Nuclear forces and ab initio calculations of atomic nuclei

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Abstract

Nuclear forces and the nuclear many-body problem have been some of Gerry Brown’s main topics in his so productive life as a theoretical physicist. In this talk, I outline how Gerry’s work laid the foundations of the modern theory of nuclear forces and ab initio calculations of atomic nuclei. I also present some recent developments obtained in the framework of nuclear lattice simulations.

1. Prologue

Although I have been a student of Gerry, I might be the only one who never published a paper with him. In fact, my first project as a fresh grad student was to work out the $\rho$-meson coupling to the chiral bag, a hot topic in 1982. In these days, various groups tried to develop a microscopic theory of the so successful boson-exchange models of the nuclear forces, based on bag, quark or Skyrme models. I became interested in this topic through the lectures Gerry gave at the 1981 Erice school and he offered me to do my PhD in his group. I arrived in April 1982 at Stony Brook and when Gerry gave me this topic to work on, he said that we would finalize it in front of the fire place in the winter. Well, when I handed him a first draft of the paper in August, he did not even look at it in detail, just saying: “You are too fast for me, do your own stuff”. So I was pretty discouraged and shelved the manuscript. I thought to publish it in these proceedings, but unfortunately it seems to have been lost over the years. Therefore, in this talk I will try to give a personal recollection of Gerry’s understanding of the nuclear force and how it influenced modern nuclear structure calculations. Clearly, I can only touch upon some issues here, topics like nuclear forces from bags or Skyrmiions or the $V_{\text{low}-k}$ approach are left to other speakers. Also, to avoid duplication, for more personal recollections I refer to my contribution “Chiral symmetry, nuclear forces and all that” to the Festschrift in honor of his 85$^{\text{th}}$ birthday, see Ref. [1].
2. How to build a serious nuclear force model

This is a condensation of the work Gerry did with many collaborators over decades, so it is neither intended to be complete nor exhaustive. As a matter of fact, Gerry knew all the ingredients how to model the nuclear force [3]. These are (I also give a few pertinent papers on these topics co-authored by Gerry):

1) Chiral symmetry [4, 5, 6, 7]: Chiral symmetry fixes pion interactions to pions and matter fields and thus relates seemingly unrelated processes, like pion-nucleon scattering with the two-pion exchange potential and the leading three-nucleon force of two-pion range. Gerry was one of the pioneers of exploring the consequences of chiral symmetry in nuclear physics. All this is now firmly rooted in the spontaneous and explicit chiral symmetry breaking of Quantum Chromodynamics (QCD).

2) Three- and four-body forces [4, 5, 8]: A precise description of few-nucleon systems requires three-nucleon forces (3NFs), see e.g. Ref. [2]. As examples, I mention the minimum in the differential cross section of low-energy neutron-deuteron scattering or the $^3$He–$^3$H binding energy difference. Four-nucleon forces (4NFs) become relevant in heavier nuclei and nuclear matter, see the discussion in Sec. 5.

3) Two-pion exchange form pion-nucleon scattering [9, 10, 11, 12]: A model-independent determination of the two-pion exchange contribution to the nuclear force is possible using dispersion relations, that allow one to connect the processes $\pi N \rightarrow \pi N$ and $NN \rightarrow \pi\pi$. This connection was utilized in the Paris [13] and the Stony Brook [14] potentials. The method is discussed in great detail in one of Gerry’s textbooks [15].

One central ingredient in a potential constructed along these lines is the generation of the $\sigma$-meson, that parameterizes the central intermediate range attraction in boson-exchange potentials, through pion rescattering. For a modern look at this problem, I refer to Ref. [16]. Also, there is of course a strong overlap between these issues, as e.g. three-nucleons forces are strongly constrained by chiral symmetry. In fact, one must admit that almost all the ingredients for an Effective Field Theory (EFT) approach were already available at the time I did my graduate studies, except for a power counting that was only formulated for multi-nucleon systems based on chiral pion-nucleon Lagrangians by Steve Weinberg in 1990 [17].

3. Nuclear forces from chiral EFT

Chiral effective field theory as originally proposed by Weinberg has become a precision tool in nuclear physics. Here, I only display its main ingredients without detailed discussion. For an introductory review with many references,
Figure 1: Contributions to the effective potential of the 2N, 3N and 4N forces based on Weinberg’s power counting. Here, LO denotes leading order, NLO next-to-leading order and so on. Dimension one, two and three pion-nucleon interactions are denoted by small circles, big circles and filled boxes, respectively. In the four-nucleon contact terms, the filled and open box denote two- and four-derivative operators, respectively. Figure courtesy of Evgeny Epelbaum.

