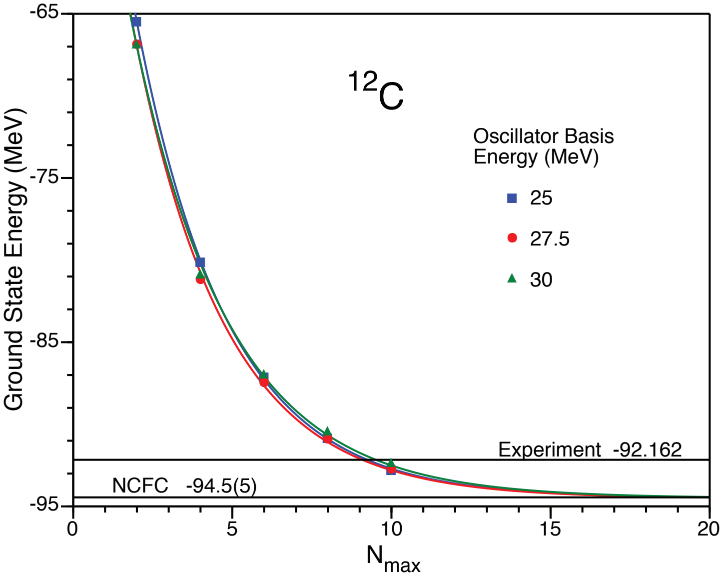

Fig. 1. Calculated ground state (g.s.) energy of ^{12}C for $N_{\max} = 2$–10 (symbols) at selected values of $\hbar\Omega$. For each $\hbar\Omega$, the results are fit to an exponential plus a constant, the asymptote, constrained to be the same for all $\hbar\Omega$ [11]. Horizontal lines indicate the experimental g.s. and the NCFC result (uncertainty = 0.5 MeV).

I show in Fig. 1 results for the ground state (g.s.) of ^{12}C as a function of $N_{\max}$ obtained with a realistic NN interaction, JISP16 [15]. The smooth curves portray fits that achieve asymptotic independence of $N_{\max}$ and $\hbar\Omega$. The NCFC g.s. energy (the common asymptote) of -94.5 MeV indicates overbinding of $\sim 2.5\%$ indicating TNI must play a role. The assessed uncertainty in the NCFC result is 0.5 MeV shown in parenthesis in the figure. The largest calculations correspond to $N_{\max} = 10$, with a matrix dimension near 8 billion. $N_{\max} = 12$ produces a matrix dimension near 81 billion which we hope to solve in the future.

One of the current ambitious undertakings seeks to develop a symmetry-adapted no core shell model approach [19]. In this approach, called the Symplectic No Core Shell Model (Sp-NCSM), one augments the conventional spherical harmonic oscillator basis with the physically relevant symplectic Sp(3,R) symmetry-adapted configurations of the symplectic shell model that describe naturally the monopole–quadrupole vibrational and rotational modes, and also partially incorporate α-cluster correlations. The potential savings in basis space dimensions are enormous but there is a price — increased complexity of the Hamiltonian matrix elements. Current projections indicate a net large gain in the scope of physics problems that may be addressed with the Sp-NCSM.

Another ambitious program seeks to extend the Monte-Carlo Shell Model (MCSM) to the no core regime and to greatly increase the number of active shells [20]. Since the MCSM has superior scaling properties with the number of nucleons, once validated, we envision this will be a very fruitful avenue for addressing heavier nuclei — possibly the entire periodic table. However, there are daunting challenges to overcome such as developing a load-balanced and scalable code.

3. Recent progress

It is worth recapping the recent achievements of the *ab initio* NCSM and NCFC approaches. Let me simply focus on those achievements that rely on either traditional TNI or the ChPT Hamiltonians including TNI. To date, we have:

- Explained the measured ^{12}C $B(M1)$ transition from the g.s. to the $(1^+, 1)$ state at 15.11 MeV and showed more than a factor of 2 enhancement arising from the TNI. Neutrino elastic and inelastic cross-sections on ^{12}C were shown to be similarly sensitive to TNI and their contributions significantly improve agreement with experiment [21].
- Explained the spectroscopy and a set of electroweak properties of $A =$ 10–13 nuclei. In particular, showed a major role of TNI for predicting the correct g.s. spin of ^{10}B [14].
- Working in collaboration with experimentalists, uncovered a puzzle in the GT-excited state strengths in $A = 14$ nuclei. The resolution, after further work, may lie in the role of intruder state admixtures [22].
- Advanced our understanding of the microscopic origins of the ^{14}C anomalous long half-life [23].