I refer to Ref. [18]. Also, I do not want to enter the issues related to the inclusion of ∆–isobars or vector mesons or some on-going attempts to improve upon Weinberg’s original work, see Ref. [19] for a recent discussion. In the Weinberg scheme, the power counting is applied to the few-nucleon potentials and not to the scattering amplitudes directly. The resulting contributions to the 2N, the 3N and the 4N forces are depicted in Fig. 1 up-to-and-including-next-to-next-to-leading order (N^3LO). First, this scheme is rather predictive. While in the 2N force, one has 2, 7 and 15 low-energy constants (LECs) at leading order (LO), next-to-leading order (NLO) and at N^3LO, respectively, to be determined by a fit to data, there are only two LECs in the 3NF at N^2LO and none in the 4NF. Isospin breaking through the light quark mass difference and the electromagnetic force can also be included systematically and precisely in this framework. Further, note that - consistent with phenomenological observations - three-nucleon forces appear only two orders after the dominant NN forces and four-nucleon forces are even further suppressed, appearing only at N^3LO. These forces have been successfully applied and tested in a plethora of calculations in few-nucleon calculations and are also frequently used (within some approximations) in many-body calculations. There are a number of challenges remaining, like e.g. the elusive A_y data in nucleon-deuteron scattering, see e.g. Ref. [20], or more calculations of the electroweak response to light nuclei with currents consistently constructed from chiral EFT, see e.g. Refs. [21, 22]. The interested reader might want to consult the reviews [23, 24].
4. Quark mass dependence of the nuclear forces

In an interesting but not much cited paper in 1987, co-authored with Herbert M"uther and Chris Engelbrecht, Gerry tackled the problem of how nuclear binding depends on the number of colors, $N_C$, and the light quark masses, $m_q$ \[25\]. For that, a one-boson-exchange model with varying $N_C$ and $m_q$ was constructed. In particular, in the scalar-isoscalar central channel, the spectral function was reconstructed from two-pion exchange and represented by an effective $\sigma$-meson, with mass $M_\sigma(N_C, m_q)$ and coupling constant $g_{\sigma NN}(N_C, m_q)$. Nuclear binding was then calculated employing Brueckner-Hartree-Fock methods. The conclusion was that “our world is wedged into a small corner of the two-dimensional manifold of $m_q$ versus $N_C$”. It is interesting to re-analyze this question in chiral EFT, which allows for a more systematic approach to possible quark mass variations. For recent works on nuclear forces at large-$N_C$, I refer to Refs. [26, 27, 28] and references therein.

As discussed before, nuclear forces in chiral EFT are given in terms of pion-exchange contributions and short-distance multi-nucleon operators. The ingredients to work out the quark mass dependence of these forces can be easily understood from the LO potential shown in the left panel of Fig. 2. First, there is an *explicit* pion mass dependence through the pion propagator in the one- and two-pion exchanges $\sim 1/(q^2 - M_\pi^2)$ and, second, there is a variety of *implicit* quark mass dependences through the nucleon mass, $m_N(M_\pi)$, the pion-nucleon coupling, $g(M_\pi)$, and the LECs accompanying the multi-nucleon operators, $C(M_\pi)$. Note that because of the Gell-Mann–Oakes–Renner relation, $M_\pi^2 \sim m_q$ (we work in the isospin limit $m_q = m_u = m_d$), one can use the notions quark and pion mass dependence synonymously. To discuss the quark mass dependence of hadron properties, one introduces the so-called $K$-factors, $\delta O_H/\delta m_f = K_H^f (O_H/m_f)$, with $O_H$ some hadronic observable and flavor $f = u, d, s$. The pion and nucleon properties (masses, couplings, etc.) can be obtained from lattice QCD data combined with chiral perturbation theory, for details see Ref. [29]. For the contact interactions, one has to resort to modeling, using the fairly successful concept of resonance saturation of the LECs. This should eventually be overcome by corresponding lattice simulations. Putting all this together, one finds for the NN S-wave scattering lengths and
the deuteron binding energy (see the right panel of Fig. 2)

\[ K_{a,1S0}^2 = 2.3^{+1.9}_{-1.8}, \quad K_{a,3S1}^2 = 0.32^{+0.17}_{-0.18}, \quad K_{B(\text{deut})}^2 = -0.86^{+0.45}_{-0.50}. \] (1)

A few remarks are in order. First, these \( K \)-factors are of natural size. Second, the sizeable uncertainties are due to the modeling of the contact terms by resonance saturation. Third, as Gerry told us, the nuclear forces are very sensitive to variations in the quark mass. Interestingly, the deuteron appears to be stronger bound as the light quark mass decreases, consistent with the expected binding energy in the chiral limit, \( E \sim F^2_\pi/m_N \sim 10 \text{ MeV} \). Using the \( K \)-factors given in Eq. (1) combined with corresponding \( K \)-factors for light nuclei\(^{30}\), one can deduce limits on the possible quark mass variations from the abundances of the elements generated in the Big Bang, \( \delta m_q/m_q = (2 \pm 4)\% \) (in the isospin limit). However, as pointed out in Ref.\(^{30}\), the neutron lifetime, that is sensitive to isospin-violating effects, leads to an even stronger constraint. Under the sensible assumption that all lepton and quark masses vary with the VEV of the Higgs field \( v \), one finds \( |\delta v/v| = |\delta m_q/m_q| \leq 0.9\% \)\(^{29}\), which lends some credit to anthropic considerations in nucleosynthesis.

5. Ab initio calculations of atomic nuclei

There are two different venues to tackle the nuclear many-body problem, that is nuclei with atomic number \( A \geq 5 \). Either one utilizes the forces from EFT within a conventional, well established many-body technique (no-core-shell-model, coupled cluster approach, etc.) or one develops a novel scheme that combines these forces with Monte Carlo methods that are so successfully used in lattice QCD. This novel scheme is termed “nuclear lattice simulations” and has recently enjoyed wide recognition as the first ever \textit{ab initio} calculation of the Hoyle state in \(^{12}\text{C}\) has been performed\(^{31}\). Space is too short for a detailed exposition of this method, so I rather make some general remarks and discuss some very recent results obtained in this framework.

In the nuclear lattice EFT approach, space-time is discretized in Euclidean time on a torus of volume \( L_s \times L_s \times L_s \times L_t \), with \( L_s(L_t) \) the side length in spatial (temporal) direction. The minimal distance on the lattice, the so-called lattice spacing, is \( a \) (\( a_t \)) in space (time). This entails a maximum momentum on the lattice, \( p_{\text{max}} = \pi/a \), which serves as an UV regulator of the theory. The nucleons are point-like particles residing on the lattice sites, whereas the nuclear interactions (pion exchanges and contact terms) are represented as insertions on the nucleon world lines using standard auxiliary field representations. The nuclear forces have an approximate spin-isospin \( SU(4) \) symmetry (Wigner symmetry)\(^{32}\) that is of fundamental importance in suppressing the malicious sign oscillations that plague any Monte Carlo (MC) simulation of strongly interacting fermion systems at finite density. For this reason, nuclear lattice simulations allow access to a large part of the phase diagram of QCD, see Fig. 3, whereas calculations using lattice QCD are limited to finite temperatures and small den-
Figure 3: Nuclear phase diagram as accessible by lattice QCD and by nuclear lattice EFT. Figure courtesy of Dean Lee.

sities (baryon chemical potential). Here, I will concentrate on the calculation of the ground state properties and excited states of atomic nuclei with $A \leq 28$.

Without going into any further details, I now present some recent results concerning the spectrum and structure of $^{12}$C, the fate of carbon-based life as a function of the fundamental parameters of the Standard Model, the ground-state energies of the alpha-chain nuclei up to $^{28}$Si and the spectrum and structure of $^{16}$O:

**Structure and rotations of the Hoyle state** [33]:
The excited state of the $^{12}$C nucleus with $J^P = 0^+$ known as the “Hoyle state” constitutes one of the most interesting, difficult and timely challenges in nuclear physics, as it plays a key role in the production of carbon via fusion of three alpha particles in red giant stars. In Ref. [33], ab initio lattice calculations were presented which unravel the structure of the Hoyle state, along with evidence for a low-lying spin-2 rotational excitation. For the $^{12}$C ground state and the first excited spin-2 state, we find a compact triangular configuration of alpha clusters. For the Hoyle state and the second excited spin-2 state, we find a “bent-arm” or obtuse triangular configuration of alpha clusters. The calculated electromagnetic transition rates between the low-lying states of $^{12}$C have also been obtained at LO (higher order corrections still require improved codes).