There are many additional successes using Hamiltonians of ChPT. One particularly noteworthy recent success is the *ab initio* calculation of the ^{17}F proton halo state and resonances in the $A = 17$ nuclei using the Berggren (Gamow) basis in the coupled cluster (CC) method [12]. Here, both resonance locations and widths are well described using only the NN interaction of ChPT. Indeed, one may argue that, for the low-density physics regime, the TNI is less important though this remains to be confirmed.

4. Future prospects

Recently, the US Department of Energy, Advanced Scientific Computing Research Division, convened a number of workshops to address how next-generation computational facilities may be critical for propelling scientific breakthroughs. The nuclear physics workshop produced a white paper, available online [25], detailing projected breakthroughs as computational resources increase over the next 7–9 years.

There are five focus areas of the report which is titled “Scientific Grand Challenges — Forefront Questions in Nuclear Science and the Role of Computing at the Extreme Scale”: (1) Cold Quantum Chromodynamics and Nuclear Forces; (2) Nuclear Structure and Nuclear Reactions; (3) Nuclear Astrophysics; (4) Hot and Dense Quantum Chromodynamics; and (5) Accelerator Physics. Each area presents a set of consensus views on the current status of the field and priority research directions that will be impacted by significant growth in computational resources, estimated to be 1000-fold over this period.

Within Nuclear Structure and Reactions, we have presented detailed plans and justifications for concerted efforts in (1) *Ab initio* Calculations of Light Nuclei and Their Reactions; (2) Reactions That Made Us: the Triple-Alpha Process and $^{12}\mathrm{C}(\alpha,\gamma)^{16}\mathrm{O}$; (3)Weak Nuclear Structure — Nuclei as Laboratories for Neutrino Physics; (4) Microscopic Description of Nuclear Fission; and (5) Physics of Extreme Neutron-rich Nuclei and Matter. One way of summarizing these plans is presented in the “riser chart” shown in Fig 2. Here we see a sequence of nuclear structure and reaction milestones presented as a function of computational resources that serve as a proxy for a timeline.

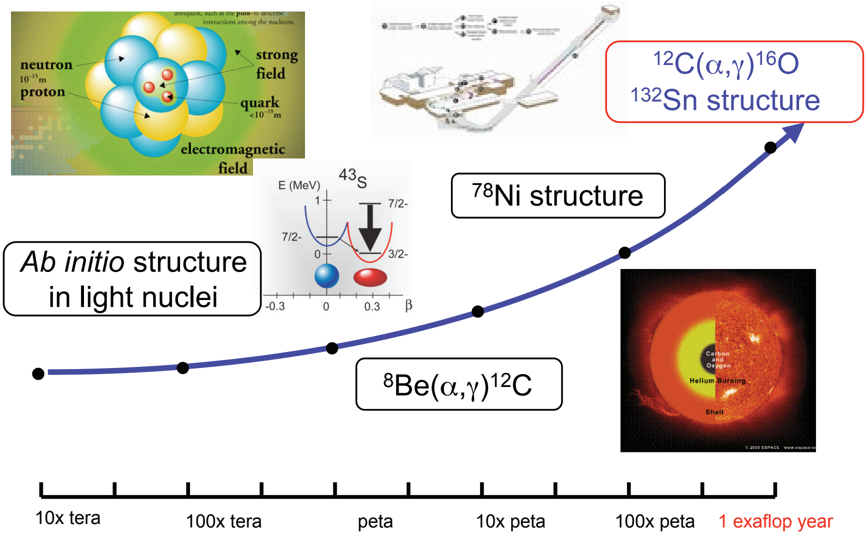

Fig. 2. Sample of consensus grand challenge goals for computational nuclear structure and nuclear reactions as a function of growth in computational resources [25].

Are these plans realistic? Of course, the answer depends on the creativity of the researchers as well as on the resources provided. Looking at recent progress there are ample reasons to be optimistic that both will become reality. We are entering a new era of "predictive nuclear physics", one that is replacing the traditional era of "descriptive nuclear physics", and recent breakthroughs, such as finding critical roles played by TNI, indicate we are slated for an exciting period of discoveries.

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