**The fate of carbon-based life** [34, 35]:
An ab initio calculation of the quark mass dependence of the ground state energies of $^4$He, $^8$Be and $^{12}$C, and of the energy of the Hoyle state in $^{12}$C have been performed. The sensitivity of the production rate of carbon and oxygen
in red giant stars to the fundamental constants of nature was investigated by considering the impact of variations in the light quark masses and the electro-magnetic fine-structure constant on the reaction rate of the triple-alpha process. We find strong evidence that the physics of the triple-alpha process is driven by alpha clustering, and that shifts in the fundamental parameters at the $\simeq (2-3)\%$ level are unlikely to be detrimental to the development of life. Tolerance against much larger changes cannot be ruled out at present, given the relatively limited knowledge of the quark mass dependence of the two-nucleon S-wave scattering parameters, cf. Eq. (1). As carbon and oxygen are essential to life as we know it, these findings also have implications for an anthropic view of the Universe.

Towards medium-mass nuclei [36]:
We have also extended Nuclear Lattice Effective Field Theory (NLEFT) to the regime of medium-mass nuclei. To achieve that, a method which allows to greatly decrease the uncertainties due to extrapolation at large Euclidean time was implemented. It is based on triangulation of the large Euclidean time limit from a variety of SU(4) invariant initial interactions. The ground states of alpha nuclei from $^4\text{He}$ to $^{28}\text{Si}$ are calculated up to next-to-next-to-leading order in the EFT expansion. With increasing atomic number $A$, one finds a growing overbinding as shown in Fig. 4. Such effects are genuine to soft NN interactions and also observed in other many-body calculations, see e.g. Refs. [38, 39, 40]. While the long-term objectives of NLEFT are a decrease in the lattice spacing and the inclusion of higher-order contributions, it can be shown that the missing physics at NNLO can be approximated by an effective four-nucleon interaction. Fitting its strength to the binding energy of $^{24}\text{Mg}$, one obtains an overall excellent description as depicted in Fig. 4.
Spectrum and structure of $^{16}$O:

Very recently, we have performed lattice calculations of the low-energy even-parity states of $^{16}$O. We find good agreement with the empirical energy spectrum, cf. Tab. 1, and with the electromagnetic properties and transition rates (after rescaling with the corrected charge radius as detailed in [37]). For the ground state, we find that the nucleons are arranged in a tetrahedral configuration of alpha clusters. For the first excited spin-0 state, we find that the predominant structure is a square configuration of alpha clusters, with rotational excitations that include the first spin-2 state.

| $J^p$   | LO     | NNLO (2N) | +3N    | +4N$_{\text{eff}}$ | Exp     |
|---------|--------|-----------|--------|---------------------|---------|
| $0^+_1$ | -147.3(5) | -121.4(5) | -138.8(5) | -131.3(5) | -127.62 |
| $0^+_2$ | -145(2)  | -116(2)   | -136(2)  | -123(2)  | -121.57 |
| $2^+_1$ | -145(2)  | -116(2)   | -136(2)  | -123(2)  | -120.70 |

Table 1: NLEFT results and experimental (Exp) values for the lowest even-parity states of $^{16}$O (in MeV). The errors are one-standard-deviation estimates which include both statistical Monte Carlo errors and uncertainties due to the extrapolation $N_t \to \infty$. The combined statistical and extrapolation errors are given in parentheses. The columns labeled “LO” and “NNLO(2N)” show the energies at each order using the two-nucleon force only. The column labeled “+3N” also includes the 3NF, which first appears at NNLO. Finally, the column “+4N$_{\text{eff}}$” includes the effective 4N contribution as discussed before.

I just mention some other topics under investigation within this framework, like e.g. calculations of the equation of state of neutron matter and the pairing gap, a method to achieve a further reduction of the sign problem or setting up methods to calculate nuclear reactions on the lattice.

6. Some final words

As it should have become clear, Gerry’s work laid the grounds for the modern theory of the nuclear forces and the application of these forces in nuclear structure calculations. In his ground-breaking paper on the chiral EFT to the nuclear force problem, Steve Weinberg gives only three references, one of them being the review Gerry had written in 1985 with Sven-Olaf Bäckman and Jouni Niskanen [41], and also, he explicitly thanks Gerry for “enlightening conversations on nuclear forces”. So clearly, Gerry has been one of the “eagles” of nuclear theory [42] and his legacy will live on.

